CHED 1

Demonstrations guaranteed to get ooohs and ahhhs! How to turn ordinary activities into unforgettable learning experiences

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The secret to developing a great science demonstration is not to overlook the importance of the presentation. This program represents a collection of highly visual demonstrations and presentation ideas that help students build connections between scientific concepts and real-world applications. Learn how to add a new twist to some classic demonstrations, and how to integrate new demonstrations, teaching techniques, and hands-on activities with your present curriculum. Whether you use demonstrations to reinforce concepts with your students or as a means to stimulate public interest in science, there’s something in this collection of activities and teaching ideas for you.

Using some of his favorite chemical demonstrations as a catalyst (pun intended), Steve shares his techniques and strategies for turning an ordinary “demo” into an unforgettable learning experience. You will uncover the secrets of developing your own unique presentation style that makes students of all ages want to learn more. You’ll laugh a little and learn a lot… guaranteed.

About Steve Spangler - @stevespangler

Steve Spangler brings charisma, energy and new ideas to the education profession. His online science videos get more than 30 million views each year. Steve is a frequent guest on the Ellen DeGeneres Show where she dubbed him “… the teacher you always wanted to have in school because he makes learning so much fun.” His passion is to find the most creative ways to make learning fun. The Wall Street Journal said it best… “Steve Spangler parlayed his talents as an educator and master communicator into a career where he turned television – and now the internet – into his world-wide classroom to inspire a new generation of STEM leaders.” For more information, visit about.me/stevespangler
CHED 2

Writing across the curriculum: Concept journals as a means to teach the metric system

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The teacher must introduce the metric system to the student in a clear and rational way. Traditional methods of teaching the metric system use dimensional analysis, proportional reasoning, or mnemonics — all of which can easily confuse the chemistry student and are easily forgettable. Teaching the metric system as the simple manipulation of sound mathematical principles enables the student to understand the metric system in a way that stands on its own. By calling upon basic mathematical knowledge the student already has, he or she becomes more confident in his or her ability to use the metric system. Through a concept journal, the teacher guides the student toward his or her own definition of the metric prefixes.

CHED 3

A few insights into classroom and lab safety

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Two "experienced" teachers will relate some of their classroom stories and tips on topics from GHS to chemical storage to answering your questions about personal & student safety issues.

CHED 4
Spectroscopy of natural resources


Molecular spectroscopy is a technique used by scientists, educators and students to determine the chemical structure of a wide range of natural materials. From pharmaceuticals to food and beverage to illicit drug formulations, spectroscopy is primary tool to analyze, qualify and quantify these materials. Spectrometers play an important role in new product development, applied research and forensic science.

CHED 5

Spark student’s interest in chemistry with resources from the American Chemical Society

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The ACS Education Division serves learners and educators by building communities and providing effective chemistry education products, services and information. The ACS encourages students to explore and excel in the chemical sciences, by providing resources that complement formal high school curriculum. This presentation will provide an overview of resources and programs from the ACS that are open to all teachers and students. Learn about the free lesson plans, videos, and other activities to use in your classroom, and explore a number of ACS programs like ChemMatters, ChemClubs, and the ACS-Hach grants.

CHED 6

Replicating peer-led team learning in cyberspace: Research, opportunities, and challenges

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This presentation will describe the mixed methods study that examined the transfer of a well-established pedagogical strategy, Peer-Led Team Learning (PLTL), to an online workshop environment (cPLTL) in a general chemistry course at a research university in the Midwest. The null hypothesis guiding the study was that no substantive differences would emerge between the two workshop settings. Students in the PLTL condition were more satisfied with their workshop and earned statistically significantly higher course grades, yet earned comparable standardized final exam scores. They also had lower
incidence of students’ earning D or F course grades or withdrawing from the course (DFW rates) than students in the cPLTL setting. Interviews with 10 peer leaders and 2 faculty members, as well as discourse analysis of workshop sessions, revealed more similarities than differences in the two conditions. The final exam scores and discourse analysis support the null hypothesis and use of both face-to-face and synchronous online peer-led workshops in early science courses.

CHED 7

Insights into how students learn from molecular visualizations through the lens of variation theory

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The purpose of this talk is to share findings from work reported in the JCE paper, “Using Variation Theory with Metacognitive Monitoring to Develop Insights into How Students Learn from Molecular Visualizations.” In this study, first semester General Chemistry students’ prior knowledge of substances tested for electrical conduction was assessed before students were shown several short molecular visualizations of substances tested for electrical conductivity. After the visualization treatment, students completed a metacognitive monitoring exercise in which they were asked how similar and different their understanding or mental models were from the visualizations. The theoretical framework, variation theory, was used to examine students’ responses to the exercise, as well as their drawn changes to pictures they constructed before and after the treatment. Findings from the study provide deeper insight about why students often retain imperfect understanding and convey these flaws in their explanations. It also sheds light on the challenges encountered when trying to study how students learn from visualizations.

CHED 8

Looking for links: Examining student responses in creative exercises for evidence of linking chemistry concepts

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Assumptive Learning Theory values the active process of linking concepts to promote meaningful over rote learning. To promote meaningful learning, assessment practices that encourage the linking of concepts needs to be developed and utilized. Creative Exercises (CEs) have the potential to encourage such links. CEs are an open-ended assessment technique where students are given a single prompt and are asked to describe, as many statements as they can that are distinct, correct and relevant to the prompt. This presentation describes a qualitative investigation into student responses to CEs. The results show considerable interconnections of content in student responses.
Further, students’ efforts toward making connections revealed multiple student misunderstandings of the limits of models that were unlikely to be shown in traditional assessments. Implications for teaching practice, particularly related to how students are assessed, will be discussed along with potential future research projects to further explore the predictions of Assumptive Learning Theory.

CHED 9

Argumentation and participation patterns in general chemistry peer-led sessions

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This presentation reports on a publication from the *Journal of Research in Science Teaching* focused on the use of Toulmin’s argumentation framework to examine group interactions through a lens of argumentation. The study was conducted in a Peer-Led Process Oriented Guided Inquiry Learning (POGIL) setting in a college general chemistry course. Two small groups were video and audio recorded for a semester during weekly peer-led POGIL sessions. For this study, student discourse without peer leader intervention was analyzed for the presence of argumentation, argument strength, and evidence of argument co-construction using a modified framework from Erduran et al. (Erduran, Simon & Osborne, 2004). This study had three major findings: 1) students did construct arguments and were able to resolve incorrect claims on their own without peer leader intervention; 2) most arguments were co-constructed, although not all students contributed to the construction in the same way; and 3) evidence and explanations were common features of student arguments, but explicit linkages to prior examples and/or fundamental principles were rare. The presentation will briefly describe the study methods and highlights of the findings but will also incorporate a description of a subsequent application of this research to teaching. Salient features of the historical development of the study and the publication process will also be presented. The research has implications for instructors who wish to develop student argumentation skills via small group activities as well as for those who work with peer leaders.

CHED 10

Cultivation of creative thinking ability in the course of Food Engineering Operations

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In food engineering operations courses, the cultivation of creative thinking is important for the improvement of students’ interests in academic learning and the enhancement of
the professional identity, which would accordingly cultivate students’ abilities of self-learning, discovering and solving problems. In order to greatly improve teaching effect, teachers should do creative thinking, leave room for exploration and focus on the construction of multi-level training in experimental teaching process. In this way, students would be able to complete the transition from knowledge-based ones to practical ones and also from imitative ones to creative ones.

**Key words**: Food engineering operations; Explorative teaching; Creative thinking ability

### CHED 11

**Seven courses, two exams: Designing the ACS Inorganic Chemistry Exams for a diverse undergraduate curriculum**

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One of the strengths of the undergraduate inorganic chemistry curriculum is that it isn’t standardized. There is diversity in both the placement of and the content covered in the undergraduate inorganic coursework. The Inorganic Chemistry Supplement provided by the American Chemical Society Committee on Professional training suggests many topics that could be covered and explicitly recognizes that it is not possible to cover all of these topics. This diversity makes it challenging to design an ACS Exam in inorganic chemistry. The latest Inorganic Chemistry Exam and a new Foundations of Inorganic Chemistry Exam were both influenced by survey data from the inorganic community that defines the content most likely to be covered in undergraduate courses. The construction of these exams and observations related to item success and coverage in the curriculum will be discussed.

### CHED 12

**ACS examination in organic chemistry at Hampton University**

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A comprehensive ACS exam in organic chemistry has been used as the second-semester organic final exam at Hampton University for over thirty years. The influence of unit exam construction, test-anxiety reducing strategies, review books, and homework on student performance on the ACS exam will be discussed. A rational scale for the conversion of exam raw scores into comparable unit exam scores for course grade calculation will be described.

### CHED 13

**Assessment of nontraditional students in organic chemistry**
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A population of college students that have not received much attention in the past in regard to assessing their academic performance in terms of cognitive and non-cognitive measures have been students over the age of twenty-two that are enrolled in Organic Chemistry classes. The following assessment takes an initial look at this population with the ACS National Organic Chemistry Final as the dependent variable using a Multiple Regression/Correlation Analysis. The five independent variables (IV) were: an Achievement Motivation (S-Mot) survey, participants sex, age, participants final grade in Organic Chemistry II lecture, and GPA (Grade Point Average).

CHED 14

Creating the Exams Data Analysis Spreadsheet (EDAS) as a tool to help instructors conduct customizable analyses of student ACS exam data and compare the results to national normative statistics

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As a result of feedback from chemistry professors, the American Chemical Society Examinations Institute (ACS-EI) has developed the Exams Data Analysis Spreadsheet (EDAS) as a tool to help professors analyze student data from ACS exams. The EDAS will conduct calculations such as descriptive statistics (mean, standard deviation, median, etc.), histograms of students’ total scores, percentiles based on the national normative dataset, difficulty & discrimination indices, and the percentage of students’ responses to individual exam questions. Since the ACS-EI acknowledges that individual professors teach different content in their classrooms, the EDAS allows professors to customize their analyses by choosing specific sets of questions that are relevant for individualized classrooms. EDAS also has the option of choosing specific sets of questions based on the Level 1 statements (i.e. ‘Big Ideas’) of the Anchoring Concepts Content Map. Professors may then compare their students’ results to the national normative results, which are also calculated based on the set of exam questions chosen by the professor. The EDAS is intended to be a user-friendly tool which may help professors better understand their students’ performance on ACS exams and could potentially be used as a means of programmatic assessment within chemistry departments. This presentation will provide a discussion of the development of the EDAS for the 2012 First Term General Chemistry Exam (GC12F), which includes instructor feedback during EDAS trial tests. Further, a visual demonstration of the features provided by the EDAS will be presented. Future goals include creating versions of the EDAS for multiple ACS-EI exams.

CHED 15

Use of American Chemical Society examinations as assessment tools
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One of the ongoing challenges in chemical education is assessing the effectiveness of our courses. This is especially true at two-year institutions where the need exists to provide evidence that courses are taught at the same level of rigor as equivalent courses at four-year institutions. In addition, most courses at two-year schools are split into multiple sections, many of which are taught by adjunct instructors. There is a need to ensure that all sections are taught at the same level of rigor. At McHenry County College, we use American Chemical Society Examinations as our primary method of assessment. The results after fifteen years of using these examinations as measures of student learning will be discussed as well as how grading scales are determined.

CHED 16

Chemical thinking: Exploring the impact of a new general chemistry curriculum

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We have developed a new curricular approach for General Chemistry for science and engineering majors focused on teaching students how to apply chemical thinking to answering relevant questions in our world. The curriculum introduces core concepts and ideas in chemistry as needed to answer essential questions that drive research and development in our discipline. For example: How do we differentiate substances? How do we control chemical processes? How do we harness chemical energy? Instructors in the classroom use a learning cycle instructional model in which students analyze data, build models, and apply their understandings to solve questions and problems in a variety of relevant contexts. The new curriculum has been tested in different General Chemistry sections over the past five years. Analysis of students’ performance in ACS standardized tests and in subsequent Organic Chemistry courses shows a significant positive effect on student understanding and achievement. In this talk we will describe the core components of the new curriculum and discuss central findings on the effect of the "Chemical Thinking" curriculum on student learning.

CHED 17

Exploring the use of the Anchoring Concepts Content Map as a programmatic assessment tool

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The American Chemical Society (ACS) Exams Institute has been developing and vetting the Anchoring Concepts Content Map (ACCM) as a tool for programmatic assessment for undergraduate chemistry curricula. Currently, the general chemistry and
organic versions of the ACCM have been published and used to analyze content coverage over time. Additional ACCM are being developed for inorganic, analytical, physical, and biochemistry. Each ACCM has identical Anchoring Concept statements (Level 1, “Big Ideas”) and Enduring Understanding statements (Level 2). Each sub-discipline map varies at the subdisciplinary articulation statements (Level 3) and the content details (Level 4). In order to explore the use of the ACCM as a programmatic assessment tool, ACS exams across the different sub-disciplines of chemistry were mapped to the first two levels of the ACCM. For example, while the different courses may teach different content details for “Bonding”, underlying concepts as described in the enduring understanding statements remain stable. Therefore, it would be possible to track students understanding of bonding across the different chemistry courses based on their performance on the various bonding questions found on ACS exams. In order to explore the relationship of selected areas of content across the different sub-disciplines of chemistry, ACS exams from organic, analytical, biochemistry and inorganic, and general chemistry have been mapped to the Level 2 statements. Content coverage (or lack thereof) will be presented in order to show the applicability of the crosscutting use of the ACCM. Data from a lateral study of chemistry curricula as measured by content coverage on ACS exams will be presented.

CHED 18

Synthetic investigation and application of a substituted 4,6-dimethylcyclohexene compound

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The growing resistance of pathogenic fungal strains to current fungicides used in agriculture and medicine creates a desire to synthesize new compounds capable of inhibiting fungal growth. Common classes of fungicides encompass an array of organic products which include sulfur and copper based compounds. More recently, studies have suggested that highly substituted cyclohexenes with reactive acyl groups have potential antimicrobial properties. The focus of this work is to synthesize similar cyclohexene compounds and test their fungitoxicity. Recently, we have synthesized a highly substituted ketone product in a 91\% yield using microwave and solvent free conditions. In addition, preliminary studies suggest that this compound, in concentrations as low as 7.4 µM, can prevent fungal growth. The synthetic method and fungicide studies for this compound will be presented.

CHED 19

Chemistry for chiral skeletons: Building chiral fragments from enantiopure 1,2-amino alcohols
Chemical biologists seek to explore human biology through the use of small molecule therapeutics and biological probes. One approach to this is fragment-based drug discovery (FBDD), where biologically active molecules are built from core fragment scaffolds. Currently, most of the chemical libraries used in FBDD are dominated by sp²-rich aromatic compounds. Building an expanded library containing sp³-rich chiral fragments would allow the exploration of a larger chemical space which in turn would open avenues for unexplored biological space. In this project, we seek to exploit the power of modern organic chemistry to create a pilot library of 86 sp³-rich, highly soluble chiral fragments derived from 1,2-amino alcohols. These fragments will be synthesized using the principles of Diversity-oriented Synthesis (DOS) to generate a set of molecules diverse in chemical and structural properties.

To begin building our sp³-rich chiral fragment library, we focus on optimizing and devising reaction conditions for the synthesis of sulfamidites and sulfamidates fragments derived from 1,2-amino alcohols. Once synthesized, these chiral fragments will be characterized, and their solubility and stability in phosphate-buffered saline (PBS) will be assessed. The results of this pilot study will serve as a blueprint in designing, evaluating and building more focused libraries of chiral fragments. In turn, this will lead to building more structurally diverse fragment libraries which will expand the scope of fragment-based drug discovery.

CHED 20

Evaluation of a new rhamnosidic donor containing a sulfonyl directing group for the formation of beta-rhamnosidic linkages

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β-rhamnosidic and β-mannosidic linkages are critical components of bacterial and mammalian glycans. However, the generation of these linkages remains an ongoing challenge for glycoscientists. Our current research focuses on improving our access to these linkages. Recently, we synthesized two novel rhamnosyl donors (electrophiles) containing sulfonyl directing groups as model systems to study β-selectivity in the rhamnose and mannose series. The sulfonyl group was selected because it has been shown to have electronic properties that favor formation of the β-linkages. In this poster we describe the total synthesis of these donors, as well as several preliminary glycosylation reactions with glucose based nucleophiles. Future extension of this
methodology to biologically relevant β-rhamnosidic linkages, as well as β-mannosidic linkages will also be discussed.

CHED 21

Regioselective opening of propenylbenzene oxides via intramolecular N-H activation

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β- and γ-amino alcohols have been used extensively in the synthesis of therapeutics due to their structural similarities to neurotransmitters and hormones. We aim to produce β- and γ-amino alcohols regioselectively by utilizing an unexplored epoxide opening of E- or Z-propenylbenzene oxides activated by an intramolecular N-H bond. This chemistry could be applied to the synthesis for derivatives of PRC200, an experimental triple reuptake inhibitor. Application to other CNS active amino alcohols will also be demonstrated.

![Diagram showing the reaction of racemic cis-epoxide to racemic syn-stereoisomer and racemic trans-epoxide to racemic anti-stereoisomer.]

CHED 22

Novel hydroxyproline methodology involving an auxiliary salicylaldehyde capture followed by imine-induced intramolecular rearrangement to achieve chemoselective ligations at difficult proline site

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Since the advent of native chemical ligation, broadening the scope beyond cysteine-site ligations has been actively studied in peptide chemistry. Proline-site ligation, owing to intrinsic electronic properties, is putatively the most challenging site, indicated both by the longest reaction times and the paucity of methodologies to address this problem. In this study, salicylaldehyde is first installed at phenolic site, furnishing the aldehyde for capture of 4-hydroxyproline’s amine. Upon capture, through a Schiff’s base-type mechanism, an iminium species is formed, inducing the 4-hydroxyl group to attack. This frees the amine to attack the N-term carboxyl, brought into proximity by the phenolically attached salicylaldehyde. The hemiaminal reforms the aldehyde of salicylaldehyde, liberating the amine of hydroxyproline and the newly ligated fragments. Salicylaldehyde is acidolyzed from the 4-hydroxyl position, yielding native peptide product. This approach was successfully demonstrated on various syntheses of oligopeptides, as verified by NMR, elemental analysis, and mass spectrometry.

CHED 23

Why does the acetaldehyde enolate favor reaction at the O atom during gas-phase nucleophilic substitution? Contributions by resonance and inductive effects

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Enolate anions are bidentate nucleophiles that can undergo reaction at the O atom or the alpha C atom. In solution, the C atom is usually the preferred reaction site, but in the gas phase, the O atom is. To better understand this preference in the gas phase, we carried out density functional theory calculations at the MPWPW91/6-311++G(3df,3pd) level of theory to determine the contributions by resonance and inductive effects toward the enhanced reactivity at O over C for the SN2 reaction between the formate anion and CH3F. To separate the contribution by resonance from that by inductive effects, we applied the vinylogue extrapolation method. Our results suggest that the dominant factor is the loss of resonance from the enolate nucleophile upon going to the transition state. That loss of resonance serves to disfavor both C attack and O attack, but C attack is disfavored significantly more than O attack.

CHED 24

Investigating the mechanism of cyanoacrylate polymerization in latent fingerprint development

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Cyanoacrylate fuming, or superglue fuming, is a widely used technique in laboratories all over the world used to reveal latent fingerprints. Cyanoacrylate fuming has been used for decades with little to no knowledge of the polymerization reaction for ethyl cyanoacrylate and the components in fingerprints. Fingerprints are composed of amino acids, sugars, oils, water, and many other constituents. Our research is focused on isolating which fingerprint constituent results in the most polymerization through fuming of isolated and mixed solutions of different constituents such as alanine, serine, and oils. Through this research, the mechanism for the polymerization reaction can be better understood at a molecular level. The understanding of the polymerization reaction can result in better substituted cyanoacrylates that proved more detailed results for fingerprints.

CHED 25

Methods towards the synthesis of Stachybotrin D

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Stachybotrin D is a novel phenylspirodramine isolated from Stracybotrys Chartarum MXH-X73. Stachybotrin D exhibits anti-HIV properties by acting as a non-nucleoside reverse transcriptase inhibitor (NNRTI) on wild type HIV-1 and 5 NNRTI resistant strands. The structure of Stachybotrin D is distinct from the other available NNRTI drugs, and is a potential new chemotype for NNRTI drug treatments. Our research group has developed a synthetic method towards a total synthesis of Stachybotrin D. The retrosynthetic analysis developed incorporates synthesized phenyl and sesquiterpene moieties which are assembled together through a furan ring. We will discuss our efforts towards this synthesis, with a focus on utilizing greener chemistry methods. This includes using a Vilsmeier-Haack reaction as a milder condition rather than a Gatterman reaction which uses hydrogen cyanide for a formylation step. Additionally, we utilize a microwave reactor for some of the steps rather than exhaustive heating to reduce the energy usage and time. The paper presented demonstrates the strategy taken by our group and the current work towards this synthesis.
Rapid synthesis of N-(2-hydroxybenzyl)acetamide

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Recently, we developed a rapid procedure for the synthesis of various benzylformamides. We also investigated acetamide as an alternative solvent for the reaction. Interestingly, in the reaction conducted on 4-chlorobenzaldehyde, N-(4-chlorobenzyl)formamide was produced only as a minor product. The use of acetamide resulted in a substantial shift towards N,N-di-(4-chlorobenzyl)formamide and N,N,N-tri-(4-chlorobenzyl)amine that were produced with the isolated yields of 33.5% and 12.4%. N,N-di-(4-chlorobenzyl)formamide appeared to be the main product of the reaction. We hypothesized that the successful formation of the dibenzyl and tribenzyl products should correlate with electron density on the nitrogen atom of the respective benzylformamides. Therefore, the reaction conducted on benzaldehydes with electron-donating substituents should result in even larger shifts towards dibenzyl and tribenzyl products. In this work this hypothesis was tested on 2-hydroxybenzaldehyde. The reaction was conducted on 10 mmol scale at 189°C. Column chromatography was used for the isolation of the products of the reaction. NMR-spectroscopy and elemental analysis were used to determine the structure of the products. The reaction was fully completed in 7 minutes. Surprisingly, N-(2-hydroxybenzyl)acetamide appeared to be the main product of the reaction with an isolated yield of 32.9%. N,N-di-(2-hydroxybenzyl)formamide was produced as the second major product with an isolated yield of 22.9%. The reaction provides an important step towards a new rapid method for the synthesis of N-(2-hydroxybenzyl)acetamide. Research reported in this publication was supported by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103442.

Synthesis of trehalose-based oligosaccharides for medicinal applications

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Trehalose, an α,α-linked disaccharide first isolated in 1832, has been found in over 80 species of plants, bacteria, fungi, insects, and algae. Interestingly, despite the prevalence of trehalose in these systems, it has not been found in any mammalian systems. Trehalose possesses several interesting structural and physical properties
which have been shown to play an important role in cell integrity and maintenance. For example, trehalose and trehalose-based oligosaccharides play a critical structural role in the cell wall of *Mycobacterium tuberculosis*. More recently, trehalose and trehalose-based oligosaccharides have been shown to play a unique role in the stabilization of proteins under high-stress conditions. The importance of trehalose and trehalose-based oligosaccharides in these examples makes it an ideal target for further structure/function studies. Here we present the complete chemical synthesis of a series of trehalose-based oligosaccharides. Our work will be presented in the context of using these compounds as probes to study the molecular mechanisms behind MTB cell wall biosynthesis. We will also discuss our ongoing studies assessing the unique properties of these compounds and their possible use for protein stabilization.

**CHED 28**

**Comprehensive chemistry: An efficient approach**

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The fundamental problem of a senior review course is efficiency for students and instructor alike. Our course is based on weekly multiple-choice exams, stepping chapter by chapter through a General Chemistry textbook. Students regain half the credit lost from missed questions by submitting a complete explanation of the correct answer. Every examination period is preceded by an oral presentation or two by a student whose submitted explanation(s) were judged to be weak. The procedure keeps students motivated and focused on their areas needing improvement. There are 10 weekly examinations keyed to the text. This is then followed by an oral examination given by three chemistry faculty and the ETS Major Field Test for Chemistry. In addition to their positive effect on student outcome these latter two experiences allow the department to determine the effectiveness of this course and the program in general.

**CHED 29**

**Introductory investigation into the substituent effect on regio-selectivity of bromination across vinyl systems: A culmination of undergraduate chemical education**

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For students at the University of Colorado Denver campus, the honors organic synthesis lab is the culmination of multiple semesters of undergraduate chemical education. The lab consists of an independent research project which requires the utilization of student's chemical intuition, advanced laboratory techniques, collaboration
with peers, as well as introducing students to the finer points of research and literature searches.

An example project required a three step synthesis in order to investigate the para-substituent effect on the regio-selectivity of bromination across vinyl systems. The synthesis utilized many benzaldehyde derivatives where substituents varied in their electron donating/withdrawing nature. The first step consisted of the formation of homoallylic alcohols from their corresponding carbonyl compounds, an allylhalide, and various organometallic catalysts. The second synthetic step resulted in the formation of a vinyl system by performing an adapted base catalyzed dehydration of the aforementioned alcohols. Finally, the vinyl system was brominated by elemental bromine and characterized by $^1$H NMR and mass spectroscopy.

This project not only allowed students to gain insight into organometallic chemistry, but required students to development procedures to obtain the desired vinyl intermediates based on the substituent present. The project also facilitated proficiency in complex characterizations by $^1$H NMR and mass spectroscopy.

CHED 30

Shippensburg University undergraduate research grant writing experience

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Shippensburg University’s Chemistry program currently provides an undergraduate research experience that provides students with a highly individualized capstone project. Students participating in research for credit are assigned a faculty mentor based on their research interests at the end of their junior year. Shippensburg University annually supports undergraduate research by providing a total of $60,000 in grants with individual students eligible for up to $2000. Chemistry research students are required to apply for this grant to obtain funds to travel and present their research at the National ACS Meeting. The grant application requires students to write a 3-page narrative that addresses the relevance and significance of the project, a budget and letter of support from a faculty mentor. The department finds this to be an excellent way for students to begin their undergraduate research experience providing them with an opportunity to exercise their writing skills and to gain an understanding of the grant process. After students are funded, they are expected to order any supplies provided by the grant and make expenditures for travel. Most students present their poster in the undergraduate research poster session at the spring National ACS meeting. The grant also requires that they present this same research at our campus wide Celebration of Student Research Conference. As the students have already presented a poster at the ACS meeting, the department uses this opportunity to require students to participate in a Chemistry Department symposium and present a 15-minute talk about their research. Thus, the entire undergraduate research program within our department provides students with many culminating experiences important to being research scientists.
including reading journal articles, writing a grant, administering a grant, traveling to meetings, and giving both a poster and an oral presentation.

CHED 31

Senior capstone experiences at Stevenson University: Everybody’s doing it

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A senior capstone experience at Stevenson University is completed by all science majors in their fourth year. Students are allowed to choose between a research or an internship experience, depending on their unique Career Architecture™ plans. A full time internship coordinator is on staff in the School of the Sciences to serve as a liaison between student interns and placements. The experience culminates in the capstone course, where students author a substantive research, project, or issue based paper. In the course, the students also produce a poster presentation of their capstone work, which is presented at a University-wide event. This is accompanied by their professional portfolio, highlighting their accomplishments at Stevenson University’s School of the Sciences. The capstone is a positive, productive and meaningful experience for our graduates, who are well sought-after in their post graduate pursuits.

CHED 32

Ups and downs of a two-semester independent research project

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For over 40 years, our institution has required all graduating seniors to complete a two-semester independent research project under the direct supervision of a departmental faculty member. Alumni routinely cite this experience, known as the senior tutorial, as the defining characteristic of their undergraduate education. As graduates from a women’s college, they also commonly report that this in-depth research experience gave them the confidence to persevere in the field and an important initial advantage over many of their peers. In the face of increased budgetary pressures, elevated demands for faculty-originated scholarship and a greater diversity of career-goals amongst our students, we are now evaluating a number of alternative student research models. In this process, we are seeking to retain the best of what we have created to date while still adapting to our current realities. The lessons and insights gained through this process will be discussed.

CHED 33

Chemistry and biochemistry capstone course at Messiah College: A holistic interdisciplinary approach
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The overarching goal of the capstone course at Messiah College is to help students think carefully and critically about connecting a vocation in chemistry, biochemistry, or other sciences to a larger worldview. At Messiah College, student worldviews fall generally, but not exclusively, within a variety of Christian traditions. Consequently, the capstone course focuses on exploring the connections between science, Christian theology, and philosophy. The course is discussion oriented and organized around the following major areas: 1) the nature of science, 2) the nature of religion, 3) models for the relationship between science and religion, 4) three central episodes in the history of science (Galileo, Newton, and Darwin), 5) origins (creation-evolution issues), 6) modern science and religion issues (God's action in the world, natural theology, the mind-body problem, etc.), and 7) science, religion, and society (including race and gender issues, environmental issues, genomics and medical science, etc.). Students are evaluated by written responses to course readings, exams, class participation, and a culminating autobiographical paper on the relationship between the student's vocational calling to a science career and his or her larger religious worldview. The course is designed to educate not indoctrinate students, such that topics are presented from a variety of perspectives and the instructor's views on issues are not imposed on the discussion or generally provided until the very end of the course as part of a course retrospective.

CHED 34

Electrifying the capstone chemistry experience

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Capstone courses have become the culminating chemical experience for many ACS undergraduates, yet course content and designs are widely variable. To enhance students’ critical reflection of their undergraduate training in chemistry and biochemistry, we developed a capstone course that emphasized the role of their education in professional goals and ethical development using modern tools of communication, including electronic portfolios, chemical blogs and Khan Academy-style, interactive teaching videos. Electronic portfolios proved essential to the capstone course by providing a unique and versatile creative space for students to not only post variable media artifacts, but also to engage in timely student-driven peer-review. Students also developed their personalized professional electronic portfolio pages tuned to chosen target audiences, which ultimately enhanced the summative reflection of their undergraduate chemistry experience. As a result of this capstone course, students produced dynamic, integrative teaching videos of such high quality that some are being used as a resource library for introductory chemistry courses. In addition, students learned the importance and challenge of communicating chemical fundamentals to a broad public audience using interactive media, as well as communicating their professional goals and intentions using innovative electronic platforms.
CHED 35

Measurement of phosphates in soft drinks: A general chemistry experiment using NMR

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Marymount University recently acquired a Bruker Avance 400 NMR Spectrometer, and to fully integrate it into the laboratory curriculum a new laboratory was developed for general chemistry students. Unlike many published experiments using advanced NMR techniques, which have been developed for upper level courses, this experiment is a simple introduction to NMR for a freshman level general chemistry course. The phosphate concentration was determined for various soft drinks using phosphorous NMR. The students run the samples themselves and perform the Fourier transformation on the Free Induction Decay (FID). After this, the spectra contain only one peak, and if the pH of the samples is the same, the peak also appears at the same position in all of the spectra. The students then integrate the peak and compare the integrated are of the peaks to determine the concentration of phosphate in their samples. The simplicity of the data analysis allow the emphasis of the experiment to be the NMR instrumentation, sample preparation and data processing.

CHED 36

Free-radical chlorination of alkanes in the undergraduate organic chemistry laboratory: Application of $^1$H and TOCSY NMR experiments to the analysis of reaction products

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We have shown that NMR spectroscopy can provide a versatile approach to quantitating and identifying the products resulting from the free-radical chlorination of alkanes. We have found that the most deshielded signals arising from certain substrates are sufficiently resolved to be integrated, allowing for the calculation of relative reactivity values. If identifying chemical shift information is not provided, these same deshielded signals can be used in 1D TOCSY experiments to provide clear spectra of each isomer. We have also found that when the deshielded region of a spectrum is particularly congested, $^1$H NMR pureshape experiments provide an attractive method for increasing resolution while still allowing for quantitation. Finally, since instrumental conditions do not need to be optimized for each substrate, we have found that this approach allows students to work with a variety of substrates, allowing them to pool their data and collectively analyze trends.

CHED 37
Implementation and assessment of a multi-week discovery based unit in the organic chemistry laboratory

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A number of laboratory experiments have been published that are discovery-oriented for the general chemistry labs, with fewer reported for the organic chemistry laboratories. One multi-week experiment developed at our institution exposes students to distillation, chromatography and spectroscopy as one multi-week, related experiment. Steam distillation of herbs and spices is done in the first week, followed by liquid-liquid extraction to obtain essential oils. In the second week, the oils are purified by column chromatography and NMR/IR spectra are collected. The third week is devoted to data sharing and analysis of the identification of isolated individual compounds.

The analogous traditional labs involve three unrelated experiments: distillation of a two-component mixture, isolation and chromatography of caffeine, and NMR/IR identification of unknowns. Students in multiple sections of both the discovery-oriented and traditional labs were given a survey at the end of the semester measuring ability to interpret NMR as well as attitudes regarding the lab. Comparison of the two lab procedures and analysis of the students test results will be presented here.

CHED 38

Unequivocal assignment for all PMR and CMR signals of unknown butyl and pentyl acetate esters from Fischer esterification using 2D NMR experiments

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Unknown butyl and pentyl acetate ester synthesis by Fischer esterification produces twelve potential products. Physical methods of analysis (boiling points and refractive indexes) provide limited identification information since the values are often similar for the various unknown esters; GLC affords purity data but does not contribute to ester identity. Spectrometric analysis using electron-impact mass spectrometry provides fragmentation data; however, lack of a discernible molecular ion makes this of limited and complicated use for ester identification. Infrared spectroscopy validates ester production but does not afford specific ester identity. Identification of every potential butyl and pentyl acetate ester can be accomplished using a compilation of PMR spectral data (number of signals/sets of signals, chemical shift data, integrals, and splitting patterns) and CMR spectral data: CMR (number of carbon signals and chemical shift data), gated-decoupled CMR (carbon signal-splitting data), and DEPT (methyl, methylene, methine, and quaternary-carbon signal identification). 2D NMR experiments are, however, required to provide unequivocal assignment for all PMR and CMR signals of the unknown esters. The necessary 2D NMR experiments include HSQC (1-bond C,H), INADEQUATE (1-bond C,C), COSY (2- to 3-bond H,H), HMBC (2- to 3-bond
C,H), and TOCSY (spin system related H,H). This study provides a plethora of experiences in the laboratory for advanced organic chemistry students. These include (1) synthesis and purification of unknown butyl and pentyl acetate esters, (2) conclusive identification of the unknown esters using a combination of physical (bp, η, GLC), spectrometric (MS), and spectroscopic (IR, 1D NMR and 2D NMR) techniques, and (3) utilization of both 1D NMR and 2D NMR experiments to afford unequivocal assignment for all PMR and CMR signals of the unknown esters.

CHED 39

Real-time classroom comparison of structures and NMR spectra using Jmol/JSpecView and nmrdb

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One of the most important learning goals for sophomore-level organic chemistry is for students to make the connection between chemical structure and spectroscopy. Recent collaborative work involving St. Olaf College, the University of the West Indies, and École Polytechnique Fédérale de Lausanne allows for the first time for chemistry students and teachers to use a chemical name or drawn chemical structure to retrieve an infinite variety of associated 2D chemical drawings, 3D chemical structures, and simulated 1H-NMR spectra in seconds. Structures can be known compounds such as Tylenol or 3-bromotoluene or totally unknown structures invented on the fly just for the sake of illustration. The retrieved model and spectrum are automatically correlated such that highlighting atoms on the structure highlight the corresponding peaks on the spectra, and vice-versa. Modification of the structure illustrates trends in the resulting spectrum. Active, adaptive learning strategies can be utilized to involve students on their own or in groups to explore the relationship between structure and chemical shift in order to solidify understanding. As with other pages developed using Jmol, either pre-designed classroom-ready web pages already on the web or pages customized by the instructor can be used.

CHED 40

Students using esters to construct for themselves the concepts of chemical shift correlation and spin-spin coupling

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NMR is an indispensable tool for structure analysis. Foundational concepts used to determine molecular structure by NMR include chemical shift correlation and spin-spin coupling. We have developed student-centered, active learning tools based on a
logically selected set of 34 esters suited to $^1$H NMR analysis by undergraduates that allow these students to construct for themselves a transitive meaning for these foundational concepts. Students are then better prepared to apply the foundations of NMR analysis to more complicated spectroscopy problems. These learning tools rely both on knowledge of electronegativity and nuclear spin as foundational concepts used to determine molecular structure by NMR and on the comparative analysis of actual NMR data. The ester functional group provides excellent chemical shift dispersion so that in all but one case to be discussed all of the peaks are resolved and first-order coupling is observed. In this presentation we will explicate our in-class and in-laboratory, hands-on methods in which students construct concepts of correlation, experience all examples of spin-spin splitting for $N = 0$-$6$, and, as a bonus, practice ester nomenclature and line-angle drawing.

CHED 41

Measuring structural and electronic effects on keto-enol equilibrium in 1,3-dicarbonyl compounds

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Nuclear magnetic resonance (NMR) spectroscopy is an integral part of the undergraduate chemistry curriculum. In addition to structure determination NMR is used to analyze chemical reactions and equilibria in situ. Determination of the position of equilibrium is well-suited to NMR analysis in the undergraduate laboratory as an extension of peak identification and signal integration. For many years we have successfully implemented the classic experiment in which students measure the position of equilibrium for a set of structurally interrelated 1,3-dicarbonyl compounds. Several factors affect the position of keto-enol equilibrium, defined here as $K_{e/k} = [\text{enol}]/[\text{keto}]$, including structure (steric bulk, conjugation, electron withdrawing/donating groups, resonance), temperature, and solvent. We present a logically selected set of compounds that have a common 1,3-dicarbonyl moiety with progressively changing ligands at the 1 and 3 positions. We also present structurally related control compounds that do not readily (e.g., monocarbonyl) or cannot (e.g., dialkylated methylene) undergo keto-enol tautomerization. These experiments fill a gap in the literature: with these controls for comparison students may gain a clearer understanding of both the role of the 1,3-dicarboxyl moiety in activating the central methylene group and the limits of detection of the NMR method. In summary, this array allows students to investigate structure-function relationships that affect keto-enol equilibrium in a cumulative fashion and affords instructors a broad selection of compounds for study in both introductory and advanced laboratory courses using a variety of pedagogic approaches. In addition, we contextualize our selections within a summary of the literature of related experiments so that those interested in implementing this type of experiment may know the range of approaches taken by colleagues at other institutions.
CHED 42

NMR-based activity assays to characterize enzymes in the biochemistry laboratory and in undergraduate research

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$^1$H and $^{19}$F NMR-based activity assays are being used increasingly in the pharmaceutical industry to complement high-throughput screening (HTS) methods. They provide orthogonal, uncoupled assays useful for HTS hit triage, and are also perfectly suited to high concentrations of test compounds used in fragment screening. In the undergraduate biochemistry laboratory setting, NMR-based activity assays are a logical extension from prerequisite organic chemistry NMR analyses. Relationships between chemical structure and chemical shift, and between peak area and quantity, are extended to distinguish between substrate and product resonances, and to determine their corresponding concentrations, respectively. Compounds can be quickly tested for inhibition, and the equilibrium constant for a reaction can be determined by integrating peak areas. The project-based biochemistry laboratory course at Adelphi has students work in small groups to purify and characterize a protein of their choosing. NMR spectroscopy is a required component of the characterization. This typically involves developing and validating a $^1$H NMR-based activity assay. Recent enzymes include amylase, lactate dehydrogenase, and malate dehydrogenase. Student groups that decide to purify a protein that lacks enzymatic activity are required to use NMR spectroscopy to monitor the methanol-induced denaturation of their protein. In the undergraduate research setting, NMR-based activity assays are being developed and used to identify inhibitors of nucleoside ribohydrolases from Trichomonas vaginalis. These enzymes are important components of purine and pyrimidine salvage pathways used by the parasite and represent novel drug targets. One assay uses $^{19}$F NMR to monitor the conversion of 5-fluorouridine to 5-fluorouracil and ribose catalyzed by uridine nucleoside ribohydrolase (UNH), while another uses $^1$H NMR to monitor the conversion of adenosine to adenine and ribose catalyzed by adenosine/guanosine nucleoside ribohydrolase (AGNH). The UNH assay has been used to screen the NIH Clinical Collection and identified several compounds with μM inhibition.

CHED 43

Award Address (James Bryant Conant Award in High School Chemistry Teaching sponsored by Thermo Fisher Scientific). Through generations X, Y and Z, learning never ends

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The James Bryant Conant Award is given to recognize, encourage and stimulate teachers of high school chemistry. The journey of sharing the passion and knowledge of
chemistry with twenty plus years of high school students has been rewarding in numerous ways. While these specific generations of students are categorized according to their ideas, actions, and beliefs, they all continue to love anything related to fire, explosions and crazy chemistry jokes. But through the student years of X, Y & Z, there have been changes in the ways students think about, study, and do chemistry. Meeting the challenge to grow and learn with them has proven to be the greatest resource available for sustaining a passion for teaching and professional growth. Sharing this journey is a way of encouraging, inspiring and stimulating other educators as they live the saga: Learning Never Ends.

CHED 44

ChemSource, the NGSS, and the particle nature of matter: How to develop classroom-ready templates

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In this paper, the identification, adaptation, and development of classroom-ready templates and lesson plans allied with the NGSS (Next Generation Science Standards) will be demonstrated. The basic material will be selected from the ChemSource module, Basic Chemical Reactions, and the NGSS performance expectations for the high school level. The templates will focus on the introduction of the particle nature of matter into secondary school chemistry instruction. The particle nature of matter and chemical reactions have been chosen for illustrative purposes because of their importance to chemistry education and emphasis in the NGSS which illustrates the development of a core concept or learning progression. Although the NGSS are described in this paper, the process is useful for constructing any standards-based instructional materials.

CHED 45

Engaging chemistry resources from the Journal of Chemical Education and ChemEd X>

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The presenter will share “ready to use” resources from the Journal of Chemical Education (JCE) and Chemical Education Xchange (www.ChemEdX.org). Participants will experience inquiry activities related to the theme and related topics. Modeling, Socratic Questioning techniques and Student Discourse will be highlighted within the presentation.

CHED 46
Think safety = work safely

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There have been numerous accidents in the chemical community that could have had more positive outcomes if safety had played a greater role in the demonstration or experiment. To reduce these incidents, safety must be integrated into the curriculum. Come and learn techniques and do activities that will make safety a way of life for you as a teacher/demonstrator and for your students in the lab and beyond.

CHED 47

Using Popular Science Magazine articles to improve students’ critical thinking and scientific literacy

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Magazine articles on scientific topics can be a great way to develop students’ scientific literacy and encourage their critical thinking. In this presentation, we will describe how science-related magazine articles can be integrated into instruction to stimulate students interest in the science behind everyday life and increase their scientific knowledge. We will mention ChemMatters magazine as one source of such articles and introduce a new resource from the American Chemical Society that will include lesson plans based on the mostly highly ranked ChemMatters articles in the past 30 years. The purpose of these lesson plans will be to integrate the Common Core State Standards and the Next Generation Science Standards into instruction through the ChemMatters articles.

CHED 48

How effective is lecturing in a high school chemistry class?

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It is difficult to measure the effectiveness of lecturing in chemistry. We, as teachers, have so much material to cover and so little time to do it. Lecturing seems to be the most practical way to achieve this goal. We spend a considerable amount of time preparing our lectures and those students who are interested in learning seem to be engaged. But what do we know about lecturing and how it dovetails with the way the human brain operates? Can students pay attention for an entire lecture? If students hear a coherent, logical presentation, do they internalize it? Is lecture the most effective way to spend our class time? How can we test its effectiveness? This presentation will
review what we know about how the brain operates, how long students can pay
attention in lecture and what alternatives are available for teaching.

CHED 49

Using the ACAST to characterize high school chemistry teachers’ data-driven
inquiry practices

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High school chemistry teachers have daily access to student assignments via formative
assessments. How teachers use those assessments to evaluate student understanding
and inform their teaching practice is described by the process of data-driven inquiry,
although not in a content- or context-specific manner. Based on a previous qualitative
study, a survey called the ACAST (Adaptive Chemistry Assessment Survey for
Teachers) was developed to probe chemistry teachers’ beliefs and self-reported actions
regarding their data-driven inquiry practices. This survey was designed to make
comparisons between responses from general and chemistry-specific probes. The
chemistry-specific probes mimic real classroom scenarios, such as setting learning
objectives, choosing items that align with that objective, and making conclusions based
on example student data. The probes are adaptive to teachers’ responses, adding
interesting analytic challenges balanced by the potential for a richer description of their
assessment beliefs and practices and more robust interpretation of responses. Results
will characterize the process that high school teachers use to inform their teaching via
formative assessment results through the use of inferential statistics. Meaningful
comparisons will be made from domain general to chemistry-specific items and also
within the chemistry-specific items. Suggestions to improve the use of data-driven
inquiry in high school chemistry along with key implications for research will also be
presented.

CHED 50

Uncovering high school students’ chemistry self-concept with cluster analysis

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Student beliefs and attitudes have been shown to affect learning and persistence in an
area of study. Self-concept is a domain-specific measure of a person’s beliefs about his
or her abilities. This study used the Chemistry Self-Concept Inventory to measure high
school students’ chemistry, math, and academic self-concepts. Student scores were
calculated based on the subscales that emerged from an exploratory factor analysis. To
further explore the data a cluster analysis was performed on four variables: Chemistry
self-concept, math self-concept, academic capability self-concept, and academic enjoyment self-concept. Four distinct groups were discovered with a hierarchical clustering technique. A rich description of the four clusters based on their characteristics, including teacher, sex, and academic track, will be presented. Findings have important implications for teachers as understanding the profiles of the groups may help us better identify and assist students who may be less likely to succeed and persist in chemistry. Implications for research will also be discussed.

CHED 51

Tool trouble: Challenges with using self-report data to evaluate long-term chemistry teacher professional development

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Science professional development (PD) programs with increased duration have demonstrated sustained instructional reform with respect to teachers’ use of inquiry-related methods. Such sustained reform, however, requires teachers to transform their beliefs about teaching and learning science. Yet, the development of instruments that longitudinally, comprehensively, and accurately measure teachers’ transforming beliefs has lagged behind increasing calls for long-term science PD programs. Using the Reformed Teacher Observation Protocol (RTOP), we have documented the effectiveness of Target Inquiry (TI), a two and half year, research-based PD program designed to reform chemistry teachers’ classroom practices. However, the use of several established teacher self-report instruments in studying the impacts of TI have yielded somewhat conflicting results. Self-report tools used in the study of TI were the Science Teaching Efficacy Belief Instrument (STEBI), Teaching of Science as Inquiry (TSI), and Inquiry Belief Teaching (ITB). These three instruments, along with the RTOP, were used to collect data before, during, and after TI PD from three teacher cohorts over six years. RTOP and interview data were consistent with teachers’ practice having increased and sustained alignment to reformed instruction. Contradictorily, these findings of increased and sustained alignment occurred alongside teachers’ apparent decreased knowledge and affect towards reformed instruction as measured by the STEBI, TSI, and quantitative component of the ITB. These conflicting results, their resolution, and implications for the longitudinal measurement of science teachers’ beliefs will be discussed.

CHED 52

Target Inquiry at Miami University (TIMU): Uncovering novel relationships among affective and cognitive measures of high school chemistry students
Target Inquiry at Miami University (TIMU) is a 2.5-year, intensive professional development program designed to meet the needs of high school chemistry teachers. The program is centered on implementing high-quality inquiry teaching in the chemistry classroom through immersion in authentic science practices, the design and implementation of inquiry activities, and an action research project. Data presented are from students whose teachers completed the first two years of TIMU. Results show the relationships between measured variables (scientific reasoning, chemistry conceptual understanding, metacognition, and self-efficacy) for the students of the TIMU teachers and comparison teachers. Additionally, few observed differences on cognitive and affective measures were found between TIMU and comparison teachers due to the time it takes to change teachers' beliefs and then have those beliefs transform their practices. However, exploring the affective domain of high school students gives a finer grained description of how students' attitudes and orientations toward chemistry influence achievement in the course. Qualitative data discussing the role of the summer research experience and the effects it had on teachers' content knowledge and beliefs about scientific inquiry and teaching will also be presented. The extent to which these interview data was found to explain the relationships observed in the student data can provide valuable insights into the effect of teachers' beliefs on their students' beliefs. Implications are abundant for professional development programs and high school chemistry instruction.

CHED 53

Efficacy of the connected chemistry curriculum

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The Connected Chemistry Curriculum (CCC) is a series of nine units (Matter, Solutions, Reactions, Gas Laws, Kinetics, Thermodynamics, Equilibrium, Acids & Bases, and Nuclear) that teach chemistry concepts at the submicroscopic and subatomic level using molecular-level simulations and corresponding workbooks. CCC utilizes guided-inquiry activities in which students investigate simulations and connect their observations to real world phenomena. Each CCC was designed by students, teachers, and researchers through several cycles of interviews, field observations, and revision cycles. The units were designed to be modular so that teachers can choose to use the activities to fit their classroom schedule needs. 9 teachers from different school types implemented a minimum of four units in their classrooms over a school year with CCC and a non-CCC classroom. Both class types were given a Unit Exam at the end of each unit. The data show that there was a main effect for class type on performance on the
Matter \[ F(1,194) = 4.695, \ p = .031, \ \eta^2 = .024 \], Thermodynamics \[ F(1,191) = 6.156, \ p = .014, \ \eta^2 = .031 \], and Acid & Bases \[ F(1,187) = 5.258, \ p = .023, \ \eta^2 = .027 \] units, with CCC student scoring significantly higher than non-CCC students. CCC students and non-CCC students performed equivalently in other units. In this talk, we present the efficacy data that was collected in a year-long study with 9 teachers in diverse settings. We propose causal mechanisms by which The Connected Chemistry Curriculum selectively improved performance in some units and offer recommendations for implementing the curriculum in ways to best improve student achievement.

CHED 54

STEM Modules: A multifaceted approach to enhancing science learning and perceptions in middle school classrooms

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It is critical that higher-ed and secondary systems partner to develop science materials that will transcend the traditional barriers (access to proper materials, restricted time periods, science equipment, etc.) that are currently limiting STEM engagement within the early learning settings. One way to address this issue is through the development of STEM modules that feature hands-on, science-based activities and 3-D simulation of science concepts through the partnership of STEM and education faculty and master teachers – a multidisciplinary team. Hence, this report describes the forging of the partnership and the development and implementation of STEM modules into middle school classrooms that were developed under this framework. Data collected before and after implementation of the STEM modules into the classrooms revealed that students’ knowledge and perception of STEM dramatically improved after completing module activities.

CHED 55

Technology integration in the undergraduate chemistry classroom

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Technological advancements have increasingly allowed chemistry instructors to integrate instructional technology into their classrooms. These technologies enable student learning by, for example, providing dynamic models of the particulate nature of matter, or providing the instructor with real-time feedback about student understanding.
However, in much of higher education, faculty receive training on the functional capabilities of technologies rather than the ways that these tools can be meaningfully and intentionally integrated with evidence-based pedagogy and specific course content. As a result, little is known about the ways in which chemistry faculty combine instructional methodologies (e.g. Peer Instruction or Just-in-Time Teaching) with digital tools (e.g. computer simulations or molecular animations) in undergraduate chemistry courses as well as the benefits to students' learning as a result of technology-enriched learning environments. The extent to which chemistry faculty integrate technology in their teaching can be described by the technological pedagogical content knowledge (TPACK) framework, which is an extension of Schulman’s pedagogical content knowledge framework. This framework has been underutilized in chemistry education research. As a first step to understanding the integration of technology with pedagogy in chemistry undergraduate classrooms, we apply the TPACK framework to the existing chemical education literature that is intended to introduce instructional technologies to instructors. In this presentation, we will describe the TPACK framework and provide the preliminary results of this investigation of the literature.

CHED 56

Building a teaching profile: Using a modified COPUS observation protocol to easily and reliably measure reformed instructional practice

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As the variety of faculty development efforts expand, there is an increasing need to quantify faculty classroom teaching practices. Stakeholders may be interested in monitoring changes over time, comparing instructional practices between instructors or courses, or mapping observed behaviors to research-defined teaching practices. Although existing observation protocols (RTOP, COPUS) may address some of these goals, their applicability is restricted by certain limitations. In this presentation, we describe our method for the reliable and valid characterization of instructional practices via easily-collected observational data. This method was developed empirically via a cluster analysis using observations of 269 individual class periods, collected from 74 different faculty at 28 different research-intensive institutions. We will describe the ten basic clusters of instructional behaviors, or “COPUS profiles,” which emerged from this analysis, including their validation with RTOP scores. In addition, a detailed breakdown of typical instructional practices by course level, class size, classroom layout, and faculty teaching experience will be provided. An interpretation of our findings, implications for faculty development efforts, and a description of available tools for implementing our method will be provided.

CHED 57
Training faculty with the Teaching Dimensions Observation Protocol (TDOP): Process and pitfalls

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As part of an NSF: WIDER funded project examining teaching practices across STEM courses at Western Michigan University, a group of faculty were trained as observers with the Teaching Dimensions Observation Protocol (TDOP). This instrument allows for data collection in two minute intervals across five dimensions: instructor actions, student actions, technology used, dialog, and cognitive engagement. In order to collect reliable data with the TDOP, inter-rater agreement must be established between observers. With a large pool of observers, this project moved outside of the scope of previously conducted training sessions with the instrument. This presented unique challenges for attaining consensus across faculty from a wide variety of disciplines. What will be presented here is a review of the TDOP, an outline of the training process used, inter-rater agreement outcomes, and an overview of how the observation data will be used in the context of the larger research project. The process of training faculty as observers, as well as the larger research goals, will be useful to the chemistry community in the development of research projects, assessment, and evaluation at departmental and university levels.

CHED 58

Creating a coherent STEM gateway for teaching and learning at Michigan State University: An AAU STEM initiative project

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The President’s Council of Advisors on Science and Technology noted in 2012 that “The first two years of college are the most critical to the retention and recruitment of STEM majors.” Researchers and faculty at Michigan State University have responded to this call from PCAST by initiating transformation of the gateway biology, physics, and chemistry courses. The MSU transformation process engages disciplinary faculty in conversations to determine the core ideas of the discipline and how students should be able to use those ideas combined with scientific practices and crosscutting concepts to explain phenomena and solve problems; that is, 3-Dimensional Learning. The emphasis on 3-Dimensional learning means that transformed instructional and assessment practices must be developed, implemented, and evaluated. Our long-term goal is to transform the gateway courses so that students learn to engage with the disciplinary core ideas, scientific practices and crosscutting concepts in the same way that scientists
Starting at the source: Foundational views about teaching influence adoption of learner-centered teaching practices

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This presentation addresses barriers to faculty adoption of engaging classroom activities and learner-centered teaching practices. Stepping back and reviewing experiences from the author’s past fifteen years in faculty development, a framework has emerged that addresses the source of resistance to change: foundational beliefs about the role of the faculty member and the role of the student in the learning process. Attitudes and beliefs about these roles greatly influence the willingness of faculty to adopt evidence-based practices and bear directly on the success of any change-related initiatives. Faculty development efforts led by the author address four foundational aspects of sustained teaching innovation and improvement. Our efforts involve working with faculty to (1) identify their own conception of what it means to teach (and what it means to be a student), (2) develop a more robust understanding of the science of learning, (3) assess their classroom climate, addressing the more relational aspects of teaching, and (4) engage in regular self reflection to help support their own experimental journey. This work is carried out through sustained consultations/conversations and peer mentoring, but most importantly, in an individualized, contextualized manner. By shedding light on existing paradigms and practices, providing resources and evidence tailored to an individual’s needs, and promoting incremental change, a stronger foundation is created on which to build a mindset of experimentation, risk-taking, and innovation in teaching practices and student engagement approaches.

Inclusive excellence in the classroom

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The changing demographics of modern day-students and the ever expanding role of technology they have been exposed to compels us to change our educational approaches to match them. We will survey some of the drivers and barriers for developing teaching tools that are accommodating to a broader audience. These considerations are critical to applicants for assistant professor positions who must write teaching plans. They are critical for new faculty writing educational components as part of early-career grant proposals. They are equally critical for all professors developing
course syllabi and teaching portfolios. Suggestions for adopting inclusive practices in the classroom useful in many of these cases will be presented and discussed.

CHED 61

VIPER faculty development workshops: Cutting edge content development and sharing pedagogical best practices

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Inorganic chemistry faculty have been sharing teaching and learning materials through the VIPER website (www.ionicviper.org) for seven years this spring. With support from the National Science Foundation we have expanded our mission to running workshops designed to help faculty create and share new content and become contributors and not just consumers of the material on VIPER. In our workshop model experts present cutting edge research and faculty take that material and adapt it for the classroom with the help of mentors from VIPER's Leadership Council. Pedagogical sessions include conversations on technological best practices and assessment techniques. We will provide evidence on how the workshops help to create stronger learning materials through collaboration and post-publication revision. We will share how the workshop experience and follow-up activities build a strong community of teaching faculty who are willing to share their both their questions and best practices. Suggestions from the workshops also feed back into the website development process to improve the features and usability of the VIPER website.

CHED 62

Cottrell Scholars Collaborative New Faculty Workshop program: Helping new faculty adopt effective approaches from day one

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New faculty often start their careers with limited teaching experience and sparse knowledge about how people learn. Only 30% of recent chemistry hires at research-intensive universities in our survey reported participating in programs, workshops, and/or courses on teaching during their training; 36% never used campus offices or centers for teaching and learning and only 15% sought teaching advice from them even occasionally. Of the 162 respondents to our surveys over the past 3 years, the vast majority had little knowledge of evidence-based teaching practices and had used only 22% of one of practices in their classrooms. The Cottrell Scholars Collaborative New Faculty Workshop was initiated in 2012 to help new chemistry hires become more effective and successful scholar-teachers. The workshop components and follow-up activities, designed using professional development research, target increasing awareness and adoption of evidence-based teaching practices. Strategies for successfully balancing and meeting expectations at research-intensive institutions are discussed. Student-centered instructional practices that can be readily implemented are modeled and practiced throughout the workshop. Participants develop and deliver teachable tidbits for their own courses. Connections are made to a broad network of colleagues and resources that can enhance faculty success. Follow-up activities, which expand the impact of the workshop, help to support individuals throughout the year following the workshop. In 2014, participants’ campus teaching and learning centers were enlisted to provide local support as well. The ultimate success of these initiatives will likely require the collaboration and the interplay between national programs and local professional development activities either within departments or through centers for teaching and learning.

CHED 63

Steering the ship from the front – how can deans change the culture to support evidence-based learning

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It’s always the faculty who are the clever ones. They work with the students and staff. They generally are so excited to try something new - but it’s always as an overload. It’s done “on their time”, while they are doing all the other things. To quote John F. Kennedy, “[they] do these things not because they are easy, but because they are
hard,” and they are moving the needle in science education. Whether it’s developing an interdisciplinary class for non-science majors or a principles of biology class that integrates major scientific concepts, supporting active engagement at a traditional large land grant university has its challenges. There are a few examples of successes and failures that suggest ways we can steer a large ship into charted but new waters.

CHED 64

Responding to barriers to and drivers for faculty adoption of evidence-based instructional practices

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Evidence-based instructional practices are well-documented by education research and the scholarship of teaching and learning to be effective in supporting student learning. Despite this, their adoption is not widespread among higher education faculty (inclusive of those in chemistry). As part of an NSF WIDER project, we have engaged all science, engineering and math faculty on our campus in a facilitated data-gathering process to learn how they perceive a proposed change to student-centered, evidence-based teaching practices. Input from faculty provided information about both driving and restraining forces (barriers) for change. This presentation will focus on the results of this data gathering effort and our initial responses, which aim to both build on the reasons faculty already have for making changes in their teaching and remove barriers to adoption of evidence-based instructional practices. Results from chemistry faculty and initiatives will be placed in the larger institutional context.

CHED 65

Development of a structured support fellowship for faculty innovation in teaching

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At Washington University in St. Louis (WUSTL), our focus on transforming how students learn about science includes changing the way in which faculty develop their knowledge of effective, evidence-based teaching. Faculty success at navigating the change to newer instructional methods requires the institutional leadership (chairs, deans, provosts) to support the infrastructure for pedagogical research, for fostering a feedback cycle of continuous improvement, and for a reward system to promote innovation in
teaching. Our programs, currently supported by the AAU Initiative on STEM Education, are creating a culture in which faculty can feel comfortable taking risks with new teaching practices—a culture in which faculty find support and the opportunity to collaborate with one another. Our programs aim to provide information on evidence-based active-learning pedagogies, assistance with implementing and evaluating these pedagogies, and the collegial support of a faculty learning community. These programs include the CIRCLE Fellowship.

The CIRCLE Fellowship has been launched via collaboration between two WUSTL centers focused on teaching and learning: The Teaching Center and the Center for Integrative Research on Cognition, Learning, and Education (CIRCLE). CIRCLE Fellows engage long term (two-year minimum) in a learning community that brings together the Fellows with a graduate-student intern, The Teaching Center, and CIRCLE to design, implement, and evaluate a teaching innovation. This project group meets during the academic year in a laboratory-research-meeting style format to discuss the project. Fellows also attend The Teaching Center’s Summer STEM Faculty Institute on Teaching (STEM FIT) in their first fellowship year and present their project at STEM FIT during their second year. Our goal is to put structures (such as the CIRCLE Fellowship) in place to accomplish institutional and sustained changes in STEM, and to establish a culture at WUSTL where teaching is a shared and collaborative endeavor (not a solitary one).

CHED 66

Mentoring junior faculty: Pedagogy is only important if you keep the job where you use it

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Mentoring programs for junior faculty can address common issues in all three portions of the academic position: teaching, research and service. Examples of effective programs include workshops, one-on-one mentoring, peer evaluation, discussion groups and grant programs with senior faculty mentors.

CHED 67

Long-term impacts of the Cottrell Scholars Collaborative New Faculty Workshop

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Chemistry graduate programs typically do little to prepare faculty to teach. As a result, assistant professors have a limited knowledge of the research on how people learn and develop their teaching skills and approaches on the job. Initiatives in physics and biology have demonstrated that short, national workshops for new faculty can significantly raise their knowledge of research-based instructional practices. Members of the Cottrell Scholars Collaborative initiated the New Faculty Workshop (CSC NFW) in order to provide a similar opportunity to chemistry assistant professors at research-intensive universities. The long-term goal of the CSC NFW is to promote the teaching identity of academic chemists, who mostly identify themselves as researchers. Along with the implementation of the workshop, a longitudinal, quasi-experimental design study was undertaken to evaluate the extent of its impact. Online surveys were collected one week before and one week after the workshop as well as one year later from CSC NFW participants and a control group that consisted of newly-hired chemistry faculty that did not participate in the workshop. Classroom video recordings from both workshop participants and the control group were collected during the fall semester following the workshop and two years later. Video recordings were analyzed using the Reformed Teaching Observation Protocol (RTOP) and the Classroom Observation Protocol for Undergraduate STEM (COPUS). These data were triangulated with the Student Evaluation for Educational Quality (SEEQ) survey which was collected from students in the observed classrooms. Teaching beliefs were measured with the adapted Self-Efficacy Toward Teaching Inventory (SETI-A) and the Approaches to Teaching Inventory (ATI). Barriers to implementation of new teaching strategies were also captured. In this presentation the impact of the CSC NFW will be discussed by sharing the results and interpretation of the longitudinal data collected from two cohorts.

CHED 68

ISSUES: Investigating student success using evidence-based strategies

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Faculty learning communities (FLC’s) have been shown to be an effective vehicle for systematic change in higher education. At CSUSB, a Hispanic-Serving Minority Institution in Southern California, the ISSUES FLC is working to initiate transformation of early STEM courses using evidence-based teaching methods. Over the past 14 months the FLC, composed of six faculty from three science departments, along with the College Dean and education/teaching enhancement personnel, has been meeting regularly to pursue our goals. After studying and discussing key references in STEM learning and teaching, each faculty participant is pilot testing one or more evidence-based teaching/learning methods during Fall quarter, 2014, and initial evaluation of the methods is underway. Keys to success for this project to date, an overview of the innovations in the FLC pilot classes, particularly successful FLC features, and plans for broadening participation within College will be presented.

CHED 69
Green extraction of lycopene from tomato (*Lycopersicon esculentum*) using 2-methyltetrahydrofuran

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Lycopene, the major carotenoid found in red-fleshed fruits, is known to have antioxidant properties that are important to human health. Breeding efforts aimed at improving lycopene content in fruits such as tomato (*Lycopersicon esculentum* Mill.) have increased as a result of the beneficial implications to nutrition. Traditional methods employed to determine lycopene content rely on the use and disposal of hazardous organic solvents. In this study, an analytical method to determine lycopene content in tomato using ‘greener’ solvents with respect to those used in traditional extraction methods was developed. Lycopene content was determined using UV/Vis spectrometry and a ‘greener’ solvent, 2-methyltetrahydrofuran (2-MeTHF), was used in place of tetrahydrofuran (THF). Green and traditional methods were performed alongside each other for each fruit sample and then compared using a paired t-test. Preliminary data suggests that the green method yields lycopene levels comparable to lycopene extracted using THF. This trend suggests the 2-MeTHF is a viable, less hazardous alternative to THF in lycopene extraction.

CHED 70

Improved protein digestion for the mass-spectrometric detection of cysteine palmitoylation

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The molecular mechanisms that regulate protein function via post translational modifications (PTMs) are largely unknown. Among the amino acid residues that provide scaffolds for PTMs, cysteine is rapidly becoming appreciated for its ability to host numerous modifications. Depending on the type and location of the cysteine based PTMs, differential effects on protein localization, function or stability can be achieved. We have previously developed methods to identify endogenous cysteine PTMs. To date 2,596 sites of cysteine PTMs have been mapped to 1,838 proteins. We aim to investigate techniques to improve the mass spectrometric identification of cysteine residues in the mouse liver proteome. Mass spectrometry techniques can only detect peptide fragments within a specific size range, limiting our ability to identify modified cysteine residues. In order to potentially increase the protein sequence coverage, we compared the fidelity of the endoproteinases Trypsin, Asp-N and Lys-C for use during enrichment of cysteine PTMs. The use of Trypsin resulted in the identification of 1,314 cysteines. Protein digestion with the alternate enzymes Asp-N and Lys-C resulted in
greater sequence coverage and detection of 440 additional cysteine residues, which represents a 25% increase in coverage. This is paramount to gaining a complete understanding of the biochemical and biological processes in which these modifications occur.

CHED 71

Degradation of estrogen: An NMR study

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Can ¹H-NMR spectroscopy be used to watch estrogen degrade in real time? In this work, two forms of estrogen, 17β-estradiol (E2) and α-ethinyl estradiol (EE2), are being investigated using NMR. The overall goal was to determine if NMR can be used to monitor the degradation of estrogens into other products. It is known that EE2 makes its way into natural water sources, and this is problematic due to the feminizing effects that estrogen compounds can have on fish and other aquatic life. Literature has shown that E2 and EE2 can be degraded in water using both biodegradation and photodegradation to form less harmful products. In research done by our collaborators (S. Mutiti, et al.) in environmental sciences, the samples of estrogen have been purposely degraded in an effort to determine the products formed. However, analysis of the degradation products has proven challenging. Hence NMR was chosen as a potential method to monitor the degradation. After determining the optimum NMR solvent for distinguishing EE2 and E2, ¹H-NMR spectroscopy was used to monitor the degradation of an EE2 sample over a given time. Results will be reported in this work.

CHED 72

Analysis of application of interpolation techniques to ultraviolet-visible spectroscopy of critical vesicle concentration

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Ultraviolet visible (UV-vis) spectroscopic analysis of vesicle formation utilizing merocyanin-540 produces a nonstandard nonlinear curve that is difficult to quantify using standard analytical techniques. Intensity of UV spectra correlates with vesicle formation, but to an unknown degree. This research uses interpolation methods to determine a function that maps changes in peak intensity to vesicle formation at varying concentrations of n-decylamine, glycerolmonodecanoate, and decanoic acid. This experiment compares several different interpolation methods against previously published data as well as experimental data generated by the authors. Lagrange
interpolation, peak intensity, peak intensity ratios, Gun method, Whittaker-Shannon
interpolation, were used to analyze uv-vis curves.
This research determined the free energy contribution to aggregation of vesicles based
on headgroup charge. It was found that ionic strength heavily impacted charged
compounds but played a lesser role in formations of structures using uncharged
molecules.
Results of this research impact understanding factors relevant in surfactant usage in oil
spill remediation, generation of liposomes for drug development, and origins of life
vesicle and cell formation theory.

CHED 73

Determining the degradation of an antioxidant, lycopene.

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The purpose of this research is to determine which factors affect degradation of
lycopene and at what rate. Lycopene is important as an antioxidant and can prevent
certain types of cancer, particularly prostate cancer. Previous literature has
demonstrated that extraction of lycopene is possible via solid-liquid extraction.
Furthermore, the extracted product can be successfully characterized via UV-vis. A lab
based off the extraction and characterization of lycopene was the original goal,
however, characterization has thus far proved problematic, despite known literature
spectra (UV-vis, NMR). Degradation of lycopene samples is suspected, thus a method
to analyze the degradation of lycopene has been developed. This work will report the
first phase of this study analyzing the effect of light on the molecule. This will be
measured by comparing the concentrations of lycopene extract in the presence and
absence of light over a given time period. Characterization and quantification will be
completed using UV-vis spectroscopy.

CHED 74

Application of ionic liquids in forensic chemistry

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Current techniques for isolating components of samples found at crime scenes by their
unique chemical properties are lengthy and often destroy important forensic evidence.
New methods aimed at forensic analysis of sensitive, minute samples are critical to the
intelligence community. In particular, successful extraction of dyes from materials found
at crime scenes will provide innumerable benefits for matching, identifying, and finding
origins of these materials and dyes. Ionic liquids possess the necessary chemical
properties to ensure efficient extractions while maintaining the forensic signatures of the
original materials. Ionic liquids, which are organic salts that are room temperature,
provide a versatile solvent to achieve single-component extraction-separation-identification of forensic analytes. Following extraction, successful identification by infrared, absorption, and fluorescence spectroscopy has provided evidence of preserved quality and complete separation of material and dye. This novel approach to forensic analysis is advantageous particularly when sample sizes are extremely limited, but it can be readily scaled to larger applications. Developing a simple and affordable method of achieving specific molecular interactions provides a solution for often unidentifiable evidence in crimes. Harnessing the versatility of ionic liquids in a high-yielding recovery and efficient single-pot methods will enhance forensic abilities for the intelligence community and forensic investigators.

CHED 75

Analysis of sol-gel processing as a controlled release method for fragrance molecules of essential oils

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As a common feature of many commercial items such as detergents and personal hygiene products, fragrances are an important aspect of a product’s design. In order to preserve the integrity of a fragrance, companies use a variety of techniques to provide a method of controlled release, one of these methods being the sol-gel process. This project involves encapsulating fragrance molecules and fragrance mixtures, particularly essential oils, within a sol-gel matrix in order to study the functionality of the fragrance overtime.

CHED 76

Integration in upper-division instructional chemistry laboratories at Regis University

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The problem of failing and withdrawing rates in STEM required courses is a major concern at small liberal colleges and universities. Oftentimes, upper division chemistry/biochemistry laboratories are taught with no apparent connection and relevance. We will present our efforts to integrate upper-division laboratories at Regis University. Our choice of cytochrome c oxidase stemmed from the following reasons: (1) electron transport chain is integral to aerobic life (mitochondrial respiration) and (2) current research has shown a link between neurodegenerative diseases, such as Alzheimer’s and Parkinson’s and a malfunction in the mitochondria, which includes the cytochrome c oxidase. The one-semester biochemistry laboratory involved the isolation, purification and characterization of the membrane-bound enzyme: cytochrome c oxidase.
In the synthesis lab, students revisited the synthesis of vanadyl bis-acetylacetonate complex. The complex was characterized by UV-Vis. spectroscopy, EPR, magnetic susceptibility (modified Gouy magnetic balance) and by $^1$H-NMR. Our efforts have led to both retention and advancement of students. As a result, many URM students have successfully completed graduate studies in chemistry/biochemistry at major universities (supported by WAESO; Hispanic Research Center, Arizona State University).

CHED 77

Integrated lab: The first year of a laboratory course integrating the sub-disciplines of chemistry and open-ended research experiences

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In this presentation we report on the first year of an integrated laboratory course designed to incorporate the essential learning outcomes from multiple upper division laboratory courses while simultaneously providing open-ended research experiences to senior undergraduates. The integrated laboratory replaces the traditional laboratory sections associated with the following courses: Physical Chemistry, Inorganic Chemistry, Advanced Organic Chemistry and Instrumental Methods. This newly created integrated laboratory course is a result of restructuring within our department and is credit neutral for our chemistry majors. In addition to integrating the content from the sub-disciplines of chemistry, the integrated laboratory infuses research into our undergraduate curriculum. The course provides an institutionally supported research incubator for faculty and student research interests, thus alleviating some of the time constraints often associated with research at undergraduate institutions. The integrated laboratory is co-taught and meets twice a week for three and a half hours per session. Students in the integrated laboratory course are assigned a research module to be completed over the course of 4 weeks, the modules rotate amongst students and evolve thought the year. Students are evaluated on their research notebook, their communication of experimental data in the form of high quality figures, and instructor observations of their laboratory practices.

CHED 78

Integrated Laboratory at Guilford College: An authentic research experience for chemistry majors

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For over 25 years, Integrated Laboratory has been the signature experience of the Guilford College chemistry major. Each spring, chemistry faculty create research teams
that include students who are taking organic chemistry and advanced chemistry laboratory courses such as physical chemistry and inorganic chemistry. Each year's lab has a general research topic at its center (such as chemiluminescence, Heck-Suzuki catalysis of cross-coupling reactions, or oscillating chemical reactions) and each team is charged with developing and executing an original research project in that area. We describe the research skills students develop in this course, with respect both to the science and to being a productive and useful member of a research group. We discuss how success in Integrated Laboratory requires much more than just basic knowledge of the science or even the ability to do good research (although both are essential components). We also focus on the intangible aspects of scientific research: the ability to be a good team member, the understanding of when it’s appropriate to take on a leadership role and how to be a strong leader, and the need to deal with the frustration when everything is not working as well as one would wish. Guilford chemistry majors are required to take Integrated Laboratory two or three times, taking on successively increasing leadership roles and thereby producing a multi-year capstone experience for the major that has at its foundation all the work done in prior chemistry courses. We discuss the setup of Integrated Laboratory, including faculty involvement in managing multiple research teams each with their own project. We also present evidence from alumni interviews about the influence the Integrated Laboratory experience has had in careers in industry, government and academia.

CHED 79

Elizabethtown College chemistry and biochemistry capstone experience

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Traditional undergraduate chemistry and biochemistry curricula are rich with content, and the increasing volume of knowledge to be gained can be daunting for both students and faculty. This often results in limitations in the content delivered, retention of knowledge, and students’ ability to communicate the science both technically and broadly. Additionally, while the practice of science has become more interdisciplinary, students have become increasingly likely to compartmentalize that which they are learning in classroom and laboratory courses. In this presentation, we will highlight ways in which the Department of Chemistry and Biochemistry at Elizabethtown College has addressed these challenges through three unique capstone experiences that are required for all chemistry and biochemistry students. The goals of the overall Capstone Experience are to expose students to topics not encountered in other courses, to highlight the interdisciplinary nature of chemistry, and to promote independent thought, creativity, teamwork, professional development, and communication skills. The experience spans the final two years of the curriculum and includes: (1) a 4-semester, topic-based seminar focused on broad interdisciplinary topics and on writing and oral communication skills for both technical and non-technical audiences (2) an independent research project which is part of a larger undergraduate research program including
inter- and intra-disciplinary investigations and (3) a 2-semester, senior-level, integrative, intra-disciplinary laboratory capstone course with a focus on novel research problems. Taken as one whole experience, this three-pronged approach emphasizes both learning and professional development through communication and experimentation. Specifically, the seminar course and the independent research project foster independent thinking and problem-solving skills while the laboratory capstone strengthens collaborative skills with a more global approach to learning. Student outcomes and the means by which the desired outcomes are measured will be discussed along with the identification of successes and challenges.

CHED 80

University curriculum meets departmental capstone: Integrating a novel seminar and research capstone into a liberal arts curriculum

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Susquehanna University has developed a forward looking liberal arts experience. Our Central Curriculum is designed to develop students who think not only in terms of their major but also perspectives from other disciplines. The goal is to integrate all facets of their education to frame their way of thinking about their eventual vocation. Given the global nature of education, industry and commerce, the curriculum topic might be approached from several perspectives and this has resulted in a refinement of the traditional courses in literature, history, and philosophy. Additionally, it has spurred the development of a whole new cadre of courses such as interdisciplinary, ethics, diversity, and team intensive courses. For example, the chemistry department offers two ethics intensive courses, Forensic Chemistry and Scientific Ethics, Fraud and Blunders.

The Chemistry Department has embraced the central curriculum goals by modifying select courses. We offer an overarching research based capstone and a novel four semester student seminar series. The research capstone is an immersive experience that is typically their senior year, but can start as early at their first semester enrolled. The students are trained and given ownership of their research projects. Research is presented during a campus celebration of scholarship and frequently at national ACS meetings.

The seminar series developed from a typical one semester seminar course. The department initiated adjustments to address to recurring weaknesses. The current iteration is four semesters long with the first semester having the students observe and participate in the Q&A sessions. The second and third semesters have the student preparing two professional seminars, first on an individual paper and the second a focused research topic, respectively. A series of graded benchmarks have been developed to guide the student in the proper steps in seminar construction and minimizing procrastination. The iterative development of our seminar series and future directions will be discussed.
CHED 81

Transitioning students to four year schools via an introduction to scientific research course

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An introduction to scientific research course has been developed to inform science majors of the opportunities they will likely have once they transfer to a four year school, and the choices they can make to gain access to these opportunities. In particular, the course introduces students to several choices for conducting scientific research: REU opportunities, internships, and undergraduate research positions at the schools to which they articulate. Successes of some of these students will be shared as well as some of the challenges that they faced.

CHED 82

Development of a pre-professional program at a rural community college

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Many of the courses required for entrance to professional programs are offered by community colleges making them a valuable asset to students seeking professional careers. SFCC has recognized the opportunity to better serve and attract the pre-professional student population. This presentation will focus on three of the tactics that have been implemented to improve the pre-professional transfer student experience: the design of advising pathways for the pre-professional students, the development of an AS in Chemistry, and chemistry course curriculum modifications.

Students need to complete a rigorous course schedule to be competitive applicants to professional programs. Since many required courses and their prerequisite courses are not offered each semester, advising sequence guides have been developed focusing on regional transfer institution program requirements. The guides are customized to each student.

The pre-professional program justified the development of an AS in Chemistry to better match transferring pre-professional student course sequencing. The degree includes courses that are typically prerequisite for the majority of professional programs. The chemistry courses in the AS program have been reviewed to better match the Workshop Summary on Chemistry Undergraduate Education published by the National Academy Press. A focus on undergraduate research, an emphasis on early introduction to organic and biochemistry, and an inclusion of pre-medical curriculum are some of the changes that have been adopted.
Advancing chemistry education in two-year college programs through self-assessment

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Two-year college programs are under increasing pressure to assess and document their progress toward programmatic and institutional goals. Moreover, programs that conduct such assessments are more likely to have successful student transitions to four-year programs and/or the workplace. The more efficient and effective an assessment tool is, the greater the likelihood it will be used. Because many two-year college chemistry faculty already have high teaching loads and departmental obligations, developing a useful assessment tool to provide this much-needed reflection can be daunting.

In 2012, a task force comprised of two-year college chemistry faculty developed an assessment tool based on the ACS Guidelines for Chemistry in Two-Year College Programs. An optional review process was also developed to give users feedback from peers in areas like curriculum, research, development of students’ skills, lecture and laboratory infrastructure, etc. to further their development. Since then, 38 institutions have used the tool, along with feedback from ACS, to determine what areas they are excelling in and those that could use some focus and attention.

In this presentation, we will address information on ACS assessment tool resources, feedback from users, and suggestions for assessing chemistry and chemistry-based technology education. In addition, we will share challenges and future direction of this resource.

CHED 84

NMR in first year chemistry

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First-year general chemistry has large enrolments at large universities and the students have diverse backgrounds. The vast majority of the students are not chemistry majors. NMR was introduced to engage the students with their learning by exposing them to up-to-date technology; and to represent modern chemistry to students for whom these subjects will be their only chemistry experience in higher education.
NMR spectroscopy was incorporated into two first year general chemistry laboratory experiments at the University of Technology Sydney in Sydney, Australia. With the advent of the bench top NMR challenges such as close access to instrumentation and high throughput have been overcome. The PicoSpin 45 NMR was moved into the student laboratory for the duration of the laboratory period each week. A pilot project in General Chemistry 2 Advanced was run to test the waters for future incorporation of NMR into all of General Chemistry 2.

The first NMR experiment involved students identifying an unknown aldehyde, ketone, or alcohol through colour tests, FTIR, and NMR. During the following laboratory experiment students synthesized an ester followed by analysis utilizing FTIR and NMR. A survey, ASCIv2 modified by Xu et al., was administered to determine students' attitudes to the experience focused on engagement and accessibility of material, in addition to a post-laboratory quiz.

CHED 85

Implementation of NMR spectroscopy into the undergraduate experience at The College of New Jersey

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The College of New Jersey (TCNJ) is highly committed to the integration of undergraduate research into its curriculum and possesses a strong institutional commitment to faculty scholarship and undergraduate research. In order to support this mission, we received funding from the National Science Foundation (MRI#1125993) and TCNJ in 2012 to purchase two high field NMR spectrometers for the enhancement of teaching and research activities in the department. This award resulted in the purchase of two 400 MHz Bruker NMRs to replace an aging 300 MHz spectrometer and support increased faculty-student research activities and the incorporation of NMR into traditional laboratory courses. To date, the instrument has resulted in: (1) 28 presentations at national meetings, 9 peer-reviewed publications, and preliminary results that were used for the submission of 6 external grant proposals, (2) the training of 52 undergraduates for research, and (3) the development of various teaching modules for multiple courses. Here we share our best practices and continued challenges for the implementation of NMR into undergraduate research activities and teaching across the curriculum.

CHED 86

New "spin" on integrating NMR spectroscopy into an undergraduate curriculum

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NMR spectroscopy has been integrated into every level of the CSB/SJU chemistry curriculum from first semester laboratories to senior capstone research projects. In the revised curriculum, the introduction to NMR spectral analysis was moved into the foundational laboratory courses. In their first college laboratory course in chemistry, students are introduced to $^1$H and $^{13}$C NMR analysis during recitation periods while simultaneously using spectroscopic techniques in the laboratory. In subsequent laboratories and research projects, students continue to use spectroscopy to determine the identity and purity of their products. In later laboratory courses, additional aspects are added such as complex coupling, 2D techniques, $^{31}$P and polymer end group analysis. The theory of NMR and advanced techniques are fully covered in an in-depth course. An overview of this implementation approach and preliminary assessment data will be presented.

CHED 87

More systematic approach to learning NMR spectroscopy

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Historically, one of the most difficult topics in organic chemistry is Nuclear Magnetic Resonance (NMR) spectroscopy. Prior assessment of student knowledge indicated students lacked a fundamental understanding of hydrogen environments, impact of functional groups, and interpreting spectra. The Supplemental Instruction (SI) program helps students to grasp the basic theory, usage, and analysis of NMR spectroscopy and previous results indicated a better understanding of NMR for students who attended a majority of SI sessions. However, results from previous research on the same topics showed that the methods used needed to be revised by using more intensive scaffolding and a more consistent systematic approach to helping students learn NMR spectroscopy. New methods, including more curricula based on scaffolding, the Socratic method, conceptual development, and group work were implemented. Students were assessed on their levels of improvement using pre and post semester tests which measured their understanding and ability to apply NMR spectroscopy.

CHED 88

Using spectra from undergraduate projects to improve higher order cognition
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For the first time since offering undergraduate chemistry degrees, the Metropolitan State University of Denver now has a 300 MHz high field NMR available to all undergraduate students. This talk will look at specific uses of the instrument in undergraduate research, in organic chemistry laboratory courses and in forensic science investigations. The impact the instrument has had on the mastery of technical writing for undergraduates, who have been using real data to evaluate their experiments will also be noted.

**CHED 89**

**13C should precede 1H NMR in teaching organic chemistry**

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Current textbooks delay teaching NMR until discussing alkyl halides or alcohols when 1H spectra become amenable to first order analysis. However 1H NMR isn't appropriate for teaching beginners as learning chemical shifts and coupling simultaneously can cause confusion with students. Proton decoupled 13C spectra deal with chemical shifts only and can be introduced early in the course prior to discussing alkanes with functional groups. Primary, secondary, tertiary and quaternary carbons are distinguished by DEPT experiments. Teaching 13C before 1H NMR has been recommended but textbooks have ignored it, most likely due to the limited access to 13C spectra in undergraduate institutions. Today 13C spectral acquisition is common even in labs with 60 MHz spectrometers thus resurrecting this idea seems appropriate now. After methane, heptane (C7H16) isomers are the simplest ones giving a signal for each C atom. Both 3-methylhexane and 2, 3-dimethylpentane are chiral so each C atom has a unique chemical shift. Students are surprised at this after previously learning that the methyl groups of an isopropyl moiety have identical shifts in pentanes and hexanes. Thus stereochemistry is introduced without reference to optical isomerism. Other examples will be discussed.

**CHED 90**

**Incorporation of benchtop NMR spectroscopy into undergraduate laboratories: An active-learning approach**

**Susanne D. Riegel**, susie.riegel@nanalysis.com. Nanalysis, Calgary, Alberta, Canada

NMR Spectroscopy is one of the most widely used characterization techniques in chemistry. Despite pedagogical shifts towards active-learning and guided-inquiry approaches, incorporation of NMR spectrometers directly into undergraduate curriculum
has remained largely limited due to mitigating factors of size, cost and availability of high-field spectrometers. As a result, students rarely gain hands-on access to this instrumentation, particularly in the beginning stages of their programs. An emergence of a new class of benchtop NMR spectrometers (42 – 60 MHz) that are affordable, portable and do not require weekly upkeep or maintenance can facilitate the introduction of this technique at all stages of chemical education. They also offer sufficient resolution and sensitivity for structure elucidation, reaction monitoring, and basic quantitation.

Herein, we describe methods for unique incorporation of the NMReady benchtop spectrometer into undergraduate laboratory experiments and illustrate how students can learn the proper technique to use an NMR spectrometer, prepare samples, monitor and characterize reaction mixtures.

CHED 91

Providing access to a million NMR spectra via the web

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Access to large scale NMR collections of spectral data can be used for a number of purposes in terms of teaching spectroscopy to students. The data can be used for teaching purposes in lectures, as training data sets for spectral interpretation and structure elucidation, and to underpin educational resources such as the Royal Society of Chemistry’s SpectralGame (www.spectralgame.com). These resources have been available for a number of years but have been limited to rather small collections of spectral data and specifically only about 3000 spectra. In order to expand the data collection and provide richer resources for the community we have been gathering data from various laboratories and, as part of a research project, we have used text-mining approaches to extract spectral data from articles and patents in the form of textual strings and utilized algorithms to convert the data into spectral representations. While these spectra are reconstructions of text representations of the original spectral data we are investigating their value in terms of utilizing for the purpose of structure identification. This presentation will report on the processes of extracting structure-spectral pairs from text, approaches to performing automated spectral verification and our intention to assemble a spectral collection of a million NMR spectra and make them available online.

CHED 92

Impact of chemical demonstrations on student interest and learning in science
In today’s culture young children are surrounded with an overabundance of distractions. It is quite a challenge to get students excited about anything that does not have an immediate reward. Demonstrations can be of great use in many fields, but the scientific field in particular can greatly benefit from the motivation and excitement that can come with the performance of demonstrations. The implementation of demonstrations in the classroom allow students to have a concrete (to some extent) example of what they are learning and often allow for inquiry learning in which the student uses what they already know as a foundation to help discover new ideas. This study was performed in an attempt to generate excitement about science, investigate the effects of performing demonstrations on student interest in science, and to teach basic chemical concepts. Students were given a questionnaire about their general interest in the field of science prior to the demonstrations. The questionnaire was divided into two sections. Questions in the first section were design to measure the student’s interest in science. The second section contained questions designed to measure the student’s knowledge of scientific facts, which were covered during the presentations. The demonstrations were performed for the students and the questionnaire was administered immediately following the performance and one week after the performance. Data from the questionnaires was collected and analyzed. The results will be presented and discussed.

CHED 93

Brewing alcoholic beverages as a means of incorporating writing instruction into an existing junior-level laboratory capstone course

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The Problems in Chemistry sequence at Mercer University is a two-semester, studio-style laboratory course that bridges a semi-independent synthesis project during the sophomore-level Organic Chemistry II laboratory and senior-level independent research. This course was originally developed to increase student exposure to instrumentation in the research lab, train students to utilize the primary literature to support their laboratory work and engage students in solving a variety of problems utilizing multiple chemical subdisciplines. Recent extramural funding has provided the department with new instrumentation to support this sequence. As a result of this funding, we have also reflected on how we teach and evaluate writing in our major. We have recently incorporated a six-week project in CHM 371 that involves the brewing of makkoli, a Korean wine made from the fermentation of rice. This project allows for the
scaffolding of a major writing assignment, class discussions about fundamental grammar and exploration of the chemical literature in a unique forum while teaching students skills they can use both in the laboratory and in their personal lives.

CHED 94

Enhancing research for students and new faculty at undergraduate institutions

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The chemistry department at Wheeling Jesuit University has developed a research model that contributes to a positive research environment and provides multiple benefits to both undergraduate students and new faculty. All faculty members have at least one project that involves the same class of molecules. The specific project depends on the specialty of the faculty member (organic, inorganic, physical, and analytical). However, all of the projects become interrelated. All research students and faculty participate in weekly research meetings where the student take turns reporting on their rec work. Benefits to students include; each student has greater contact with all faculty members, students can discuss their research with each other more readily because of the commonality, students can rotate through the faculty disciplines. Benefits to new faculty include, but are not limited to; easier initiation of projects, inclusion in grants and publications of senior faculty, potential for co-mentoring of students. This model provides very natural and non-intrusive mentoring of new faculty in their role as mentors (expectations, scope, and opportunities). The dialog during research meetings leads to generation of ideas for new research projects as faculty and students talk about on-going experiments.

CHED 95

Scientific connections: Development of a chemistry of art course for non-majors

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Ouachita Baptist University has recently begun revamping the CORE science courses offered. Previously, students took both Physical Science (physics and chemistry) and Life Science (biology). These courses sometimes focused more on content (and correcting the lack of content many of our students should have received in high school). The new sequence includes a Scientific Inquiry class, where students learn to analyze and apply data to real-world situations, and a Scientific Connections course, which focuses on connecting science to a particular real-world topic. The new Scientific Connections: Chemistry of Art course is being piloted in the Spring of 2015. This poster
will address the process of course development and approval, and the trials and victories of the first semester.

CHED 96

On the production of Chinese Purple in the art studio and chemistry laboratory

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Chinese blue (BaCuSi$_4$O$_{10}$) and Chinese purple (BaCuSi$_2$O$_6$) were two synthetic pigments prepared in China especially during the Han dynasty. Chinese purple is a metastable compound that slowly converts to Chinese blue. Both are related to the synthetic pigment Egyptian blue (CaCuSi$_4$O$_{10}$) first prepared in Egypt during the Early Bronze Age (from 3000 BC onward).

We will present results on how to prepare Chinese purple in the laboratory using readily available materials such as barite, malachite, and quartz. A flux is added to lower the processing temperature. We explore variations in stoichiometry, temperature, and processing time as well as the amount and type of flux. The equipment needed is minimal: crucibles and a programmable ceramics kiln. The latter can often be found in art departments at many primary and most secondary schools. Manufacture of Chinese purple is of special interest to students interested in art and chemistry and is a unique opportunity for collaboration between teachers of art and science.

CHED 97

Under the Dome: Student-designed evidence-based inquiry to understand and predict climate change outcomes

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High school students designed and executed a long-term project to help explore and answer questions related to the topic of climate change. A debate held on the subject brought to light many of the questions and evidence students most wanted to investigate. A scaled experiment designed to replicate earth-like conditions using model organisms was then designed by the students. Multiple sets of experiments were held simultaneously to compare possible future scenarios the earth’s atmosphere might encounter. The results of their experiments are discussed herein. This evidence-based inquiry method helped students feel more connected with what they were learning and find greater appreciation in the conclusions which were drawn.
The chemistry of Thomas Edison

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During the course of his career Thomas Alva Edison received more than 1000 patents and while almost everyone thinks of Edison as an inventor, it was his ability to understand the chemistry behind his work that allowed him to succeed in so many of his endeavors. In this presentation some of the chemistry associated with Edison’s lifetime of work will be presented including a discussion of one of his final research projects, the search for a domestic source of rubber that was actually a joint venture between Thomas Edison, Henry Ford and Harvey Firestone. The presentation will also discuss the granting of National Historic Chemical Landmark status to three of Edison’s laboratories by the ACS which occurred in 2014.

CHED 99

Application of mathematical concepts to teaching and learning of chemistry

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Mathematics is a fundamental subject in understanding our nature, our society and ourselves. Mathematics provides not only the conceptual knowledge, but also the procedural skills and logical thinking for teaching, research and service. Mathematics proficiency is the key for students to excel in chemistry. It plays an irreplaceable role in teaching and learning. The aim of this paper is to present the study of students’ abilities in understanding mathematical concepts and applying mathematical knowledge to chemistry.

CHED 100

FUTURE program: Ensuring that underserved populations become the scientific and civic leaders of tomorrow

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The FUTURE (Fellowships in the Ursinus Transition to the Undergraduate Research Experience) program at Ursinus College seeks to provide early research opportunities to members of underserved populations in science to encourage and equip them to become the scientific and civic leaders of the future. The program specifically targets underrepresented minorities (URMs), women, first-generation college students, and disabled students prior to, or immediately following, their first year at Ursinus. Students
in the program participate in a four-week summer research experience closely mentored by a faculty member and an upper class FUTURE mentor. In addition, the students participate in a team-taught course titled “Science and Mathematics in Society”, are expected to present their research findings at a regional or national conference, and are strongly encouraged to continue research in subsequent years. The FUTURE program was established in 2012 through HHMI funding as a part of the Center for Science and the Common Good (CSCG) at Ursinus College, which provides a framework for all Ursinus students to think, speak, and write about the impact of science on the common good. In addition to continuing their science education, the FUTURE students are encouraged to become FUTURE mentors and to participate fully in the CSCG. Since its inception in 2012, 16 FUTURE students, 16 FUTURE mentors, and 13 faculty have participated in the program from a wide range of disciplines (Biology, Biochemistry & Molecular Biology, Chemistry, Computer Science, Health & Exercise Physiology, Math, Neuroscience, and Psychology). Nearly all of the FUTURE students (15/16) have continued to participate in undergraduate research. In addition, results of the HHMI SURE III Follow-Up survey indicate that the FUTURE program yields above average gains in almost every category assessed. Thus, the FUTURE program is proving to be effective at ensuring that underserved students at Ursinus have the tools and opportunities to become the scientific and civic leaders of tomorrow.

CHED 101

Expansion of the Science Resource Center

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The Science Resource Center at SLCC is administered by the Division of Natural Sciences and Engineering to meet the needs of students for tutoring and other essential resources. Data on the number of students served and the associated costs is reported. The history of the center is reported, along with improvements in tutorial availability and quality. Due to success from previous years, the SRC received base funding from SLCC. The SRC will transition to a larger space and combine with the Math Lab to create a new STEM resource center.

CHED 102

With the scientific research advantages in the discipline, the construction level of chemical characteristic specialty is enhanced

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The characteristic specialty is both an important way of the innovative talent training, and an effective measure to enhance the construction level of chemical characteristic specialty. The following three aspects on the characteristic specialty have been carried out by School of chemical engineering and technology in HIT, China.

1. Translate into strong research directions of professional disciplines into the advantage of characteristic specialty. For many years the characteristic research directions are formed in our school. Theses have been translated into the advantage of characteristic specialty by our school. Our school has built characteristic professionals and high quality courses based on the subject basis and educational resources to meet the newer and higher requirements for chemical talent cultivation.

2. Convert the resources of academic research into the advantage of innovation talent training. In the idea of scientific research and teaching servicing for personnel training, scientific research laboratories are open to the undergraduates and the scientific research is transformed into the education teaching advantage. The scientific research and teaching platform are generated for students' scientific research training, curriculum design, graduation thesis (design), etc. Undergraduate tutorial system is another way to encourage students to participate in teachers' scientific research work early.

3. Change industry-university-research cooperation resources into the practice teaching advantage. Based on discipline advantage and industry market, the school has established a long-term and stable relationship with over a dozen enterprises on the scientific research and teaching cooperation, which lays a sound foundation for the student cultivation in the combination of production and study. To coordinate the campus and offcampus resources, and set up a joint laboratory with the enterprise to further strengthen the construction of practice base, the complex platform of teaching, scientific research and enterprise research is formed.

CHED 103

Cultivation of chemical engineering talents innovation ability based on the scientific research project trainin

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Students’ scientific research training is an effective way to cultivate research talents with innovative consciousness and innovative ability. Our School successfully carried out undergraduate scientific research training for many years, which has significantly improved the students' comprehensive quality and innovation ability.

1. Innovate the education idea and respect students' innovation spirit. One is to broaden the source of the scientific research project topics. All the projects are reviewed by the subject teaching steering committee before they are released to all students. The second is to strengthen the guidance to the topic selection. Before the project application, the professors are arranged to give a lecture on the related projects and the related scientific research activities and their development. The third is that the students
can freely make a team in the project.
2. To strengthen the process management, cultivate the students' academic literacy. Our school focuses on the process of strengthening training of scientific research project management. One is to make students master the methods of information retrieval through the electronic information resources retrieval lectures. The second is to complete the daily management of the project daily management. Teachers are responsible for the day-to-day management; the school concentrates on the intermediate inspection of the projects.
3. Pay attention to the concise summary, improve students' scientific spirit. Our school focuses on the final report and summary of scientific research project training. Firstly, the team needs to compose the final report; the discipline organizes the experts to check the project defense of the team. In the process of the defense, the expression, logical thinking and scientific rigor of the students are examined carefully. Secondly, the college student academic exchange platform is formed. Students are encouraged to summarize project results by applying for the patents, or composing research paper

CHED 104

The 2016 Biennial Conference on Chemical Education

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The Biennial Conference on Chemical Education will be hosted on the campus of the University of Northern Colorado the week of Sunday, July 31 through Thursday, August 4, 2016. We believe that there will be an exciting combination of plenary speakers, symposia, workshops, and exhibitors present which will encourage the elevation of chemical education research and practice for chemical educators at all levels, K-college.

CHED 105

“I want to be the inquiry guy!” How research experiences for teachers transform beliefs about teaching science as inquiry

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The current chasm between the need for reformed science instruction and teachers' nearly exclusive experiences with traditional, didactic practices has created a nationwide need for professional development (PD) programs that immerse teachers in scientific knowledge construction as it occurs in the field and laboratory. Toward this
goal, the Target Inquiry (TI) PD program at Grand Valley State University begins with a research experiences for teachers (RET) to help middle and high school science teachers develop more authentic beliefs about scientific knowledge construction. During the six week summer RET, each TI teacher works on a unique research project with a Grand Valley science faculty member where they review scientific literature, engage in data collection and analysis, and then present their findings at a regional or national conference. In conjunction with this experience, TI teachers also work to modify some of their classroom activities to more closely model for their students the activities they engaged in during their RET. Though such experiences have been found to positively impact teachers, there is still a need to understand how such opportunities affect teachers’ beliefs about science teaching and learning. To explore how TI’s RET influenced teachers’ beliefs about science instruction and their subsequent classroom practices, post-RET interviews were conducted. Using Pajares’s and Rokeach’s conceptualizations of beliefs, transcribed interviews were coded to identify and classify teachers’ changing knowledge, emotions, and classroom behaviors related to teaching science as inquiry. This poster will highlight the changes in teachers’ beliefs and attitudes about classroom reform in relation to their pathways of implementation, the features of the RET teachers cited as influential in precipitating these changes, and the implications for designing science PD programs.

CHED 106

Using Special English as a tool to engage students in chemistry lecture

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Special English was created by the Voice of America in 1959 for news broadcasts and other programming aimed at listeners in foreign countries where English is learned as a second language. It uses about 1500 words which are commonly used in everyday conversation, is spoken 1/3 slower than regular English, and uses short sentences and no idioms. Everything in the world is described or defined using the core set of 1500 words. New words can be used only after defining them using the core words of Special English.

For students in general chemistry as freshmen, chemistry can seem like a foreign language. For foreign students, the language barrier makes understanding chemistry lectures in English even more difficult. By speaking slower and by defining chemistry terms and concepts in the most simplest ways possible, students have a better chance of understanding lecture material and will do better on quizzes and exams.

CHED 107

Design, development, and delivery of the Nevada GEAR UP STEM Summer Institute
The Nevada State Gaining Early Awareness and Readiness for Undergraduate Programs (NV GEAR UP) project is a federally-funded, statewide project with a goal of increasing the number of underrepresented, low-income students who enter college. To meet this goal, NV GEAR UP supports middle school students’ learning in science, technology, engineering, and mathematics (STEM) subjects through services such as tutoring, STEM activities, academic advising, and professional development opportunities for their teachers. The University of Nevada, Las Vegas (UNLV) STEM leadership team has been tasked with providing NV GEAR UP middle school teachers with professional development opportunities, one of which is the 2014 GEAR UP STEM Summer Institute (STEM SI). The STEM SI aims to authentically integrate the Nevada Academic Content Standards in science, technology, engineering design, and mathematics by engaging the teachers in an interesting storyline as they attempt to answer the guiding question “What would an alien eat?” In this poster presentation, we will discuss the design, development, delivery, and initial evaluation of the SI.

CHED 108

PROPEL Center at Colorado State University-Pueblo: The effect of a STEM tutoring center on academic excellence

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The Providing Opportunities to Excel (PROPEL) Center at Colorado State University Pueblo is a Federally Funded initiative committed to supporting the success of STEM students. PROPEL offers a comprehensive portfolio of services, including free walk in tutoring for all STEM courses, supplemental instruction (SI) and group exam review support, assessment support for laboratory courses, Summer Academic Grade Forgiveness (SAFE) courses to help students succeed in key gate keeping courses, and sponsors diverse and engaging STEM speakers for students to learn from and network with. Additionally, the PROPEL initiative has allocated funds to update STEM research labs and classroom labs with cutting edge equipment and much needed renovations, and fund faculty to participate in a Summer Institute program, where they are tasked to focus on curricular redesign, and streamline articulation agreements with partnering community college institutions. The day-to-day operations of the PROPEL center are successful, in part, due to a highly motivated team of peer tutor mentors that are all STEM undergraduate students. Statistics garnered by the center have shown that students who regularly attend study sessions or visit the PROPEL Center have increased exam scores and are more likely to overcome gatekeeper courses in their
STEM majors. For example, the scores for an Organic Chemistry SAFE course offered by the PROPEL Center in the Summer of 2013 showed a 40% increase in passing rates compared to the same course offered by the same instructor in the Spring semester of that same year. In this poster presentation, two peer tutor mentors will share their experiences as Chemistry tutors for the PROPEL Center, and provide insights to others looking to create comprehensive Chemistry course support at their higher education institutions.

CHED 109

Revision of chemical professional undergraduate training scheme guided by "Excellence engineers education program"

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Excellence engineers education program of China aims to foster a large number of various types of engineering and technical personnel with strong innovation ability and adapt to the economic and social development needs, serving for the new type industrialization developing direction and the construction of an innovation-oriented country. "Chemical engineering and technology" specialty in School of Chemical Engineering and Technolog in Harbin Institute of Technology is the first selected to join the program in 2010. For the full implementation of the program and the active service for the national strategic needs and industry enterprise needs, our school has launched the revision work of undergraduate talent training scheme with the talents cultivation idea of “morality-oriented, ability to be focused, all-round development”. After nearly a year’s work, we have analyzed the effect of preliminary practice and formed the new training scheme of course system.

The new training scheme on knowledge structure processing is to build an organic connected professional curriculum system. In practice, the course system give full play to the "production-teach-research prominent" advantages of chemical engineering and technology discipline in the application of electrochemistry. Long-term and stable cooperative enterprise of scientific research and teaching include tens of enterprises, which lays a good foundation for student cultivation of production-teach-reasench combination. Secondly, our school has formed a big platform of scientific research and teaching. The openness of scientific research equipment and research laboratory resources to the students is strengthened gradually to make students to come into the lab early and involved in the teachers’ scientific research work. Thirdly, the teachers are encouraged to convert the achievements in scientific research into the teaching contents, which is helpful to teach the latest knowledge and skill to the students

CHED 110
High school students’ perceptions and performances on predict-observe-explain tasks in chemistry laboratory

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This study sought to understand the impact of gender and reasoning ability on students’ perceptions and performances of Predict-Observe-Explain (POE) laboratory tasks in a high school chemistry laboratory. Previous literature has reported that students at all levels have not developed the specific knowledge and skills that were expected from their laboratory work. Also, although boys have been more successful than girls in physical science and mathematics courses, this gap seems to be narrowing. This research was conducted at a mid-western, rural high school where the participants were 24 boys and 25 girls enrolled in physical science classes taught by the same teacher. The outcome variables used in the quantitative methods were POE performances and perceptions of the chemistry laboratory environment. MANOVA statistics revealed significant main effects in which formal-reasoning students outperformed their concrete counterparts, while females surpassed males on the outcome variables. Several qualitative oral and written methods were used to derive themes. The majority of these themes indicated that students both understood and enjoyed participating in the POE learning tasks. Implications and recommendations were described. The authors would like to thank Bryce Hach and Hach Scientific Foundation for their support.

CHED 111

“Building Your Science Toolkit:” Encouraging young female undergraduates to pursue science through laboratory experiences and interactive, tiered mentoring

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The minority status of women in STEM has brought attention to the necessity of instilling interest and confidence of scientific skills in women. Retention and persistence of women has improved but there still remains a paucity of women in leadership positions in the STEM industry. In order to address this, Simmons College has implemented a mentoring program that educates first years and sophomore undergraduates in biochemistry laboratory skills while providing leadership opportunities for senior students. The goal of “Building Your Science Toolkit,” is to engage students in research methods early and often to prevent them from exiting the science pipeline. Senior undergraduate research students mentor the underclassmen in the laboratory and provide a supportive learning environment. The seniors serve as roll-models of students with a clear science identity. Underclassmen will be able envision themselves in this position in two or three years time while they advance their laboratory skill set in
this program. Direct mentoring of the senior students by senior faculty enhances the “tiered” mentoring component. The faculty, seniors, and underclassmen participate in several “non-laboratory” activities designed to break down some of the significant barriers to women in science. “Building Your Science Toolkit” is peer driven and creates a challenging, but comfortable atmosphere for students to engage in foundational biochemistry laboratory experiments that encourage them to pursue science. We present here the program components and the assessment of three student cohorts.

CHED 112

Leveraging REU programs to attract talents in STEM fields: A comparison of outcomes of a discipline-based education research and a molecular science REU program

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Summer programs that provide research experience for undergraduate students (REU programs) have traditionally played an integral role in exposing students to authentic scientific research practices and transitioning those students from undergraduate coursework to research-based graduate programs in STEM fields. This model was recently applied to a program that focused on research in STEM education fields at North Dakota State University (NDSU). Coincidently, this university also run a molecular science REU program. The goal of this study was to compare the impact of these two programs on the outcomes that the National Science Foundation set for REU programs: "attracting students to and retaining them in science and engineering, and for preparing them for careers in these fields.” Identical data was collected in the form of pre and post surveys, weekly activity-log and post interviews from REU students in both of these programs over a two-year period. Our results indicate that participants in the STEM education REU program tended to have less initial knowledge of career options within the field of Discipline-Based Education Research (DBER) and fewer students in this program had been considering a research-based graduate program than those participating in the molecular sciences REU program prior to the program’s commencement. A greater change was observed in the number of students who said they would most likely continue their education beyond a bachelor’s degree in the STEM education program despite similarities in the nature of the research activities between the two programs. This would suggest that the STEM education program is more in line with the National Science Foundation’s goal of promoting research-based science among those students who would otherwise not consider it as an option.

CHED 113

Balancing “wow” and “satisfying standards” with hands-on activities and critical thinking: Developing middle school science modules
Creating a middle school science module which is engaging to students, satisfies state course of study objectives, incorporates current research techniques or results, and uses guided inquiry methods is a balancing act. This is a presentation of modules developed with a group of university professors, a middle school teacher, and undergraduate assistants as part of the project “A NanoBio Science Partnership for the Alabama Black Belt,” an NSF-funded Math and Science Partnership grant. In an eighth grade module on light bulb efficiency and a seventh grade module on the characteristics of living things, the trade-offs in achieving competing goals are discussed.

CHED 114

Test-based learning with online vs. paper tests

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Recently, it has become more common to assess students' learning in online settings. For the last several years, ACS Exams has been working to design and deliver its tests online. Even though technology is quickly establishing itself as efficient tool in education, only few studies have examined whether online assessment can offer similar learning benefits to students as traditional, paper-and-pencil tests. This study investigated the effect of test mode on the chemistry content with 660 students from introductory chemistry courses. In the present study, we measured student performance on two General Chemistry practice tests. All students took the practice tests on paper or online. Half of students took both tests in the same mode (e.g., first practice test on paper and the second practice test on paper) whereas other students switched the test mode (e.g., first practice test on paper and the second practice test online). Student characteristics and test features that provide insight why students perform differently in online versus paper-and-pencil administration will be presented.

CHED 115

When teaching chemistry and text messaging do work together in a classroom

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An instant text message method, polleverywhere.com, was introduced in a small chemistry class to be initially evaluated as a free interactive teaching tool. In the
classroom, an instructor usually decides if it is time to go into more in depth discussion or move on from the current chemistry topic base on past experience or the result of assignments. It is especially hard when question is asked and the students are not actively participated to answer it. To reveal student’s understanding level of the chemistry concept, an interactive teaching tool was studied, utilizing students’ cell phones and a skill they mastered already, text messaging. During the course of the study, students’ anonymous text messaging responses to the chemistry problems were collected in the classroom through the platform of polleverywhere.com. Instructor was able to see the result instantly using online access to the designed chemistry problem, and make instant modification and decision accordingly on the lecture content in the classroom. Students’ performance was improved by comparing two classes taught with and without the interactive method.

CHED 116

Younger Chemistry Education Scholars (YCES) committee: Who we are and what we do

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The Younger Chemistry Education Scholars (YCES) Committee was formed by the ACS Division of Chemical Education (DivCHED) in an effort to market the field of Chemistry Education Research (CER) to a broader audience, namely graduate students, postdocs, and early career (pre-tenure) faculty. The goals of the YCES committee are to aid in recruitment of undergraduate students into CER, and to support both graduate students and postdocs in their early careers as they apply for and enter into the field of chemistry education. To do this, the committee regularly organizes professional development activities and social gatherings at national meetings. These events include a CER symposium organized by graduate students for graduate students, interacting with undergraduate students at poster sessions, networking socials, and CV evaluations from CER scholars. This poster will highlight recent committee events and outreach initiatives as well as offer ways for others to get involved.

CHED 117

Frequent assessment: Does it make a difference in student learning?
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This presentation will examine the use of homework due prior to each class meeting and quizzes given at the beginning of nearly every class period in a sophomore Organic Chemistry class. Student perception of their learning via surveys and student evaluations as well as true gains in student learning via lecture exams, quizzes, homework, etc. will be assessed and compared to previous semesters where no quizzes were given and homework was submitted at the conclusion of an entire chapter.

CHED 118

New chemistry advanced placement (AP) test: Hands-on inquiry based experiment workshops

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A series of inquiry-type experiments were designed by the faculty and student members of the Florida International-Biscayne Bay Campus (FIU-BBC) Science Club to prepare high school students for the Chemistry Advance Placement (AP) Test. Over 70 students from different Miami-Dade high schools were invited. Students from Miami Norland Senior (95% African American, 5% Hispanic and 0% White); Miami Senior (3% African American, 94% Hispanic, and 3% White); Miami Southridge Sr. (41% African American, 50% Hispanic and 7% White); and North Miami Beach High (75% African American, 19% Hispanic, 3% White, and 2% Asian) attended the workshop and were presented with various experiments. This event provided AP Chemistry students with means to enhance their inquiry skills. Students investigated systems that reinforced their knowledge through inquiry-based labs allowing them to thrive in the new AP Chemistry test. Experimental stations were created in the FIU-BBC chemistry laboratories. Each station was designed to provide the students the freedom (with a logic strategy) to choose a method and materials needed to complete the task. The knowledge of many chemical concepts and the application of various laboratory techniques were required. Theories such as Le Chatelier’s principle and methods like calorimetry, colorimetric devices, titration, and basic glassware use were reviewed. The experiments utilized everyday materials in combination to Vernier apparatus and sensors. These experiments successfully prepared the students for their AP test owing to the support of the Science club members/advisors, non-Science club members, and high school teachers.

CHED 119

Using missing data methods to address the problem of incomplete national normative datasets at the ACS Examinations Institute
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As part of the process of developing nationally normed exams, the American Chemical Society Examinations Institute (ACS-EI) collects student datasets from volunteering colleges and universities from around the country. Since national data is collected on a volunteer basis, the ACS-EI may receive datasets which include students’ total scores for an exam, but not necessarily data regarding students’ responses to individual exam questions. However, several statistics calculated during the national norming process (e.g., difficulty & discrimination indices, etc.) cannot be calculated with only students’ total scores, and instead require students’ responses to exam questions. A future direction of the ACS-EI is the development of customizable exams in which instructors may choose the exam content based on a question database, and therefore, the problem of missing data intensifies since norming such exams without individual student responses would be very difficult. This poster will discuss the research methods used to address the missing data problem at the ACS-EI. Missing data methods have obvious implications for the ACS-EI, but such implications also extend into many studies in chemistry education research.

CHED 120

Incorporation and evaluation of science practices in multiple-choice items

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Students today have access to a plethora of information with the click of a button, so simple factual recall as the primary indicator of learning is no longer appropriate. Rather, the ability to use knowledge appropriately and within the proper context is of greater importance. The Next Generation Science Standards intertwine the use of science practices and cross-cutting concepts with traditional science content. In order to measure students’ development beyond content knowledge, redesign of traditional assessment items to incorporate the measure of skills beyond content knowledge will be necessary. Multiple-choice items are widely used in assessments because they are easier to score, yet they often offer fewer insights into how a student uses specific skills or practices to interact with the content knowledge. This poster presents an evaluation of instructor generated, Advanced Placement®, and ACS general chemistry exam items to inform the status of the current state of incorporation of science practices into multiple-choice assessment items.

CHED 121

Importance of demo shows in the community

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Most students receive their primary science education in a classroom setting. Although this is a viable stepping stone to learning and becoming competent in science, it can be detrimental when students try to apply their knowledge from the classroom in a setting outside school. The ACS student chapter at the University of Toledo hosts demo shows to the various community groups to enable students to think outside of the classroom and apply their knowledge in a practical, real world setting. The students are asked many questions while a demo is being performed to maintain their interest in the chemistry behind the demo. It is our goal that these questions help students expand their knowledge from the classroom. These demo shows are modified each time to present the science content at the level of the audience.

CHED 122

Fostering student success: Advanced topics and research at a community college

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Science majors at a community college ultimately transfer to a university. Success of community college science majors at a university is dependent upon the student receiving university level instruction and appropriate training in laboratory preparation, laboratory skills and use of modern instrumentation. Pima College has invested in student success by permitting the acquisition of modern instrumentation as well as putting into practice many of the suggestions presented in the “American Chemical Society Guidelines for Chemistry in a Two-Year College”. In addition, Pima College supports research and provides financial support for an American Chemical Society Student Chapter at Pima College. This Poster will highlight the efforts that Pima College East Campus Chemistry department has taken to facilitate success of community college science students and discusses the challenges and benefits of having program involving advanced topics and research.

CHED 123

Community outreach at Pima College East Campus: Summer research for high school teachers and high school students

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In addition to educating college students, community colleges also have an important role to play in supporting their local community. Pima College has supported the efforts of their chemistry department in community outreach activities. Outreach activities are varied, ranging from research programs for high school teachers as well as high school students to chemical demonstrations for grade school students being performed by college students involved in Pima’s ACS student chapter. This poster will highlight the community outreach activities that involve high school teachers as well as high school students who have engaged in chemical research at Pima College East Campus. The poster will present the challenges and benefits of Pima College East Campus reaching out to local high school teachers and high school students.

CHED 124

Introduction of powder X-ray diffraction in K-12 education

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The project team successfully designed and ran a two-week chemistry workshop funded by NSF for practicing K-12 teachers from a number of different disciplines. The goals of the workshop included: to generate transferable enthusiasm for chemistry, to encourage K-12 teachers to conduct scientific research and to cultivate teachers’ appreciation for the scientific process as the systematic, yet uncertain pursuit of new and exciting knowledge. The participants of the workshop learned how to use powder X-ray diffraction (PXRD) instrumentation and application of the instrument. Participants were given time to characterize a round of research samples using the PXRD individually. There were also opportunities for teachers and faculty to meet professionals in the industry and discuss uses of the instrument. The following instruments were used to evaluate the goals of the workshop: pre/posttest, practical assessment, student portfolios and student workshop assessment. Detailed schedule of the workshop, types of experiments, and the assessment data will be presented.

CHED 125

Investigating organic chemistry students’ ideas about nucleophiles, electrophiles, and reaction mechanisms

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Undergraduate and graduate students of organic chemistry struggle with the electron-pushing formalism used in mechanisms. Identifying nucleophiles and electrophiles is one prerequisite skill for students to master before they can attain fluency in the electron-pushing formalism, but little is known about how students think about electrophiles and nucleophiles related to reactivity in organic chemistry. Semi-structured
interviews were conducted with students enrolled in both first- and second-semester undergraduate organic chemistry. Although the second-semester organic chemistry students understand nucleophilicity better than electrophilicity, they also struggle to distinguish between nucleophilicity and basicity - a finding consistent with previous research. However, contrary to previously published research that found students failed to use mechanistic thinking even when explicitly directed to do so for a product prediction task, the students in our interviews immediately considered mechanism (without prompting) when asked to consider the presence or absence of nucleophiles and electrophiles in a variety of organic transformations. The juxtaposition of these findings suggests that students have well-defined ideas about the circumstances under which mechanistic thinking is useful. This poster will discuss these and other findings from the student interviews.

CHED 126

Developing an interdisciplinary medicinal plant research program that engages agriculture, biology, and chemistry undergraduate students across the curriculum

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Undergraduate science education has failed to meet the demand for science, technology, engineering, and mathematics (STEM) students. “Engage to Excel”, a 2012 report to the President of the United States, predicts a shortfall of 1 million STEM graduates over the next decade. The attrition rate for STEM students can be linked to many factors: lack of engaging subject matter, a disengaged learning environment, and lack of encouragement or recruitment of potential STEM students by STEM faculty. Supported by a seed grant from Tuskegee University, we are developing an interdisciplinary research based undergraduate education program that will span agriculture, biology, business, chemistry, and engineering courses and transform STEM undergraduate education. Using a discovery based, interdisciplinary research intensive learning method, we are fusing research and education to create an integrative environment where undergraduate students are engaged in impactful research while taking courses that are a part of their normal matriculation. Currently, we are integrating medicinal plant research into a number of agriculture, biology, and chemistry lecture classes and laboratories. Students will participate in original research that spans the entire medicinal plant spectrum. Students will take an active role in plant selection, plant growth and cultivation, extraction of important plant components, bioactivity testing of crude extracts, isolation and identification of active compounds, testing of active compounds for both individual and synergistic bioactivity, synthesizing derivatives of active compounds, and developing commercial applications. Because of Tuskegee
University’s land grant status and long agricultural mission to assist small farmers, medicinal plant research was chosen as the cohesive theme.

CHED 127

Connecting organic chemistry and biochemistry

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Students often fail to see the connection between the Organic Chemistry and Biochemistry. We worked with a research student on a combined lab experiment. The research project proposed examines the synthesis of two known inhibitors, difluorosuccinic acid and 2,4-dinitrophenol, and their effect on succinate dehydrogenase. The question posed is how the two synthesized inhibitors will obstruct the succinate dehydrogenase’s enzyme ability. To assess the type and the effectiveness of these inhibitors on succinate dehydrogenase in isolated yeast cells, we will utilize the knowledge of enzyme kinetics in conjunction with Succinate Dehydrogenase Activity Colorimetric Assay Kit. This proposed lab will enhance the laboratory skill for the Meredith students since so many of our organic students also take Biochemistry I. We proposed that the lab can be done in two periods in both Organic Chemistry I and Biochemistry I Labs and will give our students a real application of synthetic experience and enzyme inhibition.

CHED 128

Video instruction in organic chemistry: Student perceptions and preferences

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Research consistently shows that active, student centered environments promote learning more efficiently than traditional lecture environments. To this end, many educators have experimented with different types of video supplementation for both hybrid and flipped classrooms. In an effort to explore student preferences before large-lecture pedagogical reform, the following formats are explored: recorded classroom instruction, screen-cast PowerPoints of lecture material and tutorial shorts, screen-casts of think-aloud problem set solutions, and biologically-applied historical examples. In this study, the student perceptions of and preferences for several different video formats are assessed. Results from the student survey data will be reported.

CHED 129

Climate change outreach demonstrations
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The Illinois College chemistry club has been working with the Illinois Heartland Section of the ACS with support from the ACS Presidential Climate Science Challenge grant to engage the public on the issue of climate change. This poster will describe the interactive chemistry demonstrations used by our club that have been developed for this purpose. In this poster we will describe the experiments we use to explain the role of carbon dioxide in the greenhouse effect, the density of carbon dioxide, and the acidification of salt water by carbon dioxide. These easy to perform demonstrations allow us to explain issues associated with climate change to the public at various levels of scientific training, elementary school through college chemistry and beyond.

**CHED 130**

**Using an online assessment tool to gain insight to students’ usage of representations in chemistry**

**Jack Polifka**¹, jpolifka@iastate.edu, **Thomas Holme**². (1) Iowa State University, Ames, Iowa, United States (2) Department of Chemistry, Iowa State University, Ames, Iowa, United States

Using multiple representations in order to understand the particulate details of atoms and molecules is a necessary skill in chemistry. Recent studies suggest that college students often have more problems viewing and applying the concepts from chemistry-related representations to content material learned in the classroom than professors may anticipate. In order to yield new techniques for teaching students how to use chemistry-based representations, it is first important to understand the strategies students use when interacting with multiple representations. Use of online assessment tools create the possibility for gaining a better understanding of how students use representations in chemistry. In this study, participants solved general chemistry questions using an online application. Each question had a set of different molecules as answers. Participants had the option to switch which type of representation was displayed for a molecule and the online assessment tool tracked their actions as they did so. Data from the tracked actions in combination with interviews in which students explained how they used the application may reveal new patterns students use when solving representation-based questions. Findings regarding students’ strategies elicited by the Variable Representation Assessment tool will be presented, giving insights to student thinking.

**CHED 131**

**Practical component to a biochemistry lab final exam**

**Kyle R. Willian**, krw0018@auburn.edu. Chemistry and Biochemistry, Auburn University, Auburn, Alabama, United States
One of the fundamental skills a student in a biochemistry lab should master is the characterization of a protein, most often an enzyme. The standard measure of purity for an enzyme is specific activity. In a practical component to the lab final, students are given a protein sample and told to determine its specific activity. The students therefore need to demonstrate proficiency with total protein analysis (Bradford or Biuret with preparation of standard curves) and an enzyme activity assay. During the semester students prepare and characterize both crude protein extracts and purified samples and are exposed to several types of enzyme activity assays. Descriptions of these “training” experiments, implementation of the practical, and student outcomes will be presented.

CHED 132

Investigating cellular steady state as a threshold concept in biochemistry

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Threshold concepts (TC) are concepts that, when mastered, represent a transformed understanding of a discipline without which the learner cannot progress. Through a process of faculty and undergraduate interviews five TC’s were identified for biochemistry: steady state, biochemical pathway dynamics and regulation, the physical basis of interactions, thermodynamics of macromolecular structure formation, and free energy. A literature search revealed that little is known about what is taught and what students know related to steady state. Student free responses to questions about this concept were analyzed and responses showed wide variation in student understanding of steady state. Several themes were established when analyzing the responses. Many students believed that chemical reactions in biological systems are at equilibrium but failed to articulate how they knew this and the majority of students were unable to define steady state in a biological system.

CHED 133

Water quality education

**Brandi R. Bricker**², bbbricker@wvstateu.edu, Jade M. Weinkauf³, Michael W. Fultz¹, mfultz@wvstateu.edu. (1) Dept of Chemistry 217 Hamblin Hall, West Virginia State University, Institute, West Virginia, United States (2) Chemistry, West Virginia State University, Elkview, West Virginia, United States (3) Chemistry, West Virginia State University, Nitro, West Virginia, United States

Working in collaboration with the local Kanawha Valley Section the student group has worked to fulfill the objectives of two water quality grants. These grants involve the education in the community. The first grant was the Community Interaction Grant which focused on the education of elementary school students on the importance of chemical
properties of water that make life and society possible. The second is based on the local section Innovative Program Grant (IPG). This grant purchased equipment needed to work with the public on water purity. The probes allowed for training on how contaminants are monitored and allowed for basic data collection.

The Community Interaction Grant funded the creation of an elementary school science box with basic supplies to do water experiments in the classroom. These boxes are an important tool to help teachers conduct basic experiments with students in the classroom without the need for an extensive science background. All of the background information, procedures, and reagents were included in these boxes. Teachers across the region were given these boxes to reach more students with these boxes to reach more students with science then we as a small chapter could ever hope to educate.

The LSAC grant provided the section with the ability to purchase a water quality testing kit that allowed us to reach out to numerous high schools giving them the ability to collect information on the water that surrounds them and their schools. This information was then collected, compiled, and shared with the schools to better the teaching concepts in the classroom.

CHED 134

Development of a self-efficacy survey instrument designed to gauge the relationship between completion of AP chemistry and comfort level in first-semester general chemistry

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Students enrolled in the first semester general chemistry course at a mid-sized public university in the southeast have had varied levels of training prior to matriculation. A statewide push to increase the number of AP classrooms has increased the number of students that have taken at least one AP course. We have administered a self-efficacy survey to gauge student attitudes towards AP courses as preparation for college chemistry. The survey was adapted to student response over the course of the semester to establish validity. Students were asked to voluntarily participate twice during the course of the semester; at the start of the term and just before final exams. Surveys were built, administered, and recorded by an online learning management system (LMS). Though the pre-/post-instrument was similar for comparison of responses over the course of the term, the survey did undergo a revision prior to the second administration. This poster will present the survey items and detail the modifications made to the instrument over the course of the semester. Summaries of responses will be presented, and preliminary correlations between completion of AP courses and a number of variables (expected final grade, confidence in ability to study for exams, self-reported GPA, etc.) will be communicated.

CHED 135
Impact analysis of prerequisite incorporation toward student success in freshman-level college chemistry courses

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At the Spring 2012 American Chemical Society National Meeting, it was reported that there was a direct correlation between the success rate of students in freshman-level college chemistry courses and the score they earned on the mathematics portion of the ACT Exam. The evaluation of the data suggested improved student success if a prerequisite of a Mathematics ACT score of 21 for the General Chemistry in Health Sciences course, and a Mathematics ACT score of a 24 for the College Chemistry course was implemented with a college mathematics course co-requisite for those that did not meet the necessary requirement.

A course prerequisite was instituted to reflect these findings. Students entering either course are required to have a Mathematics ACT score of 21 or a prerequisite/co-requisite of College Algebra. In the research presented here, we will be reporting the findings associated with the incorporation of these prerequisites on student success rates.

CHED 136

Manual dexterity: assessing its role in the chemistry laboratory

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Few would argue that more than conceptual knowledge is necessary for success in a laboratory setting. However, few studies of teaching laboratories have included physical skills as part of the pre-testing regimen. Many tests for motor skills exist; some studies have shown improvements in predictions of job success when such tests are used in conjunction with tests of cognitive ability. These tests often are boring, time consuming, expensive, and require special training to administer. In addition, multiple tests might be necessary to address the aspects of manual dexterity relevant to laboratory performance. As part of another study focused on Thin Layer Chromatography, a novel test has been developed. Modified from a Hasbro Operation Rescue Kit board game, the success or failure of removing the bones is coupled with the number of times the sides were touched to assess various aspects of manual dexterity. Details on the modifications to the board, the reliability and validity of the board as a test, and the correlation of test results with student lab performance will be discussed.

CHED 137

Analysis of meaningful learning in the General Chemistry laboratory
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A review of the research on laboratory learning demonstrates the need to understand student perspectives in order to improve laboratory teaching and learning. Novak's Theory of Meaningful Learning states that the cognitive, affective, and psychomotor domains must be integrated for meaningful learning to occur. The psychomotor domain is inherent in the chemistry laboratory, but the extent to which the cognitive and affective domains are integrated is unknown. For meaningful learning to occur in the laboratory, students must actively integrate both the cognitive domain and the affective domains into the “doing” of their laboratory work. The Meaningful Learning in the Laboratory Inventory (MLILI) was designed to measure students’ cognitive and affective expectations and experiences within the context of conducting experiments in the undergraduate chemistry laboratory. The MLILI was administered online using Qualtrics survey software to general chemistry students (N=436) at the beginning and end of the fall semester. To better understand how students change from pre to post, the data was analyzed using hierarchical agglomerative cluster analysis. Cluster descriptions and implications for teaching and research will be presented.

**CHED 138**

**Teaching chemistry at a technical college through practical field work using performance based instruction: The Milwaukee River Project**

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Milwaukee Area Technical College (MATC) Chemical Technician program students collect river water samples from five predetermined sites within Milwaukee County’s watershed. Students conduct field analysis at these sites to collect data for phosphates, pH, dissolved oxygen, nitrates, nitrites, flow rate, temperature, and depth. The samples are then taken to MATC for analysis of heavy metals using Inductively Coupled Plasma Emission Spectroscopy (ICP-AES), pesticides by Solid Phase Microextraction (SPME) with Gas Chromatography Mass Spectrometry (GC/MS), UV-Visible Spectroscopy (UV-VIS) for the various forms of phosphorus, and Ion Chromatography (IC) for relevant anions in surface water environments. All field and laboratory analysis is performed by MATC’s Chemical Technician program students. This project was designed to teach two-year students the methodology of a research project by integrating hands-on work with performance-based instruction (PBI). Students learn to work and interact like a research group, applying proper techniques of surface water sampling, field analysis, data collection, data documentation, and stabilization of samples for transportation and storage. They analyze the results and prepare their findings for a conference presentation in poster format.

**CHED 139**
Fearless investigators: Teaching science through experimental design

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In a physical sciences course for non-majors, students design experiments to investigate energy-related phenomena. During whole-class discussions following each experiment, students describe experimental designs and results, as well as offer constructive criticism to their peers. When serious experimental design flaws are identified or a clear consensus does not emerge, students design and conduct fresh experiments. The course explicitly targets experimental design as well as energy content-related outcomes. As students design their own experiments to answer questions, they are able to focus on learning experimental design and energy concepts, undistracted by step-by-step procedures. Students are offered multiple and varied opportunities to demonstrate understanding of each outcome (via quizzes, lab reports, oral explanations, etc.), that is, about 40% of the grade follows a “mastery” or “outcomes-based” grading approach. We report gains in energy understanding using AAAS Science Assessment questions, gains in scientific reasoning using the Lawson’s Test of Scientific Reasoning, and discuss ongoing course development.

CHED 140

Flipping general chemistry via a highly structured teaching pedagogy: Initial conclusions

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In the 2013-2014 school year, a new assessment system was piloted and adopted for the general chemistry sequence at UC Davis. The purpose of this suite of tools was to give a faculty member, interested in adopting evidence-based teaching practices, a means to measure if their changes in practice are associated with improvements in student learning or attitudes. The assessment system has three components: content pre/post assessment, attitudes towards chemistry instrument, and systematic observations of in-class activities. The content assessment is a 35 question multiple choice exam which was designed at UC Davis to assess the learning outcomes for each quarter of general chemistry. Attitudes towards chemistry was measured by using the well validated CLASS Chem instrument (1). Classroom Observation Protocol for Undergraduate STEM (COPUS) Tool was adapted to characterize what type of activities are happening in the classroom (2). In Fall 2014, five lectures taught the first quarter of general chemistry. Four lecturers used more conventional teaching practices and one implemented a highly structured classroom pedagogy (3). This poster will show how the first attempt of this evidence-based approach compares to more conventional approaches using the new assessment system as the basis of comparison.
Using first-day assessments to determine math readiness for general chemistry

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Math readiness is essential for success in chemistry. However, many students come to General Chemistry with the inability to do the math required for standard introductory chemistry calculations. The use of a math assessment tool on the first day can serve to allay fears about math or allow certain students to identify math as being problematic, therefore increasing their chances of obtaining necessary, timely assistance. This poster presents the results of a short (10-minute) math assessment that is given in class on the first day of General Chemistry I. The assessment contains both arithmetic and algebra diagnostics. The assessment results are compared to overall success in the course at the end of the semester. The assessment has been given at three institutions with different student populations; results for two of the institutions show a strong correlation between the results on the assessment and success in the course regardless of student cohort. Results from the third institution, a 2-year public college, do not show this correlation. Possible explanations for the discrepancy are presented. The goal of the assessment is to provide awareness of mathematical deficiencies to students and to increase the number of students who seek the extra help that they need for success in chemistry.

Use of eye fixation sequence analysis to identify common cognitive processes among students solving conceptual stoichiometry problems

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This study analyzed the eye fixation sequences from students asked to solve stoichiometry problems dealing with particulate nature of matter diagrams. Fixation sequences for each question were grouped using k-means cluster analysis of similarity scores assigned to pairs of fixation sequences. Retrospective think-alouds (RTAs) were then used to identify cognitive processes that students belonging to the same cluster used in combination with visual analysis of the diagrams. Common cognitive processes among students grouped together were then identified through analysis of the RTAs.
CLP: A collaborative learning program in chemistry with benefits for both students and facilitators

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The concepts of peer-led learning and collaborative learning have been used for many years in chemistry education and the advantages of these approaches are well documented. There are many references that show that this method has many advantages. The Chemistry Department of Saint Vincent College has implemented a Collaborative Learning Project (CLP) which incorporates aspects of Supplemental Instruction and Peer-Led Team Learning (PLTL) in a unique way. Our evidence to date shows that the method not only has significant benefit for the students enrolled in the classes, but there are also positive impacts on the facilitators. A unique aspect of our program is the significant role that facilitators have in designing the details of the peer learning activities. This responsibility appears to help facilitators develop both a better understanding of the concepts used during the CLP sessions as well as how these concepts are used in upper level classes they take.

Development of a service-learning introductory chemistry course for culinary arts students

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This presentation will discuss the transformation of an introductory chemistry class designed for non-science major students into a service-learning course specifically designed for culinary arts students. An outline of the course with specific lecture and laboratory materials/examples geared towards the culinary arts will be included. The capstone project for the class was a service-learning project involving America’s Second Harvest in which students prepared recipes with ingredients that are in plentiful supply in the America’s Second Harvest pantry but difficult to find a use for in common recipes. The culmination of the project was a cook-off in which students prepared their dishes and invited the college as well as the general public to taste the dishes and vote for their favorite for a small donation. Pre and post student perceptions and attitudes about chemistry as well as service-learning will also be presented.
Transparency and electronic assessment

**Erik M. Epp**, erikepp@gmail.com. Chemistry, WebAssign, Apple Valley, Minnesota, United States

Online and electronic learning systems have provided new ways to assess student understanding and learning. Electronic learning system questions can be programmed with a wide array of randomizations for chemical formulas, reactions, structures, equations, and more that increases variety and makes it more difficult for students to plagiarize. These new assessment choices also present a challenge to confirm the validity of questions and the accuracy of the answers and solutions. This poster discusses that evaluation process along with considerations in the selection of a learning system and describes how to both analyze and edit the question programming in one particular system.

CHED 146

Constructing a consensus definition of conceptual understanding in chemistry from empirical data provided by instructors

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There is a large body of literature on the merits of conceptual learning and going beyond the more algebraic approach to problem solving as a way to understand chemistry. In 1996, the ACS Exams first released a conceptual exam for general chemistry. The ACS Exams is currently in the process of developing their fourth conceptual exam for general chemistry. In order to address a change in the nature of how concepts are incorporated in the course, a national survey was implemented which measured first what types of multiple choice questions are perceived to measure conceptual understanding followed by faculty. Definitions from approximately 1500 faculty members have been coded and analyzed. The definitions provided by faculty members have overall shown an inconsistency in how conceptual understanding is defined. The definitions are currently being used to work towards developing a working definition of what it means to measure conceptual understanding. Trends within the definitions and the responses on the survey will be presented.

CHED 147

Water quality comparison of city facilities and residences in North Miami, Florida

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The City of North Miami Water and Sewer Utility serves a population of over 70,000 people in a 13 square-mile area, including portions of unincorporated Miami-Dade County, Miami Shores and Biscayne Park. They also provide emergency interconnects to the municipalities of North Miami Beach and Opa-Locka.

The United States Environmental Protection Agency (EPA) and the State of Florida Department of Environmental Protection (FDEP) set both primary and secondary standards to ensure public water is safe to drink.

The aim of this project was to analyze whether differences exist between treatment facilities and residential tap water.

The FIU-BBC Science Club members and Upward Bound Math & Science high school students collected water samples from different residential areas within the region of North Miami during the summer 2014. The students designed an experimental matrix with a set of parameters that included: density, pH, nitrate, chloride, salinity, calcium, magnesium and total hardness, conductivity, total dissolved solid (TDS).

Each parameter was measured using both a Vernier interface with specific sensors and traditional chemistry techniques. The data was analyzed using the statistical package SPSS 19.0 for Windows. There were non-significant differences in the density and total dissolved solid among the samples, but significant differences (p<<0.05) were found in the analysis of nitrate, chloride, salinity, and calcium, magnesium and total hardness. Although, all the values were within EPA drinking water parameters, we observed differences in the quality and composition of the water analyzed. These differences were among residences and among residences and facilities.

**CHED 148**

**Lewis Misconstruction: An investigation into student’s Lewis structure drawings**

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The construction of Lewis structures serves as a vital foundation towards understanding the structure of molecules and in turn the properties those molecules exhibit. Often, students are given guidelines to follow when constructing their Lewis structures; however, many students’ resultant structures are molecules that defy even the most basic rules. To gain better insight into the strategies students use to construct Lewis structures, 16 students were interviewed using a think-aloud protocol. The students were presented with five molecular formulas that required different approaches. Of the 16 students, 3 students drew an acceptable Lewis structure for each molecule. Thus, we will present the findings from the think-aloud interviews.

**CHED 149**
Describing and characterizing the affective domain in middle and high school science students

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Students’ views of science can become more negative as they move from middle to high school and as their exposure to inquiry-based methods of teaching science decreases. As greater emphasis is placed on the need for more science literacy in a U.S. society and knowledge-based economy, greater emphasis also needs to be placed on understanding how increased use of inquiry-based instructional practices influence students’ affect towards science. Research on the affective domain of middle and high school students—how they feel, their motivation, and what they believe—can give valuable insight into maintaining student interest in science and facilitating their success in science classrooms. This study focuses on students’ affect in classrooms associated with Target Inquiry (TI), a 2.5-year professional development program at Grand Valley State University and Miami University aimed at increasing middle and high school teachers’ use of inquiry in their classrooms. We used the Students’ Adaptive Learning Engagement in Science (SALES) Questionnaire with the four subscales of self-efficacy, task value, self-regulation, and learning goal orientation, to track student affect as their teachers progressed through TI. At the beginning (pre) and end (post) of each academic year, the SALES was administered. Pre- and post-SALES data, along with data related to students’ reasoning skills and conceptual understanding were collected over two years from the teacher cohorts from each TI site. Analyses yield relationships among the SALES subscales and students’ changing conceptual understanding and reasoning skills. Results as well as implications for teaching, professional development, and research will be presented.

CHED 150

Introducing computational chemistry: A hands-on spreadsheet approach

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Computational chemistry is a powerful tool for used in chemical research and chemical education. However, often times it is seen as a black box by undergraduate students. Here we present a method that can be used in the physical chemistry lab to teach students the theory behind geometric optimization. By using simple molecules, students can perform geometric optimizations using a spreadsheet software such as Excel. The
students can then continue on to optimize their molecule using a computational chemistry software such as Gaussian, allowing them to connect their hands-on spreadsheet calculations with the “black box” of computational chemistry software.

CHED 151

Conformational analysis discovery activity using 3D potential energy surface models

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Discovery activities in chemistry can provide students with a deeper understanding and longer retention of important concepts. There have been some reports of conformational analysis discovery activities using computer models or ordinary molecular models, but those activities do not provide students with a tactile sensation of potential energy. Recently we developed three-dimensional models that represent potential energy as a function of molecular geometry. Here we report a discovery activity for introductory organic chemistry in which students combine textbook images, molecular models, and 3D potential energy models to explore conformational analysis.

CHED 152

Mathcad exploration of Fourier transforms found in physical and analytical chemistry courses

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The Fourier transform algorithm has practical applications in analytical and physical chemistry. When these courses are taken concurrently, the mathematics of the algorithm are taught through applications of quantum mechanical systems such as the particle in a box. In systems where momentum and position are the pertinent domains, the Heisenberg Uncertainty Principle is demonstrated with the Fourier transform on a linear combination of cosines, accomplished by analytical integration. Further, a linear combination of harmonic oscillator states built up to model the particle in a box is validated. The transform is also applicable to the time/frequency pair, whose primary application arises in analytical spectroscopy. Here, the transform converts a Fourier series between time and frequency domains via the Fast Fourier Transform algorithm. This Mathcad exercise demonstrates the Fourier transform on a square wave function in conjunction with the Nyquist Theorem, demonstrating the impact of sampling frequency.
Mustard: Tiny seed - unlimited possibilities

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Seeds of yellow mustard present a unique teaching tool for understanding a series of important concepts in chemistry, biochemistry, and biology. Here we present an educational module that is suitable for use in both K-12 and higher education laboratories as well as a standalone STEM workshop. Mustard seeds have a unique chemical composition that facilitates demonstration of the following concepts: acid-base equilibrium, enzymatic reactions, colloidal systems, biodiesel production, and herbicidal and antioxidant activities. The proposed module consists of six independent experiments that can be accomplished in four 45-min lab periods. Most of the demonstration reactions are monitored using colorimetric indicators and no analytical equipment is required.

CHED 154

Impact of supplemental video prelab material for a biochemistry lab practical on student overall preparedness

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Gel electrophoresis is a widely used technique for the separation of proteins in a mixture. However, reliable results require strict attention to the technique to complete the procedure. Students in an upper level undergraduate biochemistry methods course, given one chance to do gel electrophoresis, need to be well prepared in order to get good results. A three part video was developed as a pre lab preparatory tool to demonstrate proper technique to students prior to completion of the required lab experiment. The video included the processes and steps involved in making, loading, running, removing, and staining the gel. The purpose of this research is to measure the effectiveness of the video on students overall preparedness. Participants were given a brief questionnaire to measure basic chemistry knowledge. Based on responses to the questionnaire, students were divided into two groups of seven while attempting to maintain an equal chemistry knowledge base between the two groups as possible. One group of students was given access to the video. The group of students that was asked to watch the video was given 24 hour access via Blackboard and had two weeks to view it on their own schedule. Both sets of students received the normal laboratory instruction via pre lab discussion given by the graduate teaching assistant and the faculty instructor. During the experiment students completed a questionnaire about the time required to complete each step, their level of confidence in their ability with each step (on a scale of 1 to 5), and their overall confidence in their ability to repeat the lab. The questionnaires, the graded lab reports, and data retrieved from Blackboard showing if/when the students actually viewed the video, were analyzed in an attempt to measure the effectiveness of the video as a useful teaching tool.
We report here representative student data for a simple quantitative analysis of glucose using the enzyme glucose oxidase as coupled to a colorimetric reaction. A microplate reader was employed to rapidly determine absorbance values for multiple aliquots of a range of standard concentrations of glucose. A standard curve was then prepared and used to determine the concentration of an unknown glucose sample. In a separate exercise, students used a single-beam spectrophotometer to investigate enzymatic decomposition of glucose over time. Absorbance/time data were then evaluated using zero, first, and second order integrated rate equations to determine the order of reaction as well as the experimental rate constant. This experiment is most appropriate for use in an introductory (first or second year) quantitative analysis course, as it provides a correlation between biochemical catalysis and simple rate laws, as opposed to the more sophisticated Michaelis-Menten kinetic model utilized by biochemists.
Measuring silver nanoparticle concentration by inductively coupled plasma optical emission spectroscopy: A laboratory experiment for chemistry and engineering students

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The worldwide proliferation of nanoscience and nanotechnology is predicted to create by 2020 approximately six million specialized jobs in these fields. To meet this educational need, a novel nano-laboratory module was developed and successfully carried out in two upper-level laboratory courses at WSU: Experimental Nanomaterials and Nanoscience and Instrumental Analysis. The main objective was to accurately quantify the total silver content of widely-used Creighton colloids by inductively coupled plasma optical emission spectroscopy (ICP-OES). Undergraduate and graduate students estimated the total silver amount via the external calibration (16.3 ± 4.7 mg L⁻¹) and the standard addition method (14.9 ± 4.2 mg L⁻¹) at two emission wavelengths (328.068 nm and 338.898 nm). It was found that the standard additions method generates more accurate results when compared to the theoretical yield of the reaction (15.4 mg L⁻¹) due to consideration of matrix effects. An average percent error of 3.2% was observed for the standard additions approach, while the external calibration method had an average percent error of 8.3%. The assessment of basic laboratory skills and the class assignments showed that the students successfully mastered the various aspects of samples/standards preparation, the operation of modern ICP-OES instrumentation, and the data analysis. Overall, the educational aspects associated with this novel laboratory experiment for science and engineering students were highly rated in the student evaluations.
Comparison of modes of delivery for safety information in an undergraduate laboratory

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While safety in the undergraduate laboratory is of utmost importance, nothing in the literature offers concise evidence on the effectiveness of the mode of delivery for safety information. This work tests the effectiveness of three different styles used to deliver safety information to undergraduate students taking an introductory General Chemistry Laboratory Course. The three modes are via text from a lab Manual, via bold text and clip art from a lab manual or via videos. Students read or saw safety information in a particular format and answered questions based upon their understanding and memory of the safety information. All safety information and questions were interfaced with the course software module, Blackboard. Results were analyzed to determine which presentation format was better to help students remember safety information. These results will be used to optimize the introductory chemistry laboratory course and offer safety information in a suitable format.

CHED 159

Microwave-assisted dye synthesis: A more efficient approach for an undergraduate laboratory

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The amount of time an undergraduate student spends in an undergraduate laboratory is minimal compared to the time many organic synthetic reactions require to set-up, monitor, and work-up. In this project, a microwave was used to synthesize reactions of triarylmethane dyes parallel to traditional synthesis using a heating mantle. Traditional heating required up to 30 hours for synthesis of the target dye, while microwave-assisted heating only took 35 minutes. In the first step of the triarylmethane synthesis, two different conditions were used with microwave-assisted heating: 1) with isopropanol as solvent, and 2) without any solvent. The second condition yielded nearly twice the amount of the product, with no different side reactions. Although the work-up of the products generated with two heating processes was the same, the set-up for the microwave reaction was faster, less cumbersome, and cleaner. Not only does the microwave-assisted heating saves time for undergraduate students and progresses their research faster, but it also saves energy. The amount of energy used to synthesize one dye during this project via microwave-assisted heating was ~ 27 times lower than the traditional heating method.

CHED 160
Quantifying and recycling precious metals from printed circuit boards: An undergraduate laboratory

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The ubiquity of printed circuit boards (PCB) is evident by the increased use of cell phones, personal computers, and electronics. PCB contain toxic metals such as lead, mercury, chromium, antimony, and arsenic as well as precious metals such as gold, silver, palladium, and platinum. Finding safe and environmental friendly methods for recycling and reclaiming these toxic and precious metals is necessary for both environmental and resource conservation. Recently thiourea has been investigated in the literature as a safe alternative to cyanide for the leaching of metals, and most notably gold, from PCB. An advanced analytical chemistry laboratory was written to study the feasibility and success of using thiourea for leaching metals from PCB. The metals were quantified using standard addition in an atomic absorption spectrophotometer. After quantitation of the precious metals the leached copper from the PCB was recovered through electrochemical deposition. The laboratory was engaging, relevant, and practical to undergraduate students because it utilized sustainable methods for the quantitation and reclamation of precious metals from the electronic materials they use every day.

CHED 161

Use of the three levels of representation to introduce the concept of buffers

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Students have difficulty connecting and transferring information between the three levels of representation (macroscopic, submicroscopic, and symbolic) in chemistry, hindering their understanding of chemistry concepts. Investigations have found that students without a conceptual comprehension in chemistry have the tendency to solve problems based on algorithms and recalling facts rather than on analysis. In this study, a hands-on activity that incorporates the three levels of representation was developed to help students hone their understanding about buffers while they explore the concept one level of representation at the time. The activity was implemented in a four-year undergraduate institution in Puerto Rico with two undergraduate populations: students enrolled in a second-semester general chemistry course and students enrolled in a first-semester physical chemistry course. Subjects’ progress during the activity was assessed through questions developed based on objectives that follow Bloom-Anderson’s taxonomy. In addition, qualitative data from observations and students'
comments during their work on the activity was collected. A comparison between the results of the two populations will be presented.

CHED 162

Periodic Table goes live

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Although chemistry is traditionally taught at the high school and college levels, it is critical that the foundation of this subject be introduced at earlier stages – in the middle school science classes. Research reports typically identify the attrition point for interest in pursuing science as a career starts in the middle school classrooms. That is, the middle school years are very impressionable and depending on the how science concepts are displayed, students will either love it or hate it. Thus, the intent of this module is to provide middle school science classrooms with supplemental, hands-on science activities that can be used to enhance science instruction. Thus the objective of this module is four-fold: 1. The students will be able to identify characteristics of selected elements from the periodic table, 2. The students will be able to identify elements from the periodic table that are found in common household products, 3. The students will be able to identify characteristics of selected elements from the periodic table by completing a research project.

CHED 163

Concrete solar cells? An investigation into an alternative form of alternative energy

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A new method of harnessing solar energy is investigated. Components of a solar cell were embedded into a concrete matrix and solar harnessing efficiency was determined. Analysis was completed using a Xenon-lamp solar simulator paired with a Keithley Sourcemeter. A prototype concrete solar-cell was created, and tested to determine the maximum voltage output and maximum circuit amperage. Also, electrode performance as a function of distance between electrode terminals within an electrolyte solution was examined. Overall results suggest that a concrete-based solar cell is a plausible technology if optimized based on concrete composition and electrode distance/solar cell
size. This work was supported in part through a summer 2014 internship award from the Bridgewater State University Internship Office.

CHED 164

Quantum dot sensitized solar cell for the undergraduate laboratory curriculum

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A CdSe quantum dot sensitized solar cell appropriate for undergraduate instruction was developed that utilizes a procedure in the pedagogical literature for CdSe quantum dot synthesis and many of the components of the dye sensitized solar cell described in the Nanocrystalline Solar Cell Kit marketed by the Institute for Chemical Education. The latter include tin oxide coated glass, P25 colloidal TiO\(_2\) and a graphite coating on the counter electrode supplied by a pencil. Loading of the CdSe quantum dots on the TiO\(_2\) matrix was achieved by using cysteine as a linker molecule. The working solar cell uses a polysulfide electrolyte in an ethanol/water mixture. Measurements under ambient conditions using a 90W headlamp gave open circuit voltage values of 0.3-0.4 V and short circuit current values of 0.8-1.3 mA. These parameters decreased from their optimum values after about 10 minutes. Fabrication and testing of this quantum dot sensitized solar cell was incorporated in a physical chemistry laboratory module which also includes synthesis of the CdSe quantum dots and their characterization by fluorescence and UV/Visible spectroscopy.

CHED 165

Integrated upper-division chemistry laboratory: synthesis and characterization of vandyl bis-acetylacetonate complex.

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Since the early reports of insulin mimicking properties of vanadium compounds, there has been a resurgence in the study of aqueous chemistry and biochemistry of vanadium in different oxidation states. Noteworthy vanadium compounds include vandyl bis-acetylacetonate, bis-picolinato oxovanadium(IV), bis(maltolato) oxovanadium(IV), and vanadium(V) citrate

The synthesis of the title complex is simple and straightforward and has been used in many instructional undergraduate inorganic laboratories. As part of an upper division synthesis and characterization laboratory, the title complex provided us with an opportunity to integrate spectroscopic techniques with the physical chemistry principles. The characterization of the vanadium complex involved UV-Vis (square pyramidal structure, crystal field theory and ligand binding studies), and IR ((V=O stretch). The paramagnetic susceptibility of the complex was determined by a modified magnetic
susceptibility system (Eaton et al; J. Chem Ed, 1979, 56, 170-71) and by $^1$HNMR (Evans’s method). The $^{d^1}$ configuration was studied by EPR. In addition, presently, we are performing electrochemical measurements (cyclic voltammetry for redox behavior) and synthesizing new vanadium(IV) complexes using small molecule ligands such as cyclohexane1, 3-dione and 5, 5’dimethylcyclohexane 1, 3-dione (dimedone).

CHED 166

Separations of acetaminophen and caffeine by high temperature high-performance liquid chromatography

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High temperature high-performance liquid chromatography (HT-HPLC) has great potential for uses in routine pharmaceutical analyses and can often be employed with little to no organic modifier, such as acetonitrile or methanol, in the mobile phase thereby lending to a green method of analysis. The use of HT-HPLC in the analyses of acetaminophen and caffeine has been investigated because of their presence in many different pharmaceutical formulations. Using a ZirChrom Diamondbond-C18 column and 100 % 0.7 M acetic acid at 3.00 mL/min, separations of acetaminophen and caffeine at temperatures between 60 °C and 110 °C were conducted. From the van’t Hoff analysis of the chromatographic data, the $\Delta H$ and $\Delta S$ for the mass transfer of these solutes between the mobile and stationary phases were evaluated. An analytical method was developed and evaluated for acetaminophen in a children’s liquid analgesic preparation by HT-HPLC using a ZirChrom Diamondbond-C18 column, 100 % 0.7 M acetic acid at 3.00 mL/min and temperature of 100 °C. Comparisons were made with results from conventional HPLC at ambient temperature using a BAKERBOND Octadecyl (C18) column with 10% methanol/90% 0.7 M acetic acid at 2.00 mL/min.

CHED 167

$^1$H NMR Analysis of the Methylation of Oleic Acid Catalyzed by Tin (II) Bromide in the Presence of a Cosolvent

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Biodiesel made from waste cooking oil is a popular substitute for petroleum diesel. However, due to its high content of free fatty acids (FFA), waste oil must undergo an initial acid catalyzed esterification. This process typically employs concentrated $\text{H}_2\text{SO}_4$ but we chose a milder Lewis acid, tin (II) bromide, as our catalyst. This project focuses on investigating the different cosolvents that can be used with methanol for this esterification reaction. The purpose of using a cosolvent is to be able to control the kinetics of this reaction by regulating the concentrations of methanol and tin (II) bromide (in a 1:1 ratio). Previous kinetic studies have been based on just methanol being the
main solvent resulting in the inability to regulate its amount with that of the catalyst. Preliminary data suggests that dichloromethane (DCM) can be used as a cosolvent for the production of methyl ester, allowing us to regulate the amounts of methanol and catalyst for the kinetics of the reaction with respective to time and temperature. Also, DCM was found to dampen the reaction and decrease the rate of the reaction, helping us to analyze the first-order kinetics for this reaction. Current studies that are taking place are focusing on the kinetics of this esterification reaction using DCM as cosolvent with tin (II) bromide as catalyst, at various temperatures and simultaneously we are also exploring other potential candidates as cosolvents for this reaction like tetrahydrofuran. This poster will present our interpretation of the data collected using a cosolvent species like DCM with methanol and how it affects the kinetics of this reaction.

CHED 168

Determination of organic and inorganic priority pollutants in herbal teas and coffee

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In recent years consumer consumption of herbal tea and coffee has been on the rise. This growth can be attributed to the many studies that tout the health benefits of herbal tea and coffee. Tea has been shown to prevent oxidation of LDL, or "bad" cholesterol, reduce blood clotting and protect against several cancers. Coffee's benefits include including protecting against Parkinson's disease, type 2 diabetes and liver disease while also improving cognitive function and decrease the risk of depression. While the health benefits of coffee and tea are outstanding there are still potential risks associated with their consumption. These risk are associated with priority pollutants that have assimilated into the tea leaves or coffee beans during their growth. The pollutants include pesticides, polycyclic aromatic hydrocarbons (PAH's), polychlorinated biphenyls (PCP), and toxic metals (Pb, Hg, Cd, As, Cr, Se, Ba). This paper presents the priority pollutant analysis results for several commercially available herbal teas and coffees. The organic constitutes were determined using microwave extraction with gas chromatography-mass spectrometry (GC/MS) analysis, while the inorganic metals were determined by microwave digestion followed by inductively coupled plasma mass spectrometric analysis (ICP-MS). Correlations between pollutant concentration and country of origin will also be discussed as well as a surrogate calibration scheme for derivative PAH determination.

CHED 169

Organic chemistry laboratory sequence alternating experiments with guided inquiry exercises

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In the traditional organic chemistry laboratory, much of the class time is spent on teaching discipline-specific technical skills. At Muhlenberg, the laboratory curriculum was revised to better fit the educational needs of pre-health students who comprise a majority of the course. In this model, more time is dedicated to higher-order process skills which transcend chemistry and are useful in any discipline. We have accomplished this shift in emphasis by alternating experiments performed in lab with guided inquiry exercises performed outside of lab. In this two-semester alternating sequence, the activities are used as a platform to introduce new material (e.g., nomenclature) and cover biologically-relevant topics which are typically omitted from sophomore organic (e.g., proteins, DNA, UV-vis spectroscopy). Importantly, the experiments are chosen such that all techniques traditionally associated with organic chemistry lab, such as distillation, extraction, and melting point analysis, are covered at least twice. To ensure students are developing proficiency in these techniques (and to get the most out of time spent in the lab), technique videos are made available to the students, and a lab practical is administered at the end of every year. Although students enrolled in organic spend approximately half the typical number of hours in the laboratory, they spend the corresponding amount of time engaged in laboratory-oriented activities intended to develop higher-order thinking (e.g., spectral problem solving, data interpretation). The benefits of this model, improvements that need to be made, student assessment data, and informal feedback will be presented.

CHED 170

Using 3D printing to model steric interactions

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Undergraduate organic chemistry students must understand the effect steric hindrance has on nucleophilic substitution and elimination reactions as a foundational step in mastering organic chemistry. However, visualizing the effects of steric interactions in space can be difficult for novice organic chemists. 3D printing can help address this difficulty by providing high-quality models that allow students to physically observe the effect steric bulk has on reactivity and confirmation. In this presentation we will provide detailed instructions on how to use Gaussian, in combination with other computational chemistry software, to build and print 3D representations of molecules. Several sample models will be on display during this presentation.

CHED 171

Simple technique for students to assign hydrogen atom resonances in heterocyclic ligand metal complexes

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NMR is widely used in chemistry to characterize chemical compounds. But in compounds with multiple numbers of protons, it is often difficult to assign $^1$H resonances to specific hydrogen atoms. In these cases, hydrogen assignments can be made using $^1$H-$^1$H, $^1$H-$^{13}$C NMR correlations by techniques such as COSY, HSQC, HMBC, etc. Although these techniques allow one to make accurate assignments, these technique require lengthy NMR usage times, and are normally unavailable to undergraduate students. We have found a simpler technique to make $^1$H assignments by using proton coupling constant $J$ values for a limited number of derivatives of tris-(2,2'-bipyridine)ruthenium(II) complexes. The methods presented in the poster will be useful in undergraduate chemistry teaching laboratories and in undergraduate research.

CHED 172

Integration of Green Chemistry topics into the traditional Organic Chemistry experiments

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Over the past several years, the experiments in our Organic Chemistry laboratory sequence have been modified to incrementally introduce students to the multifaceted topic of Green Chemistry. Our Green Chemistry integration progresses from the simple use of greener solvents to qualitative description of solvents’ greenness to a complex qualitative and quantitative analysis of a reaction. The students begin early in Organic I Laboratory with an experiment to examine the optical activity of D-limonene extracted using liquid carbon dioxide. The students next make a qualitative comparison of three solvents used for the determination of the partition coefficients of benzoic acid and sodium benzoate. Later in the semester, the students are able to use qualitative descriptions and the quantitative measure of atom economy to compare traditional and greener methods for the bromination of trans-cinnamic acid. For the first reaction in Organic II Laboratory, teams of students collaborate to compare two methods for the oxidation of cyclohexanol. The student groups characterize the relative benefits and hazards of each reaction. Each student is then asked to calculate atom economy, experimental atom economy, and environmental factor. The small groups prepare a final report summarizing and evaluating their results.

CHED 173

Boiling point, azeotrope: A simple discovery-based experiment for organic laboratory course

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A discovery experiment designed for the first semester organic chemistry laboratory course will be presented. Students identify three unknown organic solvents by measuring boiling points of pure liquids and their mixtures and performing miscibility tests. The experiment teaches students the important concepts of intermolecular forces, vapor pressure, boiling point, distillation, and azeotrope. The procedure requires a very simple set up and three common organic solvents as the only chemicals. Detailed experimental protocol, sources of error, and experiment video will be presented.

CHED 174

How to PDB: a class exercise for professional Pharmacy Med Chem

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Teaching Medicinal Chemistry has come a long way from our use of large plastic lecture models, and continues to evolve. Every year there are about twenty new drug introductions, with at least a couple of them representing first-in-class medicines. How does one teach to prepare students for material that hasn't been discovered yet? We have developed a class exercise to encourage familiarity with the principles of hypothesis-driven structure-based drug design, which summarizes the tools required for understanding inevitable new discoveries. The number of drug receptor interactions known at atomic resolution has exploded since Kari Mullis invented PCR, most accessible on the protein data bank (pdb), which has open access freeware for visualization. We have developed class exercises which incorporate the pdb into real time visualization of drug receptor interactions in Med Chem classes at the introductory graduate and professional pharmacy levels, where we use the on-line resource in class. There are individual and team based learning components of the exercise. Its fun, bring your lap top or cell phone, because there's an app for that.

CHED 175

Novel instructional undergraduate organic chemistry laboratory experiment exploring substitution patterns of various allylic halides

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There are very few published instructional undergraduate organic chemistry laboratory experiments that require students to explore the different allylic substitution reaction pathways. This poster discusses the development and implementation of an instructional experiment that allows for clear distinction of the different substitution pathways taken by various allylic halides when reacted with acetate nucleophiles. The
instructional experiment was initially designed to specifically compare and contrast the $S_N1$ and $S_N2$ reaction pathways, but has since been expanded to become highly amenable to the study of other possible allylic substitution pathways, such as indirect $S_N2$ attack. Upon completion of the standardized synthetic procedures, all products are analyzed by use of gas chromatography under optimized conditions. Students are then asked to rationalize their observed experimental outcomes using commonly understood substitution mechanistic theory.

CHED 176

**Intermolecular forces: An organic laboratory experiment**

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Working with consultation from faculty, undergraduate students developed a new laboratory experiment to be carried-out near the beginning of a sophomore-level organic course. The primary purpose of the lab was to reinforce the theory discussed in the concomitant lecture course involving how intermolecular forces influence melting points, boiling points, and solubility. The secondary purpose of the lab was to introduce laboratory skills such as melting point and boiling point analysis, use of the Sigma-Aldrich website to gain chemical information, and waste disposal. Furthermore, the materials (types and amounts) were carefully considered to provide a financially and environmentally sustainable laboratory protocol.

CHED 177

**Profile of metal bioaccumulation in selected invertebrates from the eastern and western shores of the Susquehanna River near Hummels Wharf Pennsylvania**

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The purpose of this study was to investigate potential bioaccumulation of metals in selected invertebrates of the Susquehanna River adjacent to Hummel’s Wharf, PA. Crayfish and hellgrammites were collected from 4 sites in the river, 2 east and 2 west of Byers Island, which bisects flow south of the confluence of the West Branch and North Branch of the river, downstream of the fiber dam in Sunbury, PA. Flow on the east side of Byers Island goes past the confluence with Shamokin Creek, a stream impacted by acid mine drainage. In addition, there is an old abandoned lead-zinc mine somewhere up the slope of the eastern bank. We suspected that organisms on that side of Byers Island would be accumulating metals from those sources. The tissue concentrations of 11 metals in Susquehanna River crayfish and hellgrammites from the 4 sites were determined. All organisms were collected from rock baskets in 2009 and 2010,
preserved in 70% ethanol by researchers at Susquehanna University, and provided to us for analysis. Crayfish samples were dissected into abdomens (n = 50) and cephalothoraces (n=48), and hellgrammites (n=7) were separated into head, thorax, and abdomen. Crayfish were classified as juvenile or adult based on length from tip of head to the terminus of the abdomen. All tissue samples were lyophilized and subjected to an acid digest with 5M nitric acid in closed containers at 75°C, with crayfish abdomens and hellgrammite portions digesting for 14 days and crayfish cephalothoraxes for 8 days. All tissue samples were analyzed for metals using ICP-OES. Organisms from the eastern bank site contained elevated levels of Fe, Mn, Al, Pb, and Zn compared to the other sites, indicating that Shamokin Creek and the mine are delivering these metals to the river.

CHED 177

Isolation and identification of natural products in dried turmeric in undergraduate research

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Curcumin in turmeric is known to have anti-inflammatory, anti-oxidant, and anti-microbial activity. Traditional Indian medicine utilizes turmeric to treat joint inflammations, ulcers, skin diseases, and other disorders. Extraction, separation, quantification, and characterization of curcumin from turmeric powder allow student researchers the opportunity to utilize thin-layer chromatography, liquid chromatography, HPLC, GC-MS, and NMR spectroscopy in isolating and identifying this substance. Results from a one-semester project quantifying the amount of curcumin in turmeric will be presented, along with ideas on how to extend this exploration in future laboratory experiences.

CHED 178

Multistep drug synthesis in the sophomore organic lab: Synthesizing \textit{R}\textsuperscript{-}rasagiline, a popular Parkinson’s drug

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A synthesis and chiral resolution of the popular anti-Parkinson’s drug, \textit{R}\textsuperscript{-}rasagiline (Azilect) was developed in order to introduce the intermediate or advanced chemistry undergraduate to a medically relevant multi-step synthesis. It makes use of concepts found in the undergraduate organic chemistry curriculum, conveniently fits into approximately three 3-hr lab modules and utilizes commonly found equipment and inexpensive commercially available chemicals.
Education through an inquiry based environment in the physical chemistry laboratory:
The thermodynamic of an electrochemical cell

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The objective of this project is to improve the way of teaching Physical Chemistry Experiments integrating an educational environment in which the student, in an active way, deeply enhance the mastery of concepts behind experimentation; inquiry based learning. As an example, the experiment of Thermodynamics of an Electrochemical Cell was selected. This experiment usually required two sections of 4 hours in which: a pre-test of 15 minutes is given to guarantee their reading comprehension of the experimental manual. The collection of data for effects in temperature and concentration were done in these two sections. Two weeks after the experiment ends, the student presents a post quiz and hands-in an experimental paper. In this cycle the assessment of learning is subject only to the correction of the paper, which is not assessment but evaluation. Also, the student never shares their findings or questions because a scenario to discuss and learn was never provided. In the inquiry based environment, now provided, a previous discussion divided in small groups precede the experiment. Here the different groups share and discuss the experiment concepts and help each other with the questions that arise before the experiment. After experimentation the students share again their findings and reach to conclusions about the lab experience. This poster includes the details about the way to conduct this experiment, the results obtained by the students including a way to integrate activity coefficients in their
calculations to determine the standard potential of the cell and some comments of the students related to this way of learning.

CHED 180

Synthesis and characterization of tricarbocyanine dyes for use in physical chemistry laboratory

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Polymethine organic compounds are commonly used as fluorescent dyes to label DNA and RNA and are used in biomedical imaging. These compounds have conjugated pi systems with varying absorbance intensities and excitation wavelengths depending upon the level of conjugation within the dye. These conjugated pi systems absorb photons causing excitation of electrons which then fluoresce upon return to the ground state. The amount of light energy absorbed represents the spacing between the energy levels and can be measured through UV/Vis spectroscopy. A traditional physical chemistry laboratory has been to use dyes with various conjugation lengths in examining a particle in a box treatment of the energy levels. In this project, the cyanine family of polymethine dyes was studied with the goal of synthesizing the uncommonly used tricarbocyanine iodide in order to study the effects of extended conjugated pi systems on the observed UV-Vis absorbance levels. The three shorter cyanine dyes within this dye series are commercially available; however the tricarbocyanine iodide is unavailable and difficult to synthesize. The synthesis of 1,1'-diethyl-2,2'-tricarbocyanine iodide was attempted through the base-mediated condensation of a quaternary amine salt and a bisimine. NMR and UV/Vis characterization of the isolated product showed that the condensation reaction was occurring with only one side of the conjugated bisimine chain. While this product was not the desired product, this partial reaction showed a promising direction in future synthesis and characterization of this and other tricarbocyanine iodides.

CHED 181

Discovering pressure-volume-temperature phase relationships with 3D models

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Undergraduate physical chemistry courses discuss phase transitions and stress the interdependence of the pressure, molar volume, and temperature of the system. To explain which phase is most stable and when phase transitions occur, textbooks use two-dimensional graphs to depict the behavior of the system as a function of pairs of variables (P vs T and P vs V). Unfortunately, students often fail to appreciate the connections between these different representations. We have produced 3D models of PVT relationships for an ideal gas and a real gas (carbon dioxide) that simultaneously
depict all three variables. These models are the basis for a group exercise in which students discover the broader connections between P, V, and T and see how two-dimensional phase diagrams and condensation graphs represent different perspectives of the same underlying phase equilibria.

CHED 182

Portable X-ray fluorescence spectrometry in the undergraduate chemistry curriculum at MWSU

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As part of a building renovation and expansion project in 2010, Missouri Western State University was able to obtain a Bruker Tracer-III X-ray spectrometer for use with undergraduates. Since then, this instrumentation has been introduced into the undergraduate in three major efforts which include two uses in courses, and several environmental research projects. The first exposure for students is in the Qualitative Analysis project of the General Chemistry II laboratory, in which students use XRF spectra as a secondary technique to complement the typical wet methods to identify unknown cations in an aqueous mixture. The second exposure within the curriculum is in Instrumental Analysis, in which the student perform a project where they compare the quantitative results of a brass analysis from three different instruments: XRF, FAA, and Spectronic 200’s. This allows students to not only learn different methods of analysis, but compare the results statistically. The environmental research projects have primarily involved soil from a local wildlife refuge, and analysis of runoff waters from campus parking lots during spring thaw. These projects have offered a way to quickly gather data so that larger questions can be addressed. They have also led to projects where the development of sampling methods for difficult samples are the focus, which reinforces points of analytical course preparation that is not easily done in a simple course experiment. An overview of these projects, as well as acquisition, storage, and maintenance information will be presented.

CHED 183

Preparation of samples for introducing undergraduate students to electron paramagnetic resonance

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Traditionally undergraduate students are not exposed to the technique of electron paramagnetic resonance (EPR); AKA electron spin resonance (ESR). In the case that instrumentation is available there is a limited number of samples suitable for ESR/EPR data collection and analysis. This poster will present procedures (and data) to prepare
both organic radicals and paramagnetic inorganic samples suitable for EPR investigation.

CHED 184

Quantitative determination of kidney cancer biomarkers in urine by liquid chromatography tandem mass spectrometry

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Kidney cancer is one of the most common types of cancer in the world, causing approximately 100,000 deaths each year. Current diagnosis techniques of kidney cancer, which usually involves angiography and biopsy, tends to cause pain and discomfort in patients. In an effort to identify useful biomarkers for this disease, some recent studies have shown that 4-hydroxybenzoate, quinolinate, gentisate, α-ketoglutarate, galactitol, N-(2-furoyl)glycine, and fructose can be potentially used for the diagnosis process. In this study, we developed and validated a noninvasive method to separate and quantify these compounds in urine using liquid chromatography- tandem mass spectrometry (LC/MS/MS), with creatine as an indicator for urine dilution.

CHED 185

Research and practice of the mode of training research capacity through scientific innovation

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Colleges are important places for cultivating high-quality scientific research personnel. Students’ innovation and scientific research ability is one of the core issues of the undergraduate education. Extensive undergraduate scientific innovation activities in universities and building the mode of training research capacity through scientific innovation will greatly promote the training of high-quality researchers. Through the establishment of scientific innovation platform will encourage the students participate in the whole scientific process, promote the ability-training of college students’ research, and make the scientific activities to be a real sense of inexhaustible motive force for the country needs high-quality researchers.

Keywords: scientific innovation, research capacity, training mode

CHED 186
Discussion on characteristic specialty construction and cultivating college students' technological innovation ability

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Specialty construction is an important strategic tool for colleges and universities to win the market and competitive advantage, the core task of the specialty construction is to develop high-quality talent. The 21st century is an age of knowledge economy of which the core is science and technology, the soul is innovation. For contemporary college students, the cultivation of innovative awareness and enhancement of innovative ability are the significant content of university professional characteristic cultivation. This article is intended to combine college students’ scientific and technological innovation ability to explore a number of issues in the college specialty construction research and practice, providing a theoretical basis for the study of science and technology innovation ability.

Keywords: Specialty construction, Innovation capability, Innovative awareness, Personnel training

CHED 187

Development of a hybrid course in sustainable energy

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A recent focus in education has been the development of the online learning environment. Increasingly, students want to be able to interact with course content at their own pace, on their own time. The advent of the “flipped classroom” learning model has also been gaining ground, as students can engage with materials before class and review learned material multiple times through video lectures. This presentation details creation of a hybrid course that combines both the traditional classroom and the online course environment to teach the role of chemistry in the sustainable world. Architecture of this environment has been to scaffold the student with a foundation of knowledge so that they not only understand the material, but interact actively with it. Throughout the course, students reflected upon their learning and were surveyed as to their thoughts regarding the hybrid nature of the course. Students found the dual nature of the course to be more rewarding than a single course either online or in the classroom. Students who would normally be reluctant to contribute to discussion in person felt comfortable contributing online, which added to the richness of the course environment.

CHED 188

Using theoretical chemistry to explain $S_N2$, $E2$, $S_N1$ versus $E1$ mechanism for undergraduate organic chemistry
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A key component in undergraduate organic chemistry is the teaching of the four elementary reactions, bimolecular nucleophilic substitution (S$_{\text{N}2}$), bimolecular base-induced 1,2–elimination (E2), unimolecular nucleophilic substitution (S$_{\text{N}1}$) and unimolecular elimination (E1). Popular organic textbooks rely on a combination of product analysis and transition state theory to develop a set of guidelines that will allow for the prediction of the correct reaction mechanism yielding the major product or product distribution arising from multiple mechanisms occurring at the same time, such as S$_{\text{N}1}$/E1. Many chemists have worked to expand the teaching toolbox, while simultaneously yielding a better understanding of these mechanisms. However, experimentalists and theorists continue to debate which mechanism is more appropriate for certain reactions and product distributions. Recent developments in modeling the solvolysis step leading to the formation of the carbocation intermediate, the rate limiting step of S$_{\text{N}1}$ and E1 mechanisms, has allowed for the development of a series of figures whereby suitable reactants can be used to theoretically determine the reaction energetics for all four mechanisms to be determined. Figures such as these are typically presented in textbooks, however for a variety reasons, only plot one or at most two mechanisms to show a difference in the transition state energy leading to the major product through a brief discussion of transition state theory. Presented here will be the work done to develop a series of figures with one favoring the formation of one of the four mechanisms as the major product. The other three mechanisms will be shown in all of the figures, so that students can fully appreciate that all mechanisms are possible all the time, but products are formed based on simple thermodynamic principles. Density Functional Theory and continuum models for explicit solvation will be used to find the minimum energies for the reactants, transition structures and the products. These energies will be used in making the figures.

CHED 189

Origins

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The emphasis of research and development activities at the University of Oklahoma in the 1980s and 90s was on laboratory, technology, and the beginnings of interests in visualization of particulate matter. The focus of this discussion will be on several publications to which Vickie Williamson contributed during that time. Some of these publications have influenced the growth of visualization as an area of study in chemical education to the present day.

CHED 190

Visualization and the learning cycle: A great partnership
Visualization has always been an important aspect of my efforts to help students gain a better understanding of models that are presented in introductory chemistry class. It was, and continues to be, a challenge to provide a dynamic view of the nature of matter. For me the introduction of microcomputers in the late 1970’s provided a means to deliver a dynamic view of some chemical models. The computer-based simulations that I worked on had to be interactive to allow students the opportunity to explore. Additionally, the simulations had to be accompanied with an activity written in the form of a Learning Cycle. Such an activity allowed the student to engage with the simulation to collect, analyze and interpret data. Forty years later, the technology is much more sophisticated, the platforms are more diverse, and animations are more accurate. Is it possible to generate activities that take advantage of the same technology to help our students become independent learners?

CHED 191

Six years in: Surviving and thriving at a SLAC

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Martin Methodist College is located in south-central Tennessee. Martin is currently in a period of growth. During the last six years, the numbers of students, majors, and full-time faculty have all increased. Six years ago chemistry courses existed primarily for either general science courses or for students majoring in biology to complete. Today, we are in the second year of having a chemistry major and minor available to students and two students have graduated with a minor in chemistry.

In this presentation will be a discussion of methods and technology used in an attempt to improve student understanding of chemistry while working with a changing student population and all the hazards and pitfalls they bring. Some methods are still in use in classes and others have been abandoned for the next shiny, new method while the search continues for the Holy Grail, a method that helps all students understanding of chemistry. Other topics touched on will be the beginnings of undergraduate research now that majors are available and other ways to bring chemistry to the Martin community.

CHED 192

Molecular visualizations through the lens of research and practice

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Visualizations depicting atomic level chemistry events are useful tools for communicating with our students about abstract chemistry events. In essence, animations could be considered analogies that use a computerized medium, in which cartoon billiard ball-like structures are used to represent the abstract and unfamiliar world of atoms. Moreover, the intended purpose of animations is to explicitly convey movement and interaction among atoms by showing balls colliding, attracting, repelling and sometimes even competing with each other. Like effective analogies, animations can help students better understand complex concepts improving their mental models and reducing misconceptions. The work of Vickie Williamson has been very influential in describing the effects of computer animation on the particulate mental models of college chemistry students. In addition, her work has examined how teachers implement visualizations in their teaching, and how connections between laboratory demonstrations and animations are important for developing students’ understanding. This presentation will report on my own teaching and research arc from high school chemistry teacher to a tenured university faculty position. Specifically, I will examine how my research studies on the design and use of visualizations have evolved and how they have influenced my teaching practice.

CHED 193

Visualizations in the chemistry classroom: A visual learner’s perspective

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As a self-identified visual learner, I recognized early on the importance of visualizations in helping me to learn chemical concepts and in helping me to teach others to learn chemical concepts. In this talk, I will address several forms of chemical visualizations (static drawings, dynamic computer animations, molecular models), my experiences with teaching and learning using these types of visualizations, chemical education research involving these types of visualizations, and suggestions for other teachers and learners struggling to effectively use these types of visualizations.

CHED 194

Developing and validating a measure of linked concepts for general chemistry

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Multiple learning theories value the process of a learner linking new information with existing concepts. While instruction may emphasize how new information is related to past course content, there is a concern that traditional assessment techniques may not explicitly measure this process. This presentation describes the development of a Measure of Linked Concepts (MLC) intended to target students' efforts to link concepts throughout a first semester General Chemistry course. MLCs are built upon prior
students’ attempts to link concepts in an open-ended context and are designed to be used in the large classroom setting as a part of a traditional assessment. As part of the development process, evidence to make a case for the validity of MLCs will be presented. Implications for learning theory and teaching practices will also be discussed.

CHED 195

Innovation diffusion in a single case: Adoption and re-invention of visualization research findings to improve applied research, instruction, and teacher professional development in chemistry

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Research on visualization in chemistry, specifically at the particulate level, has been critical in drawing attention to the need for a focus on conceptual understanding. Furthermore, it has provided a foundation and evaluation platform for interventions aimed at reforming instruction and improving chemistry learning outcomes. Roger’s innovation diffusion model serves as a useful framework to examine the elements and dynamics of how innovations, such as those from CER pertaining to visualization, are invented, shared, and adopted within a social system. This talk engages the elements and dynamics of Roger’s model to demonstrate how innovations have been adopted and re-invented in one case within contexts familiar to chemistry faculty. The innovations generated by Dr. Williamson’s work will be discussed in relation to how they have manifested through adoption and re-invention in one case in multiple CER projects, classroom instruction, and in-service teacher professional development. Implications uncover how Roger’s model furnishes a structure for reflection on fidelity of implementation for both research and teaching.

CHED 196

Redesigning the hydrogen spectrum experiment for guided inquiry

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The hydrogen spectrum lab is one of the classic experiments in the physical chemistry curriculum. Despite the simplicity of the chemical system, students can gain deep insight into energy levels, electronic transitions, and spectroscopic parameters. In this presentation, we discuss our efforts in redesigning this classic experiment into a guided inquiry format. Working within the Process Oriented Guided Inquiry Learning-Physical Chemistry Lab (POGIL-PCL) project, we took an existing hydrogen spectrum experiment and overhauled it to emphasize transferrable skills and student decision-making in order to help students discover the scientific content of the experiment. We
will briefly discuss the POGIL-PCL framework in the context of redesigning this experiment, and we will highlight the guided inquiry aspects of the redesigned lab by discussing specific examples of guided inquiry questions within the experiment.

CHED 197

Using the spectrum of HCl as a model building exercise

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The rotation-vibration spectrum of HCl is a standard exploration in many physical chemistry laboratories. Through the use of an inquiry-based activity students explore this spectrum using previously obtained data. Our students often demonstrate that a classroom exploration of quantized rotational and vibrational motions and associated energies does not fully translate into understanding of spectroscopic observations. The activity is designed to challenge students’ uninformed misconceptions about molecular spectroscopy. Based on the POGIL model, the activity provides students with data that they must use to develop and redevelop their understanding of quantum rotors and oscillators. The underlying purpose of the experiment is to challenge students’ perceptions of the goals of a physical chemistry lab course. These goals, the structure of the activity, and recent observations of student work using this activity will be discussed.

CHED 198

Incorporation of single-molecule FRET measurements into an undergraduate Physical Biochemistry Laboratory course

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The ability to image cellular and molecular phenomena with single-molecule resolution has revolutionized chemistry and medicine, as exemplified by the awarding of the 2014 Nobel Prize in Chemistry for super-resolution microscopy. Single-molecule methods allow for kinetic analysis of asynchronous processes and for observation of rare events that go undetected in population average measurements. For undergraduate students, they also offer a direct glimpse into the stochastic nature of chemical and biochemical events. However, single-molecule measurements are not performed in most teaching labs due to cost and technical difficulty. We are developing a new physical chemistry laboratory course for biochemistry students at CU Denver. The capstone experiment of the course will be a single-molecule fluorescence resonance energy transfer (FRET) measurement of DNA folding kinetics using total internal reflection fluorescence microscopy. The experimental system builds on the authors’ research expertise and
existing undergraduate research projects, and is based on published experiments in the field. A pilot course is being offered Spring 2015, and a presentation of this work in progress will discuss experiment design, initial implementation, and current challenges.

CHED 199

Guided-inquiry approach for relating the fluorescence spectrum of the pyrene excimer to its thermodynamic properties

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In this guided-inquiry style laboratory the fluorescence spectra of pyrene monomers and excimers are used to explore the relationship between spectroscopy and thermodynamic parameters. Students are introduced to the concept of excimers and begin the lab with an examination of the energy diagrams for the pyrene excimer and for pyrene monomer-monomer interactions. This initial consideration of the energy diagram guides students as they develop a set of fluorescence experiments that enable them to explore the effects of concentration and temperature on the resulting spectra. Once a set of spectra has been collected at various temperatures, students use their data to calculate thermodynamic parameters of the system. The data analysis includes challenging but appropriate manipulation of equations and graphical methods to determine the enthalpy and entropy of pyrene excimer formation. Students also calculate the monomer-monomer repulsion energy and dimer binding energy, parameters which relate directly to the energy diagram that was initially analyzed in the opening exercise of the experiment.

CHED 200

Constructing a binary phase diagram for aqueous salts

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Traditional physical chemistry experiments in which students construct binary phase diagrams employ toxic and carcinogenic organic aromatic compounds. A safer and more environmentally-friendly approach utilizes aqueous solutions of common salts. A laboratory experiment will be described in which students determined the eutectic temperature and melting points of aqueous salt solutions. With their data they constructed one side of the binary phase diagram. They then compare their results to simple freezing point depression and also a thermodynamic description from the literature. This laboratory exercise functions well as a multi-week exploration in which each student chooses a salt and then develops a procedure for determining the properties of its aqueous solutions. In particular, we investigated sodium chloride, silver nitrate, potassium chloride and calcium chloride. Advantages and disadvantages of this approach as compared to the classic experiment will be discussed.
CHED 201

POGIL physical chemistry lab experiment: the vapor pressure of liquid

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We describe the details of experiments based on the NSF-funded POGIL-PCL project model. In these experiments, students are asked, “How does temperature affect the vapor pressure of a liquid?” Different ways of doing the experiments will be described so potential adopters may tailor the experiment to the equipment they have available. Students follow two learning cycles over a two lab period. The first has students make predictions and then acquire data to test the predictions. After this, students are guided to think about the data they’ve obtained and design a set of experiments that will allow them to collect a larger set of data and analyze the results. We will present typical student results and a discussion of these results using two different vapor pressure experimental set ups.

CHED 202

Using food additives to enhance traditional bomb calorimetry experiments

John B. Dudek, dudekj@hartwick.edu. Chemistry, Hartwick College, Oneonta, New York, United States

The goal of this project is to enhance a traditional physical chemistry experiment by measuring the heat of combustion of a variety of different brands and types of rice cakes. Previous works has shown that different brand and different types of potato chips have shown that regular potato chips and non-fat potato chips have the same heat of combustion even though the reported caloric content differs by about 40%. The difference is due to additives found in non-fat potato chips. This laboratory experiment investigates whether this trend continues in rice cakes due to food additives. The bomb calorimeter is calibrated by burning benzoic acid and is tested by measuring the heat of combustion of naphthalene.

CHED 203

Are the molecules that make a solution red big or small? A POGIL-PCL recasting of the cyanine dye experiment

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We present a recasting of the classic cyanine dye experiment using the development principles of the POGIL-PCL (POGIL in the physical chemistry laboratory) project. The revised dyes experiment incorporates four learning cycles that explore concentration dependence, dye mixtures, model development, and exploration of the particle-on-a-line model. These cycles build student conceptual understanding of spectroscopy and the connection between molecular structure and the quantum mechanical model. We discuss how the guided inquiry nature of these learning cycles can expose (and repair) student misconceptions about absorption spectroscopy and build better understanding of the application of quantum mechanical models to experimental data. We also describe how instructors can use a subset of the learning cycles to address learning objectives appropriate for their students.

CHED 204

Guided inquiry solid-liquid phase diagram experiment

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We describe in detail a re-invention of the traditional solid-liquid phase diagram experiment as a guided inquiry experience called “How does the composition of a mixture affect its freezing point?” This POGIL-PCL (Process Oriented Guided Inquiry Learning - Physical Chemistry Laboratory) experiment follows two learning cycles. The experiment is carried out using lauric acid and stearic acid in place of biphenyl and naphthalene. These fatty acids are safer, less expensive, and cleaner, and fatty acid mixtures have been suggested as phase-change materials for energy conservation. The experiment begins with a prediction by the students as to the freezing point of two specific mixtures of the fatty acids. Students then measure the freezing points and assess their predictions. In a second learning cycle, students make further predictions regarding the dependence of freezing point on mixture composition, select the appropriate mixtures to test their predictions, measure the freezing points, and analyze their data to construct the full phase diagram and obtain the enthalpies of fusion of the two fatty acids. In this experiment students practice hypothesis testing, experimental design, and model building while learning content and unlearning misconceptions. We will present typical student results and discussion for these experiments.

CHED 205

Developing polymer and chemistry research lessons for the high school classroom – NSF GK-12 at The University of Southern Mississippi

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The goal of the National Science Foundation sponsored “GK12 Connections in the Classroom: Molecules to Muscles” (GK12) at The University of Southern Mississippi is to improve graduate fellows’ communication and teaching skills. This is achieved through partnership with local high school science teachers. Graduate fellows work with lead teachers to develop lessons based upon their current research. Fellows employ the “Five E” methodology to develop and deliver instruction and laboratories with content based on their own research findings. The lessons are designed to engage students in experiments with relevance to the world around them and that address national science standards. Successful research-based classroom lessons will be highlighted. The graduate fellows also learn different approaches to communicate to non-scientific audiences and to relate research advances in a way that is relevant to high school students. Initiatives implemented to improve fellows’ scientific communication skills are comprised of a series of talks developed and presented by fellows to different audiences. These include two classroom activities, a scientific research update, a research summary presentation, and external presentations at education and scientific conferences. This presentation will highlight successful tools used to develop high school lesson plans/activities and targeted activities to improve the graduate fellows’ communication skills.

CHED 206

Integration of polymer research into a lab-based polymer chemistry class at a small, primarily undergraduate institution

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Development of suitable laboratory components for upper-level chemistry classes can often be a challenge at small, primarily undergraduate institutions, due to lack of resources available to buy expensive, specialized equipment. It can also often be a challenge to develop undergraduate research programs due to the aforementioned financial limitations, as well as limitations in available time and students to perform the research. This presentation gives examples of ways that continuous polymer chemistry projects can be used as the basis for the lab component of an upper-level polymer chemistry class, and also can use affordable, easily obtained equipment and other resources. By incorporating ideas such as these, it is possible not only to effectively teach an upper-level polymer chemistry lab component with varied techniques, but also to effectively teach undergraduates to how to conduct research.

CHED 207

Aerospace composites and the scientific method: Supporting high school classroom curriculum with real-world applications
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Through support of the NSF GK-12 program at the University of Southern Mississippi, a graduate research assistant and a high school chemistry teacher collaborated to develop a lesson and a lab to introduce high school students to the fundamental principles of fiber reinforced polymer composites research. The lab challenged students to design the strongest composite structure possible with the least amount of construction materials, and it guided them through scientific methodology and the process of writing formal lab reports. These activities were designed to simulate authentic research practices in academia and industry. The presenters will share their experiences in developing and implementing the unit, as well as the results of its effectiveness in the high school classroom.

CHED 208

Discovering chemicals through solid-phase microextraction gas chromatography/mass spectroscopy

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The rapid development of solid-phase microextraction, SPME, as a fast, economical and solvent-free technique has received considerable interest. Research performed over the last two decades spotlighted this analytical method as a powerful candidate for a broad field of applications. As a non-hazardous tool, SPME is welcomed in the family of green chemistry. Both qualitative and quantitative investigations can be attained because SPME matches with gas chromatography mass spectrometry, GC-MS, or high-pressure liquid chromatography, HPLC. The conceptual simplicity of SPME makes its inclusion in the undergraduate and high school curriculum appropriate. Moreover, SPME/GC-MS measures samples we can smell with our noses. Inspired by these aspects, the present work is intended to serve as a guide for teachers and students seeking to connect modern analytical instrumentation to our everyday olfactory sense.
Introducing the effect of additives on hydrogel properties

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Polymer hydrogels have been widely studied due to their potential use in wound care, drug delivery, tissue engineering, cosmetic, and agricultural industries. Hydrogels can be made by a crosslinking process through covalent, ionic, or hydrogen bond formation to completely alter the properties of the material. In order to teach students the importance of additives (i.e. calcium chloride, sodium chloride, and vinegar) in altering the properties of hydrogels, a comparative investigation between crosslinked sodium polyacrylate and sodium alginate was performed. Students learned that the addition of salts and acid to an aqueous solution of swelled sodium polyacrylate led to a collapse of the crosslinked gel. Additionally, when an aqueous sodium alginate solution was added to a solution of calcium chloride, an ionically crosslinked gel was obtained. Students were able to learn concepts such as equilibrium, ionic bonding, and the importance of proper selection of additives to alter the properties of polymer hydrogel in an exciting way.
Degredation of hydrogel integrity due to the addition of sodium chloride.

CHED 210

Integrating polymer labs into the NGSS high school chemistry classroom

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The Next Generation Science Standards (NGSS) present both a challenge and an opportunity in terms of integrating polymer research into the high school chemistry classroom. On the one hand, the standards do not specifically identify polymers in the core ideas for chemistry, raising the possibility that they could be left out of a high school chemistry curriculum. On the other hand, the standards emphasize cross-cutting concepts - concepts that bridge the life, physical, and earth/space sciences, as well as engineering, technology and applications of science. Polymers also span this bridge, and many polymer-based labs or demonstrations are well-suited for inquiry and assessment. For example, comparing the changes in properties caused by different attractions between polymer chains is an idea way to explore, reinforce, or even assess the concept of intermolecular forces. While the changes in physical properties due to the introduction of hydrogen bonds or covalent crosslinks can be measured, they are also obvious enough to be compared without measurements. Other main concepts can be explored and explained using polymers, and many existing polymer-based lessons can be adapted to fit an NGSS curriculum. The level of exploration and explanation can be adjusted for the course level, using a more conceptual approach for the basic classes, with more detailed inquiry available for the pre-AP chemistry classes. Developing additional polymer lab resources and linking existing high school polymer labs to specific NGSS performance expectations will promote the long-term integration of polymer research into high school classrooms.

CHED 211

Using polymer properties to illustrate and explain concepts in introductory chemistry

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Polymers are ubiquitous in everyday life. However, the chemistry that underlies these materials is not always presented in undergraduate or high school chemistry classes. This in part reflects the mistaken belief that the concepts that underlie polymer chemistry are too complicated or too advanced for introductory classes. While polymer chemistry principles and concepts can be complicated, they like complicated concepts in organic, inorganic, or physical chemistry, can still be part of any introductory class. Indeed, polymers and demonstrations using polymers can sometimes be more useful as examples. For example, polymers as macromolecules often have behavior that can be ascribed to entropy effects. This can include entropy effects in polymer synthesis or entropy effects that lead to seemingly novel properties of polymers. Likewise polymers have structural and stereochemical features which have analogies in common life and these analogies can be used to illustrate how molecules behave and the physical basis for chemical transformations. These and other ways polymer chemistry and the features of polymers can be used to teach chemical concepts in college and some high school courses will be discussed.

CHED 212

Polymers in biomedicine and hydrophobic surfaces: Two RET experiences at the University of Akron

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This talk will present the results of two RET experiences at the University of Akron in summer 2014. The RETs will discuss their research projects focusing on polymers in biomedicine and modifying surfaces. The use of these experiences to develop new inquiry based lesson plans will also be presented. From the biology experience a lesson focusing on comparing natural lactase and lactase supplements was developed. A lesson focusing on characterizing the surface properties of commercial hydrophobic surface treatments was developed from the surface science experience.

CHED 213

Research Experience for Teachers program at The University of Akron

\textbf{Kevin A. Cavicchi}, kac58@uakron.edu. University of Akron, Akron, Ohio, United States

This talk will discuss the Research Experience for Teachers (RET) site at the University of Akron National Science Foundation (EEC-1161732). The objective program is to expose teachers to polymer research through group professional development activities and individual research projects conducting in participating faculty members’ laboratories. Using this experience the RETs develop individual lesson plans based on their research that can be implemented their classrooms. Through this program
teachers they gain increased confidence and knowledge in performing and mentoring inquiry based science in their classrooms. This helps invigorate their classrooms and encourage students to pursue further science and engineering education in college. This presentation will discuss the structure of the program and the lessons we have learned for the effective execution and completion of the program objectives.

CHED 214

Transferring teacher research on wastewater wetlands into effective classroom activities

Aaron Glimme, aglimme@cal.berkeley.edu. Science, Berkeley High School, Berkeley, California, United States

Student participation in authentic research activities is fundamental to building long-term interest in, and understanding of, STEM careers. Teachers who gain firsthand experience in current scientific research have a valuable foundation for creating realistic lab activities. However, transferring teacher research experiences into effective classroom activities can be difficult. The resulting lessons are often limited to little more than a show-and-tell exercise. One way to increase student engagement is by coupling innovative multimedia materials with laboratory activities designed to engage students in using more advanced research tools. We present iBooks and lab activities designed to bring liquid chromatography and mass spectrometry techniques to high school students and present evidence for effective engagement in authentic practices. The interactive textbooks and activities were created as part of the NSF-sponsored Berkeley Engineering Research Experience for Teachers (BERET) at UC Berkeley in conjunction with the NSF funded engineering research center ReNUWIt also at UC Berkeley.

CHED 215

RET model for professional growth of teachers and improved student learning

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In this RET program 6 RET Teachers (RTs) conducted action research on using two innovative teaching pedagogies, Challenge Based Learning (CBL) and Engineering Design Process (EDP). Previously trained teachers, known as RET Teacher Leaders (RTLs) were deployed to prepare, train, and guide the 6 RTs. The RTs were introduced to the teaching pedagogies by 3 RTLs who had participated in either a previous NSF RET Site or an ongoing NSF MSP program. They were specifically selected based on their prior in-depth training on CBL and EDP and proficiency at writing multiple instructional units using CBL and EDP. The 3 RTLs prepared and presented 4
professional development sessions to the 6 RTs and also provided support as they developed one unit of instruction that incorporated CBL and EDP. Additional classroom support was provided to the RTs by undergraduate, senior engineering students, who received a tuition scholarship from Choose Ohio First (COF) Scholarship Program. The COF scholarship recipients, known as COF Fellows (COFFs), spent 6 hours/week working directly with the RTs in the classroom. They also taught one activity based on the academic content standards for that class and related it to their own Senior Design Capstone Project. Together these three groups, RTs, RTLs and COFFs supported the delivery of instruction based on math and science content standards, utilizing CBL and EDP pedagogies for the purpose of increasing student learning and student engagement. A dedicated RET Coordinator provided longitudinal support throughout the program for the reviewing, critiquing, and approval of the Unit produced by each RT and the Activity produced by each COFF using a standard format in the form of a template. A curricular Unit consisted of at least 2 Lessons, with each lesson including at least 2 Activities and one of the activities is an EDP challenge project. After Unit/Activity implementation, the RTs and COFFs incorporated the assessment results, documenting impact on student learning and their reflections on their implementation experience and suggestions for future changes. The program concluded with the production of 3 project deliverables by the RTs and COFFs, Unit/Activity plan, slide presentation and poster, which they showcased to a panel of external judges. The project evaluation plan included assessment of both the impact of the experience on the teacher and COFF who were trained, and on student learning as a result of their classroom implementation.

CHED 216

Make it and break it: Employing a plant starch bio plastics experiment in the high school classroom for addressing engineering education standards

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Based on previously popularized experiments of making bio plastics from plant starches, we have developed an inquiry-based experiment that introduces engineering standards through tensile-testing. Students synthesize a variety of plastics made from renewable and readily available starches of the potato, tapioca, and corn plants. Students investigate how the properties of these bio plastics differ based on the starch or mixture of starches used and effect additives such as sugar, glycerol, and glue have on their properties. Use of tensile testing to quantify the strength of the bio plastics is then performed and adds an engineering component to the experimental design. This two-day lab introduces students to the concepts of sustainable polymers through straightforward and accessible techniques and materials in the high school classroom.

CHED 217
Activities in polymer optical physics for STEM education enrichment in the K-12 environment

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The Graduate Student Fellowship Program (GK 12), funded by the National Science Foundation, was created to provide graduate students with an opportunity to improve communication through educational outreach to teachers and students at the K-12 level. A lab based lesson was developed, using the 5e’s teaching framework, to introduce the concept of refractive index and how it applies to the use of corrective lenses in order to remedy impaired vision. In this activity, high school students observed the influence of lens shape on the behavior of light, as well as the effect of lens thickness on the focal length. The lesson focus is related to current research being conducted at a graduate level at the University of Southern Mississippi.

CHED 218

Preparation and evaluation of antimicrobial films

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Due to the spread of harmful microbes and the outbreak of certain contagious diseases such as Ebola, S. aureus, and E.coli, implementing the use of antimicrobial films in hospital, gym, and everyday settings may be beneficial to prevent the spread of harmful microbes. For this lesson, antimicrobial films were prepared and evaluated by high school students. The antimicrobial films were prepared by incorporating rose bengal into a thiol-ene polymer film, and the effectiveness of the film’s antimicrobial properties was explored by varying the different light intensities and time. During the analysis, the students were introduced to the light spectrum, various monomers, and important chemistry concepts such as polarity and intermolecular forces. Preparing an antimicrobial film and observing the film’s ability to kill microbes, sparked numerous student’s curiosity towards science while enhancing their scientific knowledge. The analysis herein provides the methods employed to prepare and evaluate an antimicrobial film.

CHED 219

Computational study of disubstituted ammonia borane derivatives for hydrogen storage
Reaction energies for the loss of 2 equivalents of H\textsubscript{2} were studied on disubstituted ammonia boranes (DAB) in the XH\textsubscript{2}N-BH\textsubscript{2}Y configuration at B3LYP/6-311+G(d,p) and CBS-QB3 levels of theory. The effects of methyl, fluoro, and trifluoromethyl groups were studied on ammonia borane (AB) by permutation at positions X and Y. The most favorable system, possessing the lowest activation energy (E\textsubscript{a}) at the CBS-QB3 level of theory was found to be F\textsubscript{3}CH\textsubscript{2}N-BH\textsubscript{2}CH\textsubscript{3} with 25.9 kcal mol\textsuperscript{-1} for the initial liberation of H\textsubscript{2} and a barrier of 42.0 kcal mol\textsuperscript{-1} for the second loss of H\textsubscript{2}. The DAB that was found to be closest to a free energy of reaction of zero for the loss of two H\textsubscript{2} equivalents was H\textsubscript{3}CH\textsubscript{2}N-BH\textsubscript{2}CH\textsubscript{3} with a value of 0.1 kcal mol\textsuperscript{-1} using CBS-QB3. The known byproducts from dehydrogenation of AB, borazine (BRZ) and boron nitride (BN), have posed significant problems for the development of an efficient hydrogen storage system. Locking the rotational freedom of DAB by inclusion in 5, 6 and 7 membered aliphatic ring systems may prevent the formation of these byproducts. The predicted reaction energies of these disubstituted ammonia boranes and cyclic systems will be presented.

CHED 220

Determining the activation energy of a series of spectroscopic imines

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The goal of this project is to understand how differences in structure between three different salicylidene imines affect the activation energy of a photochromic process. This process is a phototautomerization that occurs with the molecular rearrangement from an enol to a keto form and back again. The spectroscopy of these photochromic imines is done by using 405 nm light, a tungsten lamp, and a visible spectrometer with fiber optic input. The reflectance spectrum of the imine can be monitored as it changes from the keto form back to the enol form. The salicylidene imines varied only by the para substituent, one being a moderate activator, another being a weak deactivator, and the last being a moderate deactivator. Using the Arrhenius Equation and the experimentally determined rate constant (k), the activation energies of the three compounds were found and will be presented.

CHED 221

Why do Ala, Ala, Lys tripeptides preferentially rearrange to the Lys-Ala-Ala sequence in the gas phase?

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Research is growing in the use of mass spectrometric sequencing of peptides obtained from enzymatic digestion to determine the identity of proteins. It has recently been shown that some peptides can re-arrange during the dissociation process, which can lead to incorrect peptide assignments. Ala-Lys-Ala and Ala-Ala-Lys are two peptides that are observed to rearrange to Lys-Ala-Ala in the mass spectrometer under collision induced dissociation conditions. The rearrangements are proposed to go through the same tripeptide ring structure.

Calculations are being done to determine if there is a particular bond in the intermediate rings that is easier to break and that gives Lys-Ala-Ala as product. Involvement of proton transfer from the lysine side chain in the ring opening process would suggest that the presence of the lysine is a key factor in the rearrangements of the smaller polypeptides. More research is being done to determine if this is an effect that can occur with only lysine or other basic amino acids as well.

CHED 222

Tandem substitution-cyclization-elimination reaction that can account for the mutagenicity of arylamines without the need of nitrenium ions

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Arylamines are considered to be carcinogens; however mechanistic detail of their reaction with DNA is still unknown. Currently it is accepted that the mechanism involves the highly reactive aryl nitrenium ions. Theoretical calculations support the direct reaction between guanine C8 and aryl nitreniums. While others suggest that guanine N7 first reacts with the aryl nitrenium yielding N7 adducts, which then rearrange intramolecularly to the C8 substituted product. Here, we have proposed an alternative reaction mechanism that does not involve the aryl nitrenium intermediates. In the initial step, N7 reacts with the activated arylamine through an $S_{N}2'$ mechanism. This intermediate cyclizes followed by a ring-opening elimination to yield the final C8 substituted product. Theoretical calculations were done using B3LYP/6-31+G(d) and the CPCM aqueous solvation model. Models for the guanine base; 1-methylimidazole, imidazole, guanine and 9-methylguanine were used. The highly mutagenic 2-aminothiazole was used as the model for arylamines. The rate limiting step is predicted to be the initial substitution reaction forming the N7 adduct. This N7 adduct will readily cyclize to a 5 membered ring intermediate, which is deprotonated at C8 resulting in the ring opening to form the final C8 substituted product. The maximum barrier after the initial $S_{N}2'$ rate limiting step is $16\pm10$ kcal/mol for the 9-methylguanine and 2-aminothiazole model system. Acid constants for a variety of nitreniums to the nitrene are predicted to be acidic suggesting that the lifetime of nitreniums in the cellular
environment would be exceedingly small. The acid constants and the singlet-triplet gap for the nitreniums will be presented.

CHED 223

**Novel ligands for metal oxides colloid stabilization**

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Aqueous colloids of metal oxides are commonly stabilized by one of two mechanisms, electrostatic or steric. Electrostatic mechanism is provided by small ions associated with colloidal particle, that form electrically charged shells which, in turn, cause inter-particle electrostatic repulsion. Steric mechanism engages when colloidal particles are surrounded by bulky hydrophilic surfactants that help to keep particles far apart. In this project we aimed small-molecule surfactants that on one hand can covalently bind to metal oxide surface, and on the other, can provide versatility in their steric properties, affinity to the media and conjugation capacity. Our experience with isophthalate- and hydroxycarboxylate-based ligands [1,2] has recently directed us to 2-hydroxyisophthalic acid [3] which we thought could be a backbone of novel effective capping ligands with improved ligand-to-metal binding strength (Fig.1). A series of derivatives was synthesized with $X = \text{Br}$, allyloxy-, 2-hydroxyethoxy- and benzoxy- substituents. Efficiency for colloid stabilization was evaluated by inhibiting the precipitation of iron(III) hydroxide from aqueous solutions. The results of DLS-monitored titration of Fe$^{III}$ and ligand-containing (2:3) solutions, showed colloid formation, in contrast to the reference Fe$^{III}$ + salicylic acid (1:3) system where precipitation was noticed at pH as low as 5 (Fig.2).

Development of a new method for graphene oxide thin-film growth

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The production of graphene and graphene oxide based carbon thin-films is an attractive modern industry due to their versatility and use in electronic devices, chemical sensing, polymer composites, and two-dimensional materials. Current methods for producing graphene thin-films require large and expensive UHV deposition chambers, which are difficult to scale up for larger films. On the other hand, production methods of graphene oxide, including the Hummer's method, are primarily focused on batch-wise, large-scale production of the material with little emphasis on controlling or tuning the specific properties of the product. While graphene and graphene oxide are distinctly different materials with different properties, there is significant overlap in their conceived applications making large-scale, finely controlled production of graphene oxide an important target. A new method for graphene oxide thin-film production has been developed, which inherently provides a greater degree of control over the characteristics of the product while also making the production of larger thin-films on the inch scale a reality. Basic characterization of carbon films produced using the method will be presented.
Iron-carbonyl clusters: Catalysts for hydrogen generation

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The need to develop clean and renewable fuels is of great importance for environmental, sustainability, and sociopolitical reasons. Hydrogen is considered a clean and primary energy carrier of the future. As a result, the development of cheap catalysts for the efficient production of hydrogen from water (an abundant and readily available resource) has gained a lot of attention. One approach for the design of such catalysts is biomimetic. In this talk, I will present studies in our laboratory toward making effective hydrogen producing catalysts by modeling the structure and function of the active site of [Fe-Fe] hydrogenase enzyme. We have prepared and characterized a series of diiron-carbonyl clusters coupled to polyaromatic thiolate ligands. These compounds have been structurally (X-ray crystallography) and spectroscopically (IR, UV-visible and NMR) characterized, and examined as catalysts for the electrochemical reduction of proton to hydrogen. Our catalysts generate hydrogen from acidic water at milder reduction potentials than similar complexes reported in the literature.

Synthesis of iron precursors for the development of iron-based hydrogenation catalysts

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Hydrogenation reactions are tremendously important to the pharmaceutical industry and, for this reason, numerous homogeneous hydrogenation catalysts based on transition metals such as ruthenium, iridium, and rhodium have been developed. While these catalysts are highly active and lead to very efficient reactions, the metals they contain are costly and detrimental to the environment. Over the past few decades, the application of green chemistry technologies has helped alleviate similar issues in the pharmaceutical sector, resulting in reduced waste production and resource consumption in this industry. However, there is still a significant need for more sustainable chemical practices in the pharmaceutical sector, as exemplified by its current demand for catalysts that do not contain expensive and polluting metals. Inspired by the principles of green chemistry, our laboratory seeks to develop homogeneous iron-based hydrogenation catalysts that would serve as cheaper and less harmful alternatives to more common catalysts. The application of these iron-based catalysts could possibly reduce resource consumption and toxic waste production in the pharmaceutical industry. The catalysts targeted in this research contain pyridone-based ligands that are intended to promote the key step of dihydrogen activation through a ligand-assisted heterolytic cleavage of H$_2$ (Figure 1). This strategy has been successfully used in
existing iridium and ruthenium catalysts. This presentation highlights our investigations of multiple pathways for coordinating the developed pyridone-based ligands to iron centers in order to form catalytically active species.

![Figure 1. Examples of the iron-based hydrogenation catalysts targeted in this research.](image)

**CHED 227**

**Shaped palladium nanoparticle synthesis on carbon substrates**

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Shaped palladium nanoparticles (PdNPs) have the potential to be selective catalysts. Unfortunately, there are some obstacles that hinder their use in heterogeneous catalysis, e.g., nanoparticles are difficult to remove from solution after a reaction. Attaching nanoparticles to a support addresses this issue. However, it is typically a two-step process, and the time and energy involved circumvents the energy saving goals of catalysis. Additionally, shaped nanoparticle synthesis usually occurs at high temperatures, which is also counterproductive. We have developed a method to create shaped PdNPs directly on porous carbon microspheres using coffee as a room temperature reductant. By adding ions, such as Br⁻ and Fe³⁺, the stability of different crystal faces are altered, which results in deviations from spherical nanoparticles. Other additives, such as ethylene glycol, are added to change the reaction kinetics. Analysis by SEM indicates that our synthesized PdNPs are roughly 50 nm in dimension. The size, shape, and distribution of nanoparticles varied based on the ratios of the reactants in the synthetic process. The concentration of tin chloride plays a large role in the size and distribution of the particles. Thermogravimetric analysis and SEM were used to illustrate this effect. Different ratios of reactants and adjustments in the synthetic process are being tested in hopes of maximizing the percentage of shaped particles. If successful, our PdNPs show promise in being effective, environmentally friendly selective catalysts.

**CHED 228**
Silicate nanoparticles from spray flame synthesis for lithium ion batteries

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Clean energy, as useful and renewable as it is, is inefficient if there is no effective way to store it. So far, battery capacity has been limited to the electrical capacity of the cathode, requiring a need to synthesize new cathode materials. According to Xu B, Qjan D, Wang Z, Meng YS, 2012, batteries made with multivalent nanoparticles coated in carbon have increased electrical capacity.

In our experiment, we tested whether or not increasing the amount of the carbon source (glucose) in the manganese silicate nanoparticle synthesis affects the electrical capacity of the batteries. We report on the synthesis methods, the results of the elemental analysis of the nanoparticles treated with increased glucose, and the battery capacity tests.

CHED 229

Morphological control of film structure in perovskite solar cells

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In the search for cleaner sources of energy, sunlight is arguably the most viable source of renewable, low cost power with minimal negative impact on the environment. To take advantage of this, recent research to improve the efficiency of solar cells has focused on perovskites, semiconductor materials that adopt a crystal structure of ABX³. Certain perovskites, particularly those synthesized with methylammonium lead iodide, have shown significant light harvesting properties and power conversion efficiencies approaching 20%. Because the degree of crystallinity appears to be the limiting factor in improving perovskite solar cell efficiency, it is critical to produce more highly crystalline films. This study was able to determine ideal deposition parameters, including solution preparation methods, spin-coating conditions, and levels of air exposure. These perovskite thin films were then analyzed using microscope imaging, UV-Vis absorption, and X-ray diffraction measurements. Ultimately
however, the shear forces acting upon the film during spin-coating limit the degree of crystallinity given by this technique. Therefore, this research also explores a novel solution-shearing process, which offers the possibility of depositing more highly aligned, crystalline perovskite thin films.

CHED 230

Laminar-flow reactor study of the pyrolysis of 4-vinylguaiacol

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In order to design optimal thermochemical processes for the conversion of biomass into chemicals and fuels, an understanding of the secondary vapor-phase cracking of tar compounds is crucial. Though several studies examining the homogeneous secondary cracking of biomass tar exist in the literature, its thermal decomposition process is not completely understood. Much of this lack of understanding is due to the complex, heterogeneous nature of biomass tar. A useful approach is to examine model compounds that are actual components, or are representative of compounds, found in biomass tar. In this study, we have used a laminar-flow reactor system to examine the vapor-phase cracking process of the model tar compound, 4-vinylguaiacol. We report the variation in the experimental yields of condensable products, namely oxygen-containing compounds and aromatic hydrocarbons, and light gases as functions of temperature. Based on the experimental data, we also determine pseudo first-order reaction rate parameters for the overall conversion of 4-vinylguaiacol to products. The results presented in this study are of relevance to the industrial-scale pyrolysis and gasification of biomass.

CHED 231

Using research as a tool to engage, retain and graduate STEM students at Queensborough Community College

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Queensborough Community College has successfully engaged community college students in high-caliber undergraduate research for a long time. Our experience, institutional commitment, faculty and modern laboratories have positioned us for unprecedented success. With the help of US Department of Education Queensborough MSEIP (Minority Science and Engineering Improvement Program) grant, our main goal is to use Undergraduate Research as a tool to engage, retain and graduate Queensborough students. We intend to substantially expand the depth and breadth of research opportunities for students, particularly underrepresented females. Students will be engaged in a multi-tiered research programs, allowing them to begin research
projects early in their academic careers and supporting them for increasingly rigorous research that culminates in placements at partner four-year colleges.

The program uses a multiple prong approach 1) Providing intensive summer immersion experiences for at risk high school students 2) Expanding undergraduate research experience for QCC freshman by easing them in STEM field through seminars and workshops then pairing them with research mentors for long term research projects and 3) Launch comprehensive faculty development program to train new faculty mentors. This multi-tiered model will be discussed in detail.

CHED 232

Goal, role, and soul of undergraduate research development at the Community College of Denver

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At the Community College of Denver we are interested in the role of undergraduate research as a pedagogical tool to help create and support pathways for students in transferring to four year universities and in entering the work place with specific skills. We developed and are implementing a four pronged model of research development designed to merge with the logistical and political realities of the college while affording enough room for growth and development of the program. This model is designed to develop research opportunities on the course level, the interdisciplinary level, and the interinstitutional level. This presentation will feature some examples of student’s experiences in this effort, what their outcomes have been, and the effect that the early development of research is having at the Community College of Denver.

CHED 233

Black bear research: A case study in undergraduate research at a community college

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Black Bear Management, an undergraduate research course at Finger Lakes Community College was created in response to a need for more information about the increasing bear population in our service area. The class is structured so that students participate in both a long-term research and a novel project each year. In partnership with the NYS Department of Environmental Conservation, students in this class assist professionals at black bear dens throughout Central New York. Bears are chemically immobilized, fitted with telemetry collars and released unharmed. Specifically, my students and I are charged with taking biometric measurements of cubs and recording
den characteristics. These two long-term projects were chosen in response to the needs of the state agency.

In addition, a novel project is conducted each year so students can participate in all steps of a research project. I follow Windschitl’s (2008) four-step model for authentic inquiry: Discussion of what we know and what we want to know, creation of a model that describes our current understanding of the phenomenon, data collection, revision of the model into a scientific explanation. Past projects include survey of college students’ knowledge and opinions of bears, ground marking behavior in black bears and correlating habitat characteristics at utility poles with bear bites versus those without. Students have presented our work at regional and national conferences.

Several challenges had to be overcome in order to make this course a reality. One large issue was reconciling the academic year with the field season in which den visits take place. Another is the amount of work required of this course as compared to a “normal” three credit course, especially with students of varying levels of preparation for undergraduate research. After four years, the course remains very popular and I consider the research a success.

CHED 234

Undergraduate research at Queensborough Community College: The first step for a successful transfer and eventual post-undergraduate career in STEM careers

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Since 2000 Queensborough Community College of the City University of New York has established undergraduate research opportunities for promising students as early as their first year of the college career. The results have led to multiple presentations in professional conferences as well as publications to peer-reviewed journals and successful REU experiences nationwide. Successful candidates have been accepted to post-undergraduate STEM programs and have continued with eventual careers both in academia and industry. The systematic approach of this effort will be described with emphasis on the difficulties associated with the grooming of these students.

CHED 235

Transporting an established undergraduate research program to a community college

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Undergraduate research programs have become increasingly ubiquitous on community college campuses in recent years. It should be noted, however, that the efforts required to initiate such a program are daunting at best. For this reason, faculty members may be hesitant to pursue new professional opportunities for fear of having to “start over”
with a new student body and new administration. In this presentation the transition of an undergraduate research program from one community college to another will be highlighted. Specifically, topics such as student recruitment, facilities, and administrative support will be discussed with regard to an established research program being moved to new school that does not have a research culture in place.

**CHED 236**

**Strategies for funding undergraduate research at the community college**

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Given the growing importance of the community college in the education of future STEM graduates, we have identified undergraduate research as an important component in attracting and preparing students to transfer successfully to baccalaureate programs. This paper will describe some of the approaches we have taken to fund undergraduate research opportunities at College of DuPage over the past several years. These include funding from the National Science Foundation, formation of alliances with local institutions such as national laboratories, universities and businesses, as well as funding from the college’s Foundation. We will be able to provide numerous examples of the transformative effects that research activities, particularly those involving internships, have had on the careers of community college students.

**CHED 237**

**Research-based and interdisciplinary curriculum design for general chemistry and beyond**

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North Seattle College (NSC) and Central Washington University (CWU) are collaborating to address the need to transform introductory science courses, embed research experiences early in the post-secondary curriculum, increase engagement of underrepresented students in STEM career pathways, and deeply immerse students in developing 21st century skills and thinking dispositions. This collaboration provides a model for how a two-year community college and a four-year university can work together to transform introductory chemistry and biology courses. Unlike most two-year/four-year partnerships, we provide a method for bringing a four-year university scientific research platform to a community college context through an iterative design of research-based curriculum that spans two years of introductory science courses. Prior work at NSC on a year-long interdisciplinary program (Atoms to Ecosystems), provides a springboard for current curriculum development efforts. The design of these activities will be considerably enhanced through a long-term collaboration with a four-
year university scientist who has extensive experience working with undergraduates on research pertaining to some of the largest environmental challenges facing the world today. Essential to this approach is the development of educational experiences that establish a “culture of thinking” where student voices are encouraged, valued, and driven by engagement with relevant interdisciplinary and research-based activities. This presentation will focus on our initial efforts to design and implement interdisciplinary and research-based modules for two general chemistry courses. We will also discuss the design of a year-long undergraduate research program for second year students, and provide some initial student learning results that capture how students think, learn, and problem solve in a research and interdisciplinary context early in the college experience.

CHED 238

Promoting undergraduate research at community colleges to increase STEM competency and transferability to 4 yr institutions within CUNY

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This paper describes the collaborative efforts between Bronx Community College, York College and Lehman College, all of the City University of New York (CUNY), to increase community college students’ exposure to research activities. Students are recruited through various STEM initiatives such as the Louis Stokes Alliance for Minority Participation (LSAMP) program, the Bronx STEM Scholars program and through NSF funded Research Experiences for Undergraduate (REU) grants, and the NSF funded Pathways to Chemical Technology and Careers grants. The efforts of the PI have also exposed Community College students to research activities with external partners such as the Texas Materials Institute at the University of Texas Austin, University of Rhode Island College of Pharmacy, Lawrence Berkeley National Laboratory, Joint Bioenergy Institute, Brookhaven National Laboratory, and Storm Peak Lab in Steamboat Springs, Colorado, in Chemistry, Biochemistry, Atmospheric Chemistry/Physics and Bioenergy research. Students who have been exposed to these undergraduate research programs have been retained at a higher level and have higher rates of transfer to 4 year degree programs than the ones that have not engaged in these activities.

CHED 239

The STEPS Program - a pathway from Community College to Bachelor's degree and beyond

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The history of the STEPS (Strides Toward Encouraging Professions in Science) Program, a Bridges to the Baccalaureate program funded by the NIH will be presented. The STEPS program has been a collaborative effort between Metropolitan State University of Denver (MSU Denver) and several community colleges, with assistance from various research institutions in the Denver Metro area. We will present the basic outline of our program’s best practices, with special emphasis on the early involvement in hands on research of participating students and the impact that has had on retention, persistence, matriculation to and graduation from 4 years schools and the pursuit of further education at graduate and professional institutions.

CHED 240

The Community College Undergraduate Research Initiative: A national collaborative

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Volunteer State Community College is one of 37 community college partners in a NSF funded initiative - Collaborative: Community College Undergraduate Research Initiative (CCURI). The national collaborative seeks to develop undergraduate research as a High Impact Practice. The CCURI model for integrating a research experience into a community college science program originates from a self-study at FLCC using Root Cause Analysis (RCA). The results of this study suggested (a) Adopt a Problem-Based Learning (PBL) approach to instruction (Case Study Method), (b) Create opportunities for students to explore research questions, (c) Incorporate a customized faculty development program, (d) Adopt a compatible Community College faculty model, (e) Connect, disseminate and sustain (create and sustain networks). Volunteer State Community College has developed a dynamic strategy using the CCURI model in its chemistry program, developing research experiences in Organic Chemistry I & II, General Chemistry I and Fundamentals of Chemistry. The CCURI model for integrating a research into community college includes three different solutions: CURE-Course Undergraduate Research Experience, SURE-Summer Undergraduate Research Experience and PURE-Program Undergraduate Research Experience.

CHED 241

Chemical education in India: Observations

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I was awarded a Fulbright-Nehru Fellowship to teach at Cotton College in India from August to December 2013. The purpose of Fulbright-Nehru Fellowships is to promote mutual understanding between the people of the US and India and to provide opportunities for personal, academic and professional growth of the participants. While
at Cotton College I presented lectures at the higher secondary, BS, and MS levels each week. This presentation will compare and contrast chemical education in India and in the US. Facilities, preparation of secondary students, curriculum, and assessment will be discussed. Personal experiences will also be presented.

CHED 242

General Chemistry study habits and instructional practices across borders

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For reasons well grounded in educational research, collaborative learning in its many expressions is becoming increasingly popular in US college classrooms. However, a large proportion of students do most of their learning outside the formal environment of our classrooms and laboratories—somewhere else—and away from instructors’ direct supervision and influence. Preliminary results of study habits at a large, urban, public, research-intensive institution in the US showed that 87% of students enrolled in General Chemistry 1 did most of their unsupervised learning individually. Similarly, more than half of the Physical Sciences majors who completed the US National Survey of Student Engagement in 2012 ‘never’ or ‘only sometimes’ worked with classmates outside of class to prepare assignments. Understanding situational factors such as where, when and how students learn general chemistry and what considerations lead to these decisions can be informative to design instruction that is consistent with their study habits. In a first stage this study intends to develop and administer a simple survey to gather information about general chemistry students’ study habits. Subsequently, this study compares and contrasts study habits in general chemistry student populations from the US and Costa Rica. It is a truism that social and cultural aspects influence learning environments. Nonetheless, a large proportion of chemistry professors in Costa Rica have obtained their graduate degrees abroad and their instructional practice may reflect their graduate experience. In addition to comparing and contrasting students’ study habits, this collaborative international study will explore instructors’ instructional practices in the two countries.

CHED 243

Language challenges in teaching and learning General Chemistry

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Language is a tool for communication and communication is always context-based. English functions as an international academic language while chemistry is an international scientific language. In Macau, Chinese is the native language for most people. English is commonly taught and used as a foreign language. In the University of Macau, English is assigned as the chief medium of instruction. Chemistry is a basic course for engineering, biomedical studies, and general education. When teaching and learning chemistry, teachers and students encounter a trilingual situation: English, Chinese, and the scientific language of chemistry. This paper explores how languages affect the understanding of concepts in chemistry and analyzes the causes of misconceptions found in students.

CHED 244

Chemistry: Finishing the Babel Tower together

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Chemistry is a language-free science as it defies all geographical and governmental barriers. Teaching and learning chemistry is unique in a sense that no matter which language you speak or from which background you come, the chemical formula of NaCl is always the same! The generation of the periodic table has created an International amphitheater where all chemists speak the same language anywhere on our mother earth and anywhere in our father universe. I have learned chemistry in Morocco and I have taught it in the USA to many different nationalities, and the language I spoke in all situations is always the same: Chemistry!

CHED 245

Improving quality control methods in the brewing industry through analytical characterization of hop alpha acids

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The alpha (α) and beta (β) acids from hops contribute to the bitterness, aroma, stability, and other final characteristics of beer. α-acids isomerize when exposed to high temperatures producing intensely bitter iso-α-acids. β-acids and unisomerized α-acids are the main contributors to the aroma and flavor. It is therefore crucial to know the concentration of α-acids and the extent to which they isomerize to iso-α-acids (% utilization). Some commercial brewers use a technique called whirlpooling where copious amounts of hops can be introduced while the wort is at near boiling temperatures. The increase in hop contact time at elevated temperatures facilitates the incorporation of hop acids but can also induce isomerization. It is assumed that % utilization is near zero, which is questionable considering analytical quality control
methods have not been employed. To date, the only attempts to determine hop utilization from whirlpooling have been highly subjective, relying on professional tasting panels. The goals of this study are to quantify hop acid content and determine how various whirlpool process factors affect hop utilization. Specifically, the effects of temperature and hop contact times are quantified utilizing HPLC and UV/vis.

CHED 246

Analysis of metal ion absorption compared to pH and conductivity changes in hydroponic growing systems

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The changes in pH and electrical conductivity are the most common methods to determine when to add nutrient to hydroponic systems. These two measures provide general concentration information rather than the specific concentrations for the many nutrients. Furthermore, the various nutrients are not consumed at the same rate. After addition of stock nutrient mixture to an existing system, the concentrations of those nutrients consumed at slower rates increases and can become toxic. By using atomic absorption spectroscopy the concentrations of metals such as Ca, Mg, and Fe can be determined. Weekly testing of the pH and electrical conductivity and measurement of metal ions concentration by AA provides a correlation between the general measurement and metal concentration. Lettuce was grown in two nutrient film technique tables (Crop King) with different nutrient solutions.

CHED 247

Archaeochemical analysis: Using chemistry to inform history

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Archaeochemistry is the use of analytical chemistry to verify and, in some cases, inform the social science analyses of material remains in archaeology. For this poster, the methodology and results of two different undergraduate research projects in the area of archaeochemistry are presented. In the first project, the powdered ceramic matrix from a potsherd (radiocarbon dated to 586-762AD) was analyzed using gas chromatography-mass spectrometry. The data indicate the original ceramic vessel was dedicated for medicinal use. The interpretation and implications of this result will be discussed. For the second research project, inductively coupled plasma-mass spectrometry (ICP-MS) was used to evaluate the accuracy of ethnographic and historical accounts of two 19th century West Virginia mummies. Specifically, the authenticity of the original patent for the embalming solution used by Graham Hamrick was assessed by comparing the patented “recipe” to the results of ICP-MS analyses performed on samples of the
solution. Both studies demonstrate the usefulness of chemical analyses in further informing archaeological records.

CHED 248

**Determination of chlorogenic acid and caffeic acid in fruits with evaluation of pesticide concentrations**

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Chlorogenic acid (CGA) is a secondary plant metabolite with chemotherapeutic and chemopreventative potential along with other purported health benefits. The primary objective of this study was to use microwave-assisted extraction (MAE), which was optimized in a previous study, to quantify and compare concentrations of CGA and caffeic acid (CA), a product of the decomposition of CGA, in the skins and flesh of various fruits, and ultimately to compare concentrations in organically and conventionally grown fruits. High performance liquid chromatography (HPLC) with a multi-wavelength detector was used for analysis. A spike recovery study was performed for tomatoes and peaches/nectarines, and high recoveries were achieved from MAE extraction. The third objective of this study was to optimize a dispersed liquid-liquid microextraction (DLLME) technique for extracting pesticides from fruit skins to determine if there is a correlation between pesticide levels and CGA and CA concentrations. Pesticides were analyzed by gas chromatography-mass spectrometry (GC/MS) using a selected ion monitoring method.

CHED 249

**Modifications of brewing parameters: Analysis of volatiles by SPME-GC-MS and hydrogen sulfide analysis in beer**

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Maintaining consistent flavor and aroma profiles between mass-produced batches of the same beer variety is critical for a brewery, as customers expect the same experience each time the make a purchase. The identification of volatile compound profiles in limited-release or specialty varieties of craft beer is also extremely important for breweries, as this process helps to define unique flavors, determine optimal storage conditions, and establish an ideal shelf-life of the specialty batch.
Brewery sensory programs provide qualitative analyses - performed through a combination of gustatory and olfactory perception - for a small number of chemical compounds that help assist in each of the aforementioned quality assurance scenarios. However, several additional volatile compounds are found in beer that cannot be evaluated using only sensory perception. Using SPME-GC-MS and a H₂S analyzer, several volatile compounds have been identified in beer samples beyond those historically identified using sensory perception. This research focuses on identifying additional compounds in beer from Allagash Brewing Company that are not typically evaluated by the company’s sensory division, as well as quantifying seven (7) compounds, including hydrogen sulfide, ethyl acetate, isoamyl acetate, ethyl hexanoate, phenethyl alcohol, phenylethyl acetate, ethyl octanoate and ethyl decanoate that are compounds regularly evaluated as part of batch QA/QC. Once quantified, changes in concentration and ratios of these seven compounds were evaluated as brewing conditions varied to determine which, if any, factors contributed to changes in the levels of these compounds in individual batches of beer.

CHED 250

Characterization of tissue browning products using attenuated total reflection: Fourier transform infrared spectroscopy

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The process of oxidative browning, in commercial fruits and vegetables, is a part of a defense response that occurs when a wound or infection occurs. Previously published results showed that a group of metallo-enzymes called Polyphenol Oxidases (PPO’s) play critical roles in the browning process. Although substantial research has been done on the enzyme, the products of the oxidation remain largely unexplored. Attenuated Total Reflection - Fourier Transform Infra-Red (ATR-FTIR) spectroscopy is used for qualitative and quantitative characterization of the functional groups of the organic compounds. In this research, we mapped the oxidation products of browning of three different varieties of apples. Apples were oxidized for one hour and compared with an unoxidized control. The products were isolated using various solvents and characterized utilizing the ATR-FTIR. Further, a multivariate statistical approach using “R” statistical language was applied for pattern recognition and quantitative analysis. Both qualitative and quantitative information on tissue browning will be presented.

CHED 251

Further defining acylsugar structural diversity within Petunia axillaris
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The glandular trichomes of Solanaceous plants, including the genus \textit{Petunia}, are major centers of secondary metabolite synthesis, storage, and secretion. Of the compounds produced in these trichomes, acylsugars are of particular interest because of their role in plant defense against insect attack. These acylsugars are derived from glucose or sucrose molecules by esterification of a variety of aliphatic esters on the sugar core, resulting from a multitude of metabolic transformations of organic acids (Kroumova and Wagner 2003). Within \textit{Petunia}, it has been made known that two major groups of acylsugars are produced, malonate acylsugars and neutral acylsugars. Extracts from the leaf tissue of \textit{Petunia axillaris} were used to isolate acylsugars produced in the trichomes. Selective solid phase extraction (SPE) by anion exchange, malonate acylsugars were separated from neutral acylsugars. Semi-preparative HPLC was then used to further isolate individual metabolites. The structures of individual acylsugars were then elucidated by time-of-flight mass spectrometry and various 2-D NMR techniques, resulting in a total of sixteen complete structures. From these structures patterns were observed that indicate the possibility of enzyme selectivity and chain elongation processes used in the synthesis of these metabolites.

CHED 252

Determining the effects of processing on antioxidant activity in cilantro, parsley, and rosemary

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Cilantro, parsley, and rosemary contain numerous medicinal and nutritional properties that have greatly increased the interest in herbs over the years. Studies have shown that these common culinary herbs are used as a rich and natural source of antioxidant compounds. Additional studies have established that freezing and cooking foods can alter the antioxidant activity. Bringing these two ideas together, this series of experiments analyzed the effects of different processing techniques (freezing and drying) on cilantro, parsley, and rosemary antioxidant levels. Methods utilized include diphenyl-1-picrylhydrazyl (DPPH) assay, trolox equivalent antioxidant capacity (TEAC) assay, and Folin-Ciocalteu method. Preliminary results suggest that processing, especially drying, does affect antioxidant viability in these particular herbs. Moreover, these experiments provide a model for extended studies on the effects of processing on herbs’ medicinal and nutritional values.

CHED 253
Mapping of oxidation products of tissue browning using 2,4-dinitrophenylhydrazine and high performance liquid chromatography

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Tissue browning causes major revenue loss in agricultural and horticultural production. Upon wounding, the plant tissue turn brown in response to wound stress which could be oxidative, enzymatic or both. Polyphenol oxidase (PPO) is a major player in the browning process. Ketones and higher order polyphenols are produced due to oxidation of polyphenols. In order to elucidate the mechanism of browning, ketones were characterized from apple tissues. In our study, three varieties of apples undergo oxidation for one hour followed by extraction of soluble ketones and phenolics. Ketones were initially mapped using attenuated total reflection – infra-red spectroscopy (ATR-FTIR) and further characterized by converting them to corresponding hydrazone derivative using 2,4-dinitro phenylhydrazine. Hydrazone derivatives were further separated using high performance liquid chromatography. Separation method will be discussed and characterization of quinones will be presented.

CHED 254

Using trace element signatures to determine cocoa liquor provenance

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Both consumers and manufacturers have recently become more concerned with food product provenance for a variety of reasons, including production ethics and product quality. An example of such a food product is chocolate, which is a mixture of cocoa liquor, cocoa butter, sugar, and sometimes milk. Cocoa liquor is derived from cocoa beans which have been roasted and ground to a liquid. The flavor and quality of chocolate is heavily influenced by the quality of cocoa liquor used in its production. Cocoa bean traceability has a growing importance in the cocoa value chain, not only due to quality factors but also due to increased demand for verification of ethical production practices. This project focused on single-origin cocoa liquor samples to determine if elemental signatures in the liquor could be correlated to the country of origin. Elemental analysis was performed using ICP-MS and the resulting data analyzed by chemometric approaches. Two main questions were investigated: 1) Could cocoa liquor samples from four or more countries be discriminated from each other? And 2) Would liquor samples from the same location but undergoing different processing treatments have the same elemental signature? Initial results indicate that single-origin cocoa liquors from five countries can be discriminated from each other based on their elemental signatures (Figure 1). In addition, the cocoa liquor samples that were produced from different treatment
processes (e.g. roast temperature and time), while having some differences in their signatures, were still correctly classified by country of origin. Future work will examine additional single-origin cocoa liquors and will aim to determine which elements are most significant in defining a signature that will allow the determination of provenance.

![Figure 1](image.png)

**Figure 1.** Discriminant function plot showing clusters of individual samples from each of five countries.

**CHED 255**

**Analysis of e-cigarette flavors with gas chromatography**

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Increasing number of cigarette smokers adopted electronic cigarettes (e-cigarettes) because of benefits such as the ability to use anywhere, eliminating the toxic benzopyrenes and tar associated with traditional cigarettes, and emitting pleasant smelling vapor into the air. The risks associated with e-cigarettes, however, are still unclear. There have been well-documented FDA-method for the quantification of nicotine in e-cigarette fluids. Other ingredients in these fluids are seldom analyzed; consequently the health risks to smokers are mostly unknown. The flavor materials associated with these electronic cigarettes are FEMA GRAS approved for food flavorings, but when vaporized into the lungs; their effects to the users’ health are unclear. Our study focuses on the flavor ingredients in e-cigarette fluids, particularly after they are volatized at the heating temperature for electronic burning (i.e. 200-300 °C). Some of the compounds of concern are diacetyl, acetaldehyde, isovaleraldehyde, and methyl chavicol (estragole). Through the use of Gas Chromatography/Mass Spectrometry, the analysis of different electronic cigarette flavors for these harmful compounds was performed. The spectra were compared against the multiple mass spectral libraries to check accuracy. We also use gas chromatography with flame
ionization detector and electron capture detector to quantify the identified flavor components using external standard calibration.

CHED 256

**Extraction and characterization of anthocyanins from organically grown grains**

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Anthocyanins are water-soluble flavonoids that contribute to the pigment in many plants. They are also phenolic compounds and are said to be health enhancing substances. Anthocyanins in the diet have antioxidant and anti-inflammatory properties, and may be helpful in preventing chronic disease. I will investigate extracting anthocyanins from various organically grown grains, measuring the total anthocyanin content, and the identification of individual anthocyanins present. I will also discuss storage conditions and the average shelf life of the extracted anthocyanins in solution.

![Anthocyanin structure](image.png)

CHED 257

**Comparison of eastern filbert blight resistance in two hazelnut cultivars**

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Oregon produces about twenty percent of all hazelnuts consumed. Eastern Filbert Blight (EFB) is a fungal disease that kills hazelnut trees, especially in moist climates. Most hazelnut cultivars are susceptible to this disease. In 1998, Taxol was discovered in certain cultivars of hazelnuts. Of these cultivars, Gassaway had the highest concentration of Taxol while Ennis had the lowest. In this project, we are attempting to discover whether Taxol is protecting the trees from EFB. Methyl Jasmonate (MeJA) and Salicylic Acid are also defense mechanisms of hazelnut cultivars. For this reason, we chose to challenge Ennis and Gassaway cuttings with EFB spores. Some of the inoculated cuttings were exposed to high or low concentrations of MeJA. Differences

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between the responses to EFB spores were analyzed by Electron Microscope (EM) and
HPLC-MS profiles. The EM pictures showed that some spores on Ennis cuttings could
germinate. The differences between LCMS profiles of Gassaway and Ennis extracts are
being analyzed.

CHED 258

Comparison between two extraction techniques used to isolate antioxidants from
the pith and carpellary membrane of pomegranates

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Pomegranates (Punica granatum) are native to the Middle East. They are fruits, popular
for not only their taste, but also their nutritional value. Previous studies have shown that
pomegranate seeds have exceptional antioxidant levels. Recently however, research
into other parts of the pomegranate has shown that the pith and carpellary membrane
also contain a considerable amount of antioxidants; perhaps even more. This study
aims to differentiate between two different techniques used to isolating the antioxidants
from the pith and carpellary membrane, as no prior research has been done on the
topic. A DPPH assay and a modified TEAC assay will be used to test antioxidant
activity. This project should help expedite future research involving the extraction of
antioxidants from pomegranates as well as other fruits.

CHED 259

Analysis of elements in nutritional beef bone broth

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Bone broth is traditionally prepared by boiling animal bones with water and vinegar for
many hours. Bone broth or stock is recommended by some as a mineral rich food.
Many health claims are made about the benefits of nutritional bone broth but there is
little published research on bone broth. In this study bone broth samples were prepared
in lab using beef bones and acetic acid. Then the samples of bone broth were analyzed
using ICPMS to determine element concentrations. It was determined that no elements
were present in bone broth in nutritionally relevant or potentially hazardous
concentrations (using USDA RDAs and EPA action limits as comparisons).

CHED 260

X-ray structure and variable-temperature photoluminescent properties of
isostructural lanthanide cyanometallates containing DMSO
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Preliminary studies of three isostructural compounds with the formula \([Ln(DMSO)\_4(H\_2O)\_2(Au(CN)\_2)\_2]Au(CN)\_2\) \((Ln = Eu, Gd, Tb)\), abbreviated \(Ln\text{DMSOAu}\), were performed. Crystal structures and Au-Au distances were determined with X-Ray diffraction. Both \(\text{[Au(CN)\_2]}\) and DMSO within \(Ln\text{DMSOAu}\) have the potential to transfer energy to the lanthanide, although the studies are focused on the contribution from the cyanometallate system. Such potential was studied via photoluminescence experiments with two foci. First, effect of DMSO on cyanometallate systems were drastic and were examined by comparing photoluminescence spectra with studies of \(Ln[\text{Au(CN)\_2]\_3H\_2O}\). Second, changes in those energy transfer with respect to changes in temperature were studied via temperature-dependent scans.

CHED 261

Spectrophotometric determination of ethanol concentration in beer utilizing an enzyme activity assay

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A method for the enzymatic determination of ethanol content in beer was adapted for a sophomore level analytical chemistry laboratory. This method was part of a module focused on determining ethanol content of beer by various analytical techniques, including density measurements, the current brewing industry standard technique, and gas chromatography. The results of these three methods will allow the students to use statistical analysis to compare the validity of multiple analytical techniques to the beer’s label value. A coupled enzymatic reaction with alcohol oxidase and peroxidase was used to determine kinetics by spectrophotometry. Kinetic rates were used to construct a standard curve of varying ethanol standards to determine the ethanol content of the beer samples. Key findings include a protocol appropriate for sophomore level chemistry students that is highly reproducible, the importance of an oxygen saturated chromogen solution, minimizing matrix effects and proper storage conditions for alcohol oxidase.

CHED 262

Determination of cocaine concentrations in dried bloodstains

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Blood stains are established as important evidence in crime scene investigations. Blood allows investigators to identify suspects and victims. Dried blood stains are primarily used for DNA identification and blood typing, but not often used for drug identification. Determination of quantitative drug values would allow better interpretation of an individual’s state of mind during a crime where a bloodstain may be the only evidence available. This project was conducted through a two step approach. The first step was to determine cocaine concentration of dried bloodstains. Drug analysis was completed using Liquid Chromatography/Mass Spectrometry (LC/MS). This was followed by determining iron concentrations using Inductively Coupled Plasma/Optical Emission Spectroscopy (ICP/OES). Iron levels were correlated to the volume of the bloodstain which in turn was used to determine quantitative values for cocaine. Variable parameters include drug concentrations, bloodstain volumes, and different fabrics. The findings of this study will be presented, including evaluation of the effectiveness of this method in determining blood volume cocaine concentrations.

CHED 263

Detection and extraction of date rape drugs from hair samples using liquid chromatography - mass spectroscopy

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Drug testing for Drug Facilitated Sexual Assault (DFSA) crimes has previously only been completed using blood and urine tests. Hairs have not been a major contributor due to the more complex methodology required. However, drug testing on hairs provides more evidence than just blood and urine samples. With an increased need for a less complex method for hair testing it is crucial to detect a method that does not contaminate the drugs inside the hairs but allows the hairs to be cleaned on the outside. Sample human hairs were cut into segments roughly 2 cm in length then washed using ethanol followed by pulverization. An internal standard was then added to the sample hairs as well as the control hairs and centrifuged. From there the hair samples went through liquid-liquid extraction, and were analyzed using the liquid chromatography – mass spectroscopy (LC-MS) and supercritical fluid extraction (SFE). Hairs with single dosage exposure to a drug is harder to detect than chronic usage. Consequently, the drug concentration will be low, but still detectable by LC-MS.

CHED 264

Elemental analysis of CdSe/ZnS core/shell quantum dots by AA

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Quantum dots (QDs) are semiconducting nanocrystals with unique fluorescent properties that depend on the core and shell size. The core size is determined spectroscopically. Several methods have been employed for determination of the shell size. Of these AA is a convenient method accessible to most labs. Others report using AA by dissolving the QDs in aqua regia and diluting with water but accuracy and precision were not reported. In our experience this method produced low accuracy and precision. A closer look at the chemistry shows that selenide in aqua regia (or just nitric acid) is oxidized to selenite which forms insoluble salts with Zn(II) and Cd(II). When solutions are diluted with 0.36 M HCl instead of water, the selenite salts are soluble, greatly improving the accuracy and precision of the method. Results from this improved procedure are presented.

CHED 265

Analyzing thermal degradation of iso-alpha acids by high performance liquid chromatography (HPLC)

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Hops have long been used in the brewing of beer and are a resource of particular importance to the Rocky Mountain region. Hops play several vital roles in the brewing process, such as contributing to the bitterness of beer. The bitterness from hops is largely due to the formation of iso-alpha acids in boiling wort. While iso-alpha acids impart desirable flavors in a finished beer, it is also known that iso-alpha acids degrade due to light exposure to produce unfavorable components. In addition, iso-alpha acids thermally decompose over time. As a result, our research group has been studying the thermal degradation of iso-alpha acids to better understand the decomposition chemistry. Employing HPLC and using 4-tert-butylphenol as an internal standard, our group has been able to monitor the concentration of iso-alpha acids as a function of time and temperature. Thus far, the reaction is best modeled by first order reaction kinetics and rate constants for this reaction have been measured at several temperatures. Subsequently, the activation energy has been determined using the Arrhenius equation. Information gathered from this research will give valuable insight into the ever-changing chemical composition of an aging beer.

CHED 266

pH Dependent Zn(II) binding behavior of an analog methanobactin peptide

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Methanotrophs are methane-oxidizing bacteria that produce peptides called methanobactins. Methanobactin peptides exhibit selective metal ion binding affinity making the peptide a potential therapeutic for the treatment of degenerative diseases that are related to metal homeostatic misbalance such as Alzheimer’s. Synthetic analogs of methanobactin have been synthesized to determine the effect of amino acid sequence on metal binding properties. Current research involves the study of Zn(II) binding with a new analog methanobactin peptide with the sequence acetyl-His$_1$-Cys$_2$-Gly$_3$-Pro$_4$-Tyr$_5$-His$_6$-Cys$_7$ (amb$_5$), over pH 3-11. In an attempt to optimize the Zn(II) binding, the new amb$_5$ peptide consists of two symmetric binding arms separated by a proline residue, each arm containing the Zn(II) binding sites of Cys-His. The pH dependent Zn(II) binding ability of an amb$_5$ was tested using ion mobility-mass spectrometry. The amb$_5$-Zn(II) complexes were observed as both negative and positive ions and the Zn(II) bound peptides were dependent on the pH of the solution. At pH > 6, the amount of Zn(II) bound by the peptide increased due to the deprotonation of His$_1$ and His$_6$ imidazole groups which initialized the anchoring of the Zn(II). The results indicate the new amb$_5$ peptide has a higher affinity for Zn(II) than the previously studied sequence of acetyl-His$_1$-Cys$_2$-Gly$_3$-Pro$_4$-His$_5$-Cys$_6$ (amb$_1$), which did not include the Tyr$_5$ residue.

CHED 267

New method for improving solar energy conversion: Side selective modification of Photosystem I

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Solar cell devices on the market are constructed with inorganic materials (e.g. silicon, indium, and tellurium) that are resource- and cost-limiting. Alternatively, biohybrid cells produce photocurrent when integrated with the plant protein Photosystem I (PSI)-a sterically stable transmembrane redox protein found in light-dependent photosynthesis. This approach offers extremely efficient solar conversion (approaching 100% at specific wavelengths) without resource depletion. Given that the charge separation that occurs in is unidirectional with regard to PSI’s molecular orientation, the protein must be oriented on electrodes such that the P700 chlorophylls are aligned away from the electrode. Visual inspection of the crystal structure of the protein extracted from spinach (PDB ID: 2WSF), reveals that the hydrophilic areas are similar in both basic and acidic acid compositions. This similarity allows for the protein to bind to electrodes in both upright (P700 distal from the electrode) and inverted orientations. Previous research has shown that increasing the fraction of upright oriented proteins on electrode in turn increases photocurrent produced. We can accomplish this by modifying the chemical properties of the hydrophilic regions to promote surface asymmetry so that the
stromal/luminal sides of the protein have different affinities for the underlying electrode. Side-selective functionalization of extracted PSI was performed by pre-extraction EDC/Sulfo-NHS coupling to glutamic and aspartic acids with thiol terminated adducts on the stromal side of the thylakoid. We have shown that the functionalization was successful by performing - UV-vis and fluorescence spectroscopic analysis. We have also developed a chromatographic purification procedure that would potentially remove the unmodified proteins from the bulk sample. Currently, we are performing electrochemical analysis on the effectiveness of the functionalized samples. Further optimization of this method will create a new library of ligands to adjoin allowing for many new biomolecular applications.

CHED 268

Quantitative analysis of hydrogen peroxide using crude peroxidase extract from cucumber peel

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Vegetable waste was used as a low cost source of enzyme peroxidase as an alternative to a commercial horseradish peroxidase. The effectiveness of a crude extract of peroxidase from cucumber peel for quantitative analysis of hydrogen peroxide (H$_2$O$_2$) was tested. A calibration curve was generated using 3,3',5,5'-tetramethylbenzidine as a substrate. The enzyme-substrate reaction was stopped with sulfuric acid. The varying yellow shades of the resulting solution, which correspond to H$_2$O$_2$ concentration, allow for quantitative analysis via the measurement of absorbance at 455 nm. The enzymatic method based on natural extract from cucumber peel and the published method using vanadium pentoxide (V$_2$O$_5$) as a chromogenic reagent were compared in terms of working range, sensitivity, detection limit, and safety.

CHED 269

Determination of bisphenol A in thermal receipt paper water samples and lake water samples using fluorescence spectrophotometry

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Bisphenol A (BPA) is a chemical that is commonly used in harder plastic products, in the lining of food cans, and in thermal receipt papers. The usage of BPA in common products has become a concern for humans, especially for infants and young children, because of its effects as an endocrine disrupter. BPA has been linked to diabetes, cardiovascular disease, obesity, and certain developmental disorders. Because of the possible effects of BPA on the development of infants and young children, the use of BPA in baby bottles and other baby products has been outlawed. However, BPA is still used in the lining of canned goods and thermal receipt papers. The purpose of this
experiment was to test the amount of BPA that leached from thermal receipt papers into water samples that surrounded the paper using fluorescence spectrophotometry. Also, lake water samples were tested for the presence of BPA. Concentrations of BPA were both detected and quantified in all of the receipt water samples and lake samples that were tested.

CHED 270

Determining the mechanism of high-temperature methylation of oleic acid triglyceride by tetramethylammonium hydroxide

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With petroleum reserves on the decline, there has been a growing interest in biofuel production. Traditional fatty acid methyl ester (FAME) biodiesel production using transesterification of seed oils has proven to be cost ineffective as a suitable replacement. By adding tetramethylammonium hydroxide (TMAH) to oleic acid triglyceride during the reaction, the glycerol backbone of the fatty acid is methylated, creating methoxylated glycerol esters in addition to the FAME compounds. Deuterium-labeled reagents, TMAH and methanol, were used to investigate the possible methylation mechanism taking place. The reactions took place at elevated temperatures (>200 °C) for several minutes. The incorporation of the label into the final products was monitored using a Leco 4D GC x GC TOFMS. Analysis of the GC spectra showed that direct methylation is responsible, not transesterification.

CHED 271

Determination of bisphenol-A (BPA) in canned goods from Arkansas markets using fluorescence spectrophotometry

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Bisphenol A (BPA) is a chemical widely used in production of consumer goods. It has come under study recently after being labeled as an endocrine disruptor (ED), mostly causing adverse effects in infants and young children. It has been associated with diabetes, cardiovascular disease, and abnormal maturation, among other medical problems. Because it is so commonly used in product development, humans are exposed to BPA through various means, such as ingestion or dermal absorption. It is a concern that the combined exposure could cause serious effects even in small doses. In canned foods, the chemical is made into an epoxy resin to provide a protective lining along the inside of the can. BPA migration occurs when the free BPA moves from the lining into the contents of the can. This study used a standard addition method, along with fluorescence spectrophotometry to quantify BPA concentrations in the linings of canned foods. After removing the can’s original contents and replacing it with HPLC-
grade H₂O, BPA levels ranged from 0.7 ± 0.5 to 1.2 ± 0.5 µg/mL. In the original liquid though, concentrations vacillated between 43.5 ± 0.7 and 95 ± 4 µg/mL. After the application of heat, values stretched from 39 ± 2 to 94 ± 12 µg/mL. The results confirmed the presence of bisphenol-A in all of the cans, and indicated that there was no effect on migration of BPA after heating the samples.

CHED 272

Rapid identification of designer drugs with NMR spectroscopy

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Designer drugs are a persistent problem for forensic and clinical labs. As the government bans synthetic cannabinoids, phenethylamines, and cathinones, those who produce these substances create new substances to maintain the legality of their business. The ever-changing nature of this market can be a burden to labs that receive large amounts of samples containing unfamiliar substances. Our proposed methodology expands upon our previous work in which proton and correlation spectroscopy (COSY) Nuclear Magnetic Resonance (NMR) NMR methods were developed to quickly identify and quantify synthetic cannabinoids in herbal samples in less than one hour after cannabinoids were extracted from 50 mg of herbal incense with an NMR solvent such as CDCl₃. The same simple pre-NMR sample preparation technique is preserved to rapidly obtain NMR results. The current expansion includes incorporating more NMR techniques such as total correlation spectroscopy (TOCSY) and diffusion ordered spectroscopy (DOSY). TOCSY experiments were performed on herbal samples with previously known synthetic cannabinoids. These experiments revealed that signals coming from the alkyl region of the cannabinoid molecules can be elucidated further, as this is a region where signals tend to overlap or may be hard to assign with proton NMR and COSY. DOSY experiments with herbal samples successfully separated solvent and other materials from cannabinoid signals in samples that contain only one cannabinoid. Due to signal overlap, separation based on diffusion coefficient is extremely difficult in samples containing multiple cannabinoids. As of now, two different cannabinoids cannot be separated efficiently using DOSY. The original methodology is further expanded to include additional designer drugs typically found in “Molly” and “Bath Salt” mixtures. Eleven phenethylamine and cathinone standards were characterized using proton-NMR and COSY with similar parameters compared to the synthetic cannabinoid experiments, with the exception of D₂O as the NMR solvent. Potential signature peaks were identified that could be utilized to quickly identify the components of a street sample. Compared to liquid chromatographic separation results from the same standards, NMR proves to be a much more reliable process at the identification because many of the substances are fairly similar, often isomers of each other, and therefore elute that similar times.

CHED 273
Optimization of silver shell and silica core nanoparticles as SERS active substrate

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Silver nanoparticles improve sensitivity in Surface-Enhanced Raman Spectroscopy (SERS). However, these nanoparticles have limitations due to the wavelength they absorb when applied in biological SERS analysis. To address this problem, silica-core nanoparticles have been proposed to help silver nanoparticles absorb greater wavelength. This project intends to synthesize nanoparticles that have a silica core and a silver shell, and this process involves three steps: (1) synthesis of the silica core, (2) attachment of silver seeds to the surface of the silica core, and (3) growth of the silver shell on the silica core. The size and the shape of the nanoparticles will be analyzed using scanning electron microscopy (SEM) and UV spectroscopy in order to determine the optimum dimensions. The preparation and the characterization of core and shell nanoparticles were determined as a result of this experiment.

CHED 274

Synthesis, characterization, and catalysis of halogen and nitro substituted Schiff-base organometallic complexes towards the copolymerization of CO₂ and epoxides

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Transition metal Schiff base complexes have been shown to catalyze copolymerization reactions of CO₂ and epoxides in the presence of the tetra-butyl ammonium salt. The resulting polymers present an innovative way to utilize CO₂ and can produce unique materials with have potential applications as biodegradable skin and bone grafts. The synthesis and structure of these organometallic complexes with various substituent groups on the ligand is explored in this study. We present several of these salophen catalyst complexes and focus on the substitution of halogen and nitro groups on the ligand. Thus far, four Schiff base ligands have been synthesized that incorporate a phenylene diamine backbone and salicylaldehyde arms including N,N’-bis(5-chlorosalicylidene)-1,2-phenylenediimine. Other substitutions on the salicylidene arms include 3,5-dichloro, 3,5-diiodo, 5-bromo-3-nitro. Chromium and cobalt ions were coordinated to two ligands to provide the necessary catalytic sights. These ligands and complexes were characterized using ¹H and ¹³C NMR, FT-IR spectroscopy, and X-ray crystallography. Future work will investigate the catalytic properties of the resulting metal complexes in the aforementioned system.
Preparation of hydrophobic thermally polymerized sol-gel monolithic columns for reversed-phase liquid chromatography using “single-pot” approach

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A “single-pot” approach for fast preparation of hydrophobic thermally polymerized sol-gel monolithic columns for reversed-phase liquid chromatography was studied. These columns were prepared in the presence of an aqueous acid catalyst, free radical initiator, porogen, and monomers including 3-(trimethoxysilyl)propyl methacrylate (MPTMS), ethylene dimethacrylate (EDMA), and octadecyl methacrylate (ODM). Alternatively, 1-octadecanediol (ODT) was used instead of ODM. The effects of ratio of MPTMS to ODM or ODT, and ratio of MPTMS to EDMA were examined by observing changes of morphology of the monoliths. The presence of the crosslinker (EDMA) proved to be necessary for attaining white opaque materials. The C18-EDMA-MPTMS and EDMA-MPTMS monolithic capillary columns exhibited enhanced retention factor for benzene, and better stability in the aqueous mobile phase compared to columns made from MPTMS alone. We also used the faster photopolymerization reaction for the preparation of monolithic columns. However, significantly reduced retention was observed compared to that found for columns prepared using thermal initiation. The “single-pot” approach demonstrated here confirms its potential applicability for the preparation of monoliths using a wide variety of monomers.
Garnet classification and provenance using laser-induced breakdown spectroscopy (LIBS)

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157 garnets from 92 locations worldwide were previously analyzed using laser-induced breakdown spectroscopy (LIBS) and demonstrated that LIBS has the potential to discern garnet geographic origin. In this study, an expanded suite of garnets was analyzed with LIBS and an electron microprobe to compare the technique’s capabilities for garnet classification and geographic provenance determination. The spectral data were processed using multivariate statistical pattern recognition methods (e.g., PCA, PLSDA) and the resulting classification models were used to successfully classify unknown garnet samples of a specific compositional type according to their geographic origin. Various preprocessing techniques (normalization, spectral outlier removal) were implemented to optimize the LIBS classification results. Comparison of the results demonstrates that LIBS offers a good alternative for identification of unknown garnet samples based on their geographic provenance.

CHED 277

HPLC method development for caffeine analysis with Chlorella vulgaris as a bioremediation agent for aquatic systems

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Caffeine is one of the most consumed drugs in the world and is found in wastewater and as a contaminant in tap water. While the levels identified in the tap water samples may be minor in comparison to the amounts commonly consumed in beverages or found in over-the-counter pharmaceutical products, the total amount consumed by an individual per day is unknown. To reduce the concentration of caffeine in aqueous samples, the green algae Chlorella vulgaris was explored as a bioremediation tool. The goal of this project was to validate the method for analyzing caffeine and to determine the effectiveness of C. vulgaris in bioremediation. Here we report a high performance liquid chromatography (HPLC) trace analysis method to detect changes in caffeine concentration due to the presence and growth of C. vulgaris. The samples were pre-concentrated using a solid phase extraction (SPE) cartridge. The C. vulgaris samples were grown in media initially containing caffeine concentrations ranging from 0.4 ug/L to 40 mg/L. The HPLC samples were extracted every seven days over a 21-day period. The development and validation of this method will also be discussed.
Laser-enhanced ionization–mass spectrometry for dried blood spot quantification of a biomedically important analyte

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There is need for a method of blood analysis that enables monitoring of critical analytes and provides meaningful and actionable medical assessment. By utilizing dried blood spot (DBS) cards remote and self-testing are enabled. Other attributes are, a smaller amount of blood is required and can be shipped by the patient for analysis, which can occur over international borders. DBS enables analytes in whole blood or serum to be quantified with small amounts of sample in an analytically controlled manner. Sampling of blood for DBS analysis is also simple and can be completed by the patient at home by finger or heel pricks for young children. The current study uses the technique of laser-enhanced ionization coupled to a quadrupole time-of-flight (QTOF) mass spectrometer to analyze the biomedically important peptide, glutathione (GSH). The ratio between GSH and oxidized glutathione (GSSG) is of significant importance in this study, since this ratio is a biomarker for the proper functioning of the immune and detoxification systems in human body. Laser ionization using matrix-assisted laser desorption-ionization (MALDI) can also be applied in the quantification of peptides and other analytes in DBS card analyses. Accurate quantification has not been achieved in laser enhanced ionization previously as it has attempted to use calibration curves which cannot account for the variation in sample arriving at the mass spectrometer. This is being achieved in this research without calibration curves by utilizing speciated isotope dilution mass spectrometry (SIDMS), which eliminates the use of calibration curves and allows the isotopic standards to be the calibration additive with the matrix. This is covered in EPA method 6800 update V, 2013 for Environmental Human Health assessment. The quantification of GSG enables a more robust understanding for physicians to track their patients’ metabolic conditions and eventually will enable improved treatment. The analytical methods will be focused on in this presentation demonstrating these new bioanalytical measurement advances.

Developing paper microfluidic devices to detect drugs of abuse

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The goal of this project was to develop paper microfluidic test kits for use in the presumptive detection of seized drugs. In the project a set of colorimetric reagents were adapted for use with paper microfluidic devices to improve specificity and the ease of use of the testing. The paper-based tests can provide doctors, law enforcement officers, and toxicologists with a rapid method for screening several different drugs of abuse simultaneously. Three colorimetric reagents, Scott, molybdic acid, and cobalt (II) thiocyanate, were successfully applied to the paper devices. A four-channel device was then prepared to detect common drugs of abuse. Cocaine could be detected based on a blue color with the Scott reagent. Ketamine produced a lavender color with the basified Co(SCN)$_2$, and codeine produced a red color with the molybdic acid reagent. Ephedrine produced a red color with the molybdic acid reagent but reacted inconsistently with the other reagents. The Scott and Co(SCN)$_2$ reagents were also screened against common drugs and substances that could act as interferences. Overall, the results of this work demonstrate the potential of paper microfluidic devices in detecting drugs of abuse in situations where rapid results are needed.

CHED 280

Characterization of patterned anti-fouling xerogel coatings

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Hybrid, sol gel derived, xerogel polymer coatings have demonstrated superb anti-biofouling properties as evidenced by the commercially available material, Aquafast™. While much is known about the efficacy of these materials in the aforementioned application, there is still a need for insight into the role of structure. We report the characterization of a novel xerogel material composed of varying mole percentages of a carboxyethyltriol silane (COE) and tetraethoxysilane (TEOS). Techniques used for analysis include: atomic force microscopy (AFM), scanning electron microscopy (SEM), scanning kelvin probe microscopy (SKPM), Fourier transform infrared (FTIR), and Raman spectroscopy. Characterization of these COE/TEOS hybrid xerogels reveals the formation of unique topographical features, the size, shape, and distribution of which change with varying percentages of COE to TEOS.

CHED 281

Investigation of chemical interferences in vehicle arson accelerant identification

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When investigating a vehicular fire, a primary job of arson investigators is to confirm the identity of any ignitable liquid used as a fire accelerant. This can be complicated due to the presence of the vehicle’s fuel and also because there are many objects and
materials inside and on the exterior of vehicles that, when burned, produce chemicals that interfere with the relevant chemical analyses. It is important, therefore, for investigators to be aware of the chemical characteristics of the substrates that may be involved and the products they may form when combusted. To explore these issues in a specific way, we studied the chemicals associated with the combustion of automobile seat cushions using 87-octane gasoline as a fire accelerant. Both passive headspace analysis and solvent extraction, in conjunction with gas chromatography-mass spectrometry (GCMS), were employed, and an internal standard was used to help quantify a subset of compounds. The results indicate that although analytical interferences are introduced by seat cushion combustion, the presence of relatively interference free chromatographic regions enables gasoline identification. Arson investigators can use these regions to help confirm (or rule out) the likelihood of 87-octane gasoline as a fire accelerant in seat cushion combustion.

CHED 282

Identifying more efficient methods for rare earth isobar separations

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The efficient separation of rare earth isotopes is essential for their use in everyday electronics, magnets, lasers, and batteries. Rare earth isotopes are also important for the hybrid vehicle industry as well as for nuclear medicine in imaging, diagnostics, and treatment. Due to the chemical similarity of the lanthanides, separations are challenging; especially for isobars. Traditional methods for chemical separations can involve large volumes of costly solvents and be very time-intensive. Separations using resin columns offer the potential advantages of a reusable setup using less hazardous material with improved selectivity for rare earth isobars. Inevitably, gravimetric enrichment processes for samarium-140 also yield neodymium-140 due to their equivalent mass. As the least abundant isotope of samarium, samarium-140 is the most valuable isotope, especially in highly-purified form. The stable isotopes neodymium-140 and samarium-140 were studied both individually and in combined samples in order to better understand under what conditions they separate using a specific resin. Optimal conditions of effluent concentrations and volumes were determined and SEM analysis was performed to determine the split point of these isotopes. Automation of the process is in development to further decrease the time intensity and manual nature of resin separations. Improving the efficiency of rare earth isotope separations will support the capability to meet the growing demand for highly purified rare earths.

CHED 283

Using fast-scan cyclic voltammetry to quantify serotonin release in Huntington’s disease model mice
As a fatal, neurodegenerative movement disorder for which there is no cure and no effective treatment, research of Huntington’s disease is crucial. Clinical depression, which is often identified well before a definitive diagnosis of HD is made, is a common problem in patients. Serotonin is a key neurotransmitter implicated in the occurrence of depression; despite this fact, to our knowledge, investigations of the ability of neurons to release serotonin have not yet been published in the literature. The substantianigrareticulata (SNr) is richly innervated with serotonin-releasing terminals, and is thought to play a large role in movement, as well as reward. In this work, fast-scan cyclic voltammetry (FSCV) at carbon-fiber microelectrodes was used to compare serotonin release in acutely dissociated brain slices from wild-type and R6/2 Huntington’s disease model mice. An electrochemical waveform, designed specifically to increase the sensitivity of the electrode for serotonin while decreasing sensitivity for dopamine, was used to quantify serotonin release in the substantianigrareticulata (SNr). Using this method, we were able to positively identify and quantify serotonin release. Our data reveal that release is sharply diminished in 12-week-old R6/2 mice (18 ± 3.4% of WT), while it is relatively unaffected at 6 weeks of age (61 ± 9.8% of WT). In summary, this study shows a link between serotonin release and Huntington’s disease, which warrants further investigation of the mechanisms by which serotonin release is impaired in R6/2 mice.

CHED 284

Elemental analysis of enamel and dentin in healthy, carious, and periodontal diseased permanent human teeth using inductively coupled plasma mass spectrometry (ICP-MS)

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Teeth are organized into four major components: enamel, dentin, cementum and pulp. Enamel and dentin are primarily composed of the inorganic mineral hydroxyapatite [Ca_{10}(PO_{4})_{6}(OH)_{2}]. The elemental composition of teeth can provide important information about oral hygiene, diet and environmental factors. For this study, using inductively coupled plasma mass spectrometry (ICP-MS), we present a comparison of the chemical elements found in teeth based on oral hygiene status (healthy, carious, and periodontal diseased) and an environmental factor (smoking). For this analysis, we removed each tooth sample’s restorative material and pulp tissue. The dentin and enamel were not separated and were dissolved in nitric acid. The samples were centrifuged to remove any residual fibrous material. The teeth samples (healthy, carious, and periodontal diseased) were shown to have high concentrations of Mg and Na. In comparing healthy and carious teeth, carious teeth showed a decrease in concentrations of Si, Co, and B, and increased concentrations of Mg, Al, Sr, Zn, Cu, Sn,
Ba, and Pb. Periodontal diseased teeth samples showed no concentrations of S, Cl, and Sc compared with healthy teeth. In addition, there was a significant lack of sulfur in periodontal diseased teeth compared to both healthy and carious teeth. Also, there was a decrease in concentration shown for K and Si, and the concentrations of Mg, Al, Sr, Ba, and Mn increased. Our results were compared with those in the literature and a discussion on the importance of chemical elements found in human teeth is given.

CHED 285

Extraction and concentration of caffeine from artificial saliva for GC/MS analysis

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The analysis of saliva for drug testing is a well-known technique. The nature of GC/MS for the quantification of caffeine in saliva requires that the analyte be extracted from its aqueous matrix. In this study, a simple liquid-liquid extraction using 0.200 mL of chloroform is optimized for convenience, efficiency, and speed. These types of extractions are usually microextractions that would require tedious manual-injection; however, this technique uses an amount suitable for auto-injection. The extraction is performed on artificial saliva with controlled amounts of caffeine. It was found that maximum extraction efficiency can be achieved by hand-shaking the samples for 10 s, followed by 120 s sonication in a water bath. Further investigation will examine steps, such as adding NaCl or using ethanol as a mixing intermediate, that are used in traditional microextractions. Using a simple calibration curve method for rough quantification, the detection limit was found to be 0.05 mg/L, and the quantification limit was 5 mg/L. Relative extraction efficiency between different methods were also compared using relative peak heights. This study is in cooperation with a psychopharmaceutical study entitled: “Caffeine: A Model Drug for Studying Environmental Factors in Addictions.”

CHED 286

Determination of fluoride levels in mouthwash and tap water samples

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The benefits of supplemental forms of fluoride from various sources has been investigated for years. An optimal concentration of fluoride in human systems is necessary to avoid both dental caries and fluorosis. The Department of Health and Human Services recommends a range of 0.7 to 1.2 milligrams per liter. This range minimizes the chance for dental fluorosis. Samples from different brands of
mouthwashes and from tap water from Oconee region around Milledgeville, GA, were analyzed using ion chromatography. Mouthwash samples showed levels of fluoride consistent with those listed on the bottle by the manufacturer. Analysis of tap water samples indicated which communities have fluoridated water supplies.

CHED 287

Quantitative determination of methionine sulfoximine by liquid chromatography tandem mass spectrometry

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L-Methionine sulfoximine (MSX) is a common compound used in cell culture media. For years, MSX has been used in small concentrations within cell cultures without an understanding of its effects. Recently, it has become more widely known that MSX is a potent glutamine synthetase (GS) inhibitor that, in vivo, irreversibly inhibits the GS enzyme. This can lead to the development of seizures as MSX is a convulsant. The seizures are a direct result of the inhibition of the GS enzyme causing a rise of the glutamic acid concentration in the cell. We propose a novel approach for quantitatively detecting MSX in the ppb range using a combination of liquid chromatography and tandem mass spectrometry. Our process includes the method development and method validation steps including mass optimization, liquid chromatography optimization. Further, limits of detection and quantitation, linearity, accuracy, recoveries and robustness will be determined. This method will be helpful in detecting residual MSX levels in pharmaceuticals and vaccines.

CHED 288

NMR Investigation of the effect of pH on aggregation, counterion binding, and amide proton exchange in amino-acid-based surfactants

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NMR Spectroscopy was used to characterize the physical properties of micelles formed by the single amino-acid surfactants undecanyl-(L)-alanate (UND-Ala), undecanyl-(L)-leucinate (UND-Leu), undecanyl-(L)-valinate (UND-Val), undecanyl-(L)-isoleucinate (UND-Ile), and undecanyl-(L)-phenylalaninate (UND-Phe). These surfactant molecules are composed of a long hydrophobic tail and a hydrophilic amino-acid head-group. In an aqueous environment, surfactants aggregate to form micelles, which stabilize the surfactants by shielding their hydrophobic tails and maximizing their polar head-group’s exposure to water. NMR spectroscopy was used to study the effect of solution pH on (1) micelle size and aggregation, (2) micelle binding by the amino-acid counterions (L)-
lysine and (L)-arginine, and (3) the rate of amide-solvent proton exchange. Micelles were observed to generally be larger in the pH 6.5-7 and 11-11.5 ranges, while being somewhat smaller in-between those ranges. It was also observed that arginine binds to the micelles in cationic form, but dissociates when it forms a zwitterion. Finally, the amino acid headgroup amide-proton solvent exchange rate constants were calculated for both micellar and monomeric surfactant solutions. Aggregation into micelles decreased the rate of amide NH-solvent exchange for all surfactants investigated. Further research is planned to investigate lysine binding to the micelles, and to characterize the behavior of dipeptide surfactants.

CHED 289

Effect of pH on isocynate amino acid based surfactants

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The purpose of this research is to synthesize and utilize chiral octyl isocyanates amino acid based surfactants. A mixture of an amino acid, sodium hydroxide and isocyanates solvated in a mixture of acetone and water were mixed at room temperature for one hour. The product was easily separated from the reaction mixture via addition of HCl
without the formation of any by-products. Purity of the product was confirmed using HPLC and NMR spectroscopy. A sequence of NMR water quenching studies in a predominantly basic solution showed that both amide groups were deprotonated, while a largely acidic solution showed both of the amide groups fully protonated. This amino acid isocyanate surfactant can be further investigated as to how the monomers form a micelle, how chiral ligands interact and separate in micellar electrokinetic chromatography and how their physical properties both differ from pervious amino acid terminated surfactants and kinetic interactions as a function of pH.

CHED 290

Surface immobilization of AMPs using click chemistry

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Antimicrobial peptides (AMPs) are a rising topic within research. Compared to antibiotics, AMPs are less likely to develop bacterial resistance. Surface immobilization has been widely used in biochips and biosensors. In this study, AMPs with an azide mutation at different terminus were applied using “click chemistry” for immobilization with alkyne terminated abiotic surfaces. Click chemistry forms a triazole linker, when an alkyne and an azide interact with each other to induce immobilization. Surface immobilization of AMPs was monitored via contact angle to determine the surface characteristics of the alkyne functionalized surface and circular dichroism (CD) determined the abundance of the α-helix and secondary structures of immobilized AMPs. Contact angle results indicated that the alkyne was functionalized on the surface and CD results presented that during surface immobilization the α-helix and secondary structures were protected in the process. This research provides further insight into characterization of surface immobilized biomacromolecules.

CHED 291

Analysis of nitrate content in vegetables using ion chromatography

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Nitrates and nitrites are added in food to prevent the growth of the Clostridium botulinum bacteria, but adding these ions can have the side effect of causing cancers along the digestive tract. Nitrates can also be found naturally in vegetables. Ion chromatography was used to quantify nitrates in spinach, celery, and cabbage. Samples of each vegetable were homogenized, heated to extract nitrates, and filtered. Silver cartridges were employed to remove chloride and improve the resolution of peaks. Although centrifuging is typically needed when analyzing meat using these methods, it was deemed unnecessary with vegetable samples. It was verified that there were no
nitrites in the vegetables. Spiked samples were created to ensure that no sample was lost due to error in the method. In addition to analyzing raw vegetables, common cooking methods were performed to determine if this had any effect on the nitrate concentration in the food. Given their carcinogenic properties, it is important to be able to quantify nitrates in foods.

CHED 292

Using regression analysis to determine the mechanism of solvent reactions

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Octyl chloroformate (OctOCOCl, 1) is used as a precursor for drugs that inhibit multiple enzymatic pathways to control obesity. The drug inhibits lipase which stops your body from breaking down and absorbing fat. Alkyl chloroformates in general are important precursors for many products and determining the mechanism of reaction for such substrates is extensive and tedious work. Hence, this undergraduate research project is also funded through the DE-INBRE and DE-EPSCoR programs as it trains students in the basic methodologies. In this project, the acid-base titration method has been used to study the specific rates of 1 in different concentrations of aqueous acetone, aqueous ethanol (EtOH), aqueous methanol (MeOH), aqueous 1,1,1,3,3,3-Hexafluoroisopropanal (HFIP), aqueous 2,2,2, trifluoroethanol (TFE), and in mixtures of TFE-EtOH at 25.0 °C. For 1, the specific rates of solvolysis correlate well with an extended Grunwald-Winstein (G-W) treatment. A direct comparison to G-W analyses obtained for phenyl chloroformate (PhOCOCl) in identical solvents strongly suggests that the addition step within an addition-elimination mechanism is also favored in 1.

CHED 293

Apparatus for ultratrace detection of arsenic in drinking water by hydride generation gas chromatography with photoionization detection

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The hydride generation technique is a common method to determine trace amounts of arsenic in drinking water. This method produces a considerable amount of pressure which would be unsafe if carried out in a normal closed glass reaction vessel. A stainless steel reaction vessel was machined which could handle the pressure generated in the hydride generation technique as well as provide an oxygen free environment to reduce interferences. A sample loop was also constructed to reduce systematic error and ensure a uniform sample introduction into the gas chromatograph. A very sensitive photoionization detector was used. A calibration curve was then constructed to determine the dynamic range of the instrument. This instrument was
validated by the analysis of highly characterized drinking water samples from Bangladesh.

CHED 294

Expanding and improving direct-analysis capabilities in mass spectrometry

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Mass spectrometry (MS) is a powerful analytical technique due to its combination of speed (analysis < 1 second), sensitivity (limits of detection in the femtomole regime), and selectivity. In addition, MS can provide qualitative, such as elemental composition and even structural information, as well as quantitative information of species present in a sample. These features offer advantages unmatched by other analytical techniques, however certain drawbacks have precluded more prevalent use of MS. In particular they are expensive (often costing over $200,000), large (weighing over 150 kg), and often require sample preparation techniques and/or time-consuming chromatographic methods to purify analytes. One area of research that aims to overcome these drawbacks is ambient desorption/ionization mass spectrometry (ADI-MS), which combines specially designed ionization sources with the speed, sensitivity and selectivity of mass spectrometry. Furthermore, samples can be analyzed in the open atmosphere and in their native environment without the need for sample pre-treatment.

In the present study, we are focusing on the performance of one such ionization source that desorbs and ionizes molecules directly from samples in the ambient environment. This source is the Flowing Atmospheric Pressure Afterglow (FAPA) which yields high desorption/ionization efficiencies and simple mass spectra. Our work is aimed at understanding how this source operates and "tuning" its ionization chemistry with the goal of being able to resolve multiple components in complex samples. By adjusting certain operating parameters of the ionization source, certain types of molecules can be selectively ionized. This tunable desorption/ionization approach provides an added dimensionality, which is essential for the analysis of complex sample types.

CHED 295

Investigation of β-blocker association with a chiral molecular micelle by means of molecular dynamics simulations

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Molecular dynamics (MD) simulations were used to investigate the binding of β-blocker drugs propranolol and atenolol to the chiral molecular micelle (MM), poly-(sodium undecyl-(L)-leucine-valine) poly(SULV)). The MM contained twenty covalently bonded surfactants each with a chiral dipeptide headgroup. Poly(SULV) is used in capillary electrophoresis to separate enantiomers of chiral drugs. One enantiomer of each β-blocker was docked into one of four MM binding pockets and MD simulations were carried out. Propranolol binding free energy calculations showed that (S)-propranolol associated more strongly with poly(SULV) than (R)-propranolol. Analogous calculations showed that the association of atenolol enantiomers with the MMM were very similar. Solvent accessible surface area analyses showed that in the preferred propranolol binding pockets the ligand’s rings penetrated deeply into the poly(SULV) core. Atenolol however, bound primarily near the surface. (S)-propranol was found to associate more strongly with poly(SULV) than (R)-propranolol because it experienced stronger hydrogen bonding interactions with the MM.

CHED 296

Investigation of the mechanism of chiral recognition by molecular micelles with molecular dynamics simulations

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Molecular dynamics (MD) simulations were used to investigate the intermolecular interactions between 1,1'-bi-2-naphthol (BOH) and lorazepam enantiomers and the chiral molecular micelle, poly-(sodium undecyl-(L,L)-leucine-valine) (poly(SULV)). Poly(SULV) is of interest because it is used to separate the enantiomers of chiral compounds in capillary electrophoresis. The goal of the project was to characterize the mechanism of chiral recognition in these separations. The MM is composed of twenty covalently bonded surfactants. BOH and lorazepam enantiomers interacted differently in each of four distinct MM binding sites. Analyses of the free energies of binding, solvent accessible surface area, hydrogen bonding, water shells, and ligand orientation were used to rationalize the enantiomers’ behavior. BOH enantiomers preferentially bound in pockets where they had favorable orientation with respect to the MM surface and hydrocarbon core. Similarly, the lorazepam enantiomers oriented in such a way that favorable hydrophobic interactions occurred between their aromatic rings and the MM core.

CHED 297

Examination of silica sol-gels and aerogels containing silver nanoparticles and 4-mercaptobenzoic acid using surface-enhanced Raman spectroscopy
Sol-gels and aerogels containing silver nanoparticles have been investigated for use as substrates in surface-enhanced Raman spectroscopy (SERS). 4-Mercaptobenzoic acid (4-MBA) was chosen as the probe molecule in this study, as it has been well-characterized using SERS. The orientation of 4-MBA at different coverages in gels, and at differing concentrations of silver colloid has not been well studied. For both base and acid-catalyzed sol-gels and aerogels, the concentration of 4-MBA was varied with a constant silver colloid concentration in the silica gels and the effects were measured with SERS. The effect of varying silver colloid concentration against a constant 4-MBA concentration was also investigated. The results of each process were compared.

CHED 298

Chromatographic analysis of bee propolis

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Propolis, a natural resinous substance collected by honeybees from buds and exudates of plants, is believed to be used in the beehive as a protective barrier against enemies. Depending on the season, bee species, vegetation, and the area of collection, the chemical composition of propolis are qualitatively and quantitatively variable. In this study, several propolis samples obtained from various parts of the world (Europe, Australia, USA and the Philippines) were analyzed using chromatographic techniques (HPLC, LC-MS, GC-ECD and GC-MS). Based on the results, most samples have different composition with one another.

CHED 299

Studies on the interactions of four nanoceramics (metal oxides) with serum albumin and hemoglobin proteins by spectroscopic techniques

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Nanomaterials are materials with morphological features on the nanoscale, with special properties stemming from their nanoscale dimensions. Nanomaterials are of great interest lately due to their wide variety of applications. The extremely fascinating and useful properties of nanomaterials, which can be exploited for a variety of structural and non-structural applications, made them versatile materials in various fields of science ranging from material science, energy and medicine. Because of this, knowledge on the interactions of nanomaterials with different biomolecules must be known. The interactions of four nanoceramics (aluminum oxide, silicon oxide, titanium oxide and
zinc oxide with bovine serum albumin, human serum albumin and hemoglobin proteins were investigated by various spectroscopic methods (absorbance, fluorescence, circular dichroism and line scattering). Results showed aluminum oxide reduced absorbance and emission of all proteins in comparison to the other nanoceramics. Changes in the conformations of proteins were also observed upon mixing with the nanoceramics.

CHED 300

Trace element analysis of commercially produced red wines and beers

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The purpose of our research was to determine and compare the concentrations of selected metals in commercially produced beers and red wines. Beers from twenty different countries including Australia, Belgium, Canada, China, Estonia, Ireland, Jamaica, Kenya, Thailand, and the United States were chosen for analysis. In addition, twenty-one red wines from seventeen countries such as Algeria, Australia, Chile, France, Greece, Hungary, South Africa, Spain and the United States were also analyzed. The elements quantified were copper, iron, manganese, and zinc which are known to be harmful when tissue accumulation occurs. As would be expected, these elements have maximum allowable limits in commercially produced alcoholic beverages. In this study, the concentrations of these elements were determined using flame atomic absorption spectroscopy and standard addition methods. Five additions of standard solution were made for each metal per sample and the solutions were analyzed in triplicate. The levels of the selected elements were generally low, and within recommended limits set by regulatory agencies and countries.

CHED 301

Comparing graphene oxide electrochemically reduced from aqueous and non-aqueous solutions for the purpose of serving as an electrocatalyst support material

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Considerable research efforts have focused on depositing graphene oxide via electrochemical reduction (ERGO). However most studies achieve this in an aqueous solution, but avoid addressing the difficulty in achieving complete surface coverage due to the evolution of H\textsubscript{2} gas during the reduction process. This is especially problematic when trying to coat a metallic surface such as Pt. This presentation will compare the electrochemical deposition of ERGO on platinum electrodes using non-aqueous (ERGO\textsubscript{DMF}) and aqueous (ERGO\textsubscript{AQ}) solutions to determine which delivers better surface
coverage while still retaining its electrochemical integrity. The goal of the research was to design a method that would achieve a reproducibility complete ERGO layer that was electrochemically active, which could then serve as an electrocatalyst support material. Toward this goal, ERGO$_{\text{DMF}}$ was explored as a support for electrooxidative hemin polymerization for the purpose of physiological H$_2$S detection.

CHED 302

**Dependence of surface roughness on electropolish time on 316L stainless steel**

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Stainless steel is a common metal used for biomedical devices, such as coronary stents. Standard processing protocols involve electropolishing and passivation, methods that treat the metal surface for smoothness and corrosion resistance. The goals of this work were to (i) determine the effect of varying electropolishing time (30-600 s) on surface roughness of a stainless steel sample and (ii) determine the effect of various ionic liquids on electropolishing effectiveness. White light profilometry was used to analyze surface roughness of the samples after electropolishing and passivation. Results indicate that the smoothness of the stainless steel sample will increase as electropolishing increases as well. The applied potential to obtain a corrosion-resistant surface finish depends on the choice of ionic liquid.

CHED 303

**Mass spectrometry imaging of the *Torpedo californica* electric organ using MALDI-FT-ICR MS**

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In the present work, the electric organ of the *Torpedo californica* was studied using mass spectrometry imaging (MSI) and trapped ion mobility spectrometry coupled to mass spectrometry (TIMS-MS). Molecular ion density maps (1 x 0.5 mm field of view with 25 μm pixel size) were generated using a MALDI source coupled to a high resolution mass spectrometer (7.0 T Bruker Solarix FTICR-MS). A protocol for sample preparation was developed to preserve the integrity of the sample and it was confirmed by traditional histochemical analysis. MALDI matrices were applied using a home built sublimation chamber and mass assignment was performed with a 3 ppm error tolerance. A total of 87 lipids were identified in the bundle of axons and surrounding electroplaque cells, of which 27 and 29 lipids were characteristic to the axon bundle and electroplaque, respectively. Lipid assignment was further confirmed using TIMS-MS.
from a liquid surface extraction from the same tissue region. TIMS-MS reveal the presence of multiple isobars for most of the MSI identified characteristic signals, and structural assignment was performed based on the ion-neutral collision cross section differences among the lipid classes. This work provided a workflow for the identification of molecular species from tissue samples, their identification by exact mass (formula) and structural assignment using ion-neutral collision cross section.

CHED 304

Study towards the selective digestion of glyphosate in surface water

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The transport and fate of glyphosate [N-(phosphonomethyl)glycine], a herbicide used to control weeds in agricultural and urban areas, in surface water is poorly understood. Routine monitoring of glyphosate and its degradation product [aminomethylphosphonic acid (AMPA)] in surface waters can be cost prohibitive in terms of the analytical technique selected (e.g., LC-MS/MS), sample preparation, and number of samples to be tested. This project describes a study towards a cost-effective method that utilizes flow-injection analysis (FIA) and the phosphorus containing portion of glyphosate and AMPA molecules. Orthophosphate can be generated from glyphosate and AMPA under acidic and oxidizing conditions. This study explores varying the digestion method with different acids, acid concentrations, and oxidizing environments (e.g., UV light) to selectively decompose glyphosate and AMPA into orthophosphate. The produced orthophosphate is then quantified by forming the antimony-phospho-molybdate complex for UV-Vis spectrophotometric detection (880 nm). Optimized reaction conditions for selective digestion of glyphosate and AMPA to orthophosphate are presented.

CHED 305

Method development towards quantifying marijuana consumption using sewage based drug epidemiology: Preliminary results for Treatment Plant #2

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Initiative 502 legalized retail of recreational marijuana in Washington State. This initiative provides a unique opportunity to estimate marijuana consumption before and after legal sales commence. Marijuana consumption analysis is typically based on survey data, however recently sewage-based drug epidemiology has emerged as a complimentary technique to estimate drug use. This study focuses largely on method development to quantify a main metabolite of marijuana, 11-nor-delta-9-carboxy-tetrahydrocannabinol (THC-COOH) in raw influent to a Wastewater Treatment Plant
The optimized method normalizes THC-COOH concentration values to the contributing population through the use of an anthropogenic population biomarker: a metabolite of serotonin, 5-hydroxyindoleacetic acid (5-HIAA). In the optimized method, raw influent 24 hour composite samples are obtained from WWTP #2 in a mid-sized WA city. These samples - starting in December of 2013 and continuing until the present - are concentrated and extracted using Solid Phase Extraction (SPE) and analyzed by HPLC-MS/MS. The poster will specifically discuss method optimization for 5-HIAA, as well as preliminary concentration results of THC-COOH.

CHED 306
C-arylation methods to a library of covalent modifiers

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Covalent modification has emerged as an attractive method of probing biopathways implicated in cancer, infectious disease, and immune as well as metabolic disorders. Enzymes such as phosphatases, ligases, kinases, and proteases have long been drug targets because of their critical role in these signaling pathways. Many of these enzymes have nucleophilic cysteine residues in their active sites, and lend themselves to electrophilic covalent modification. A library of electrophilic vinyl sulfonamides has been constructed with the goal of developing a probe for cysteine-activated enzymes. These amino ester-derived, fused bicyclic, Michael accepting, vinyl sulfonamides were developed by a C-arylation driven protocol. This method consisted of: sulfonylation, bromination, dehydrohalogenation, propargylation, Huisgen [3+2] and final intramolecular C-arylation to close the ring. Future work will include attenuating the Michael acceptor via a Heck reaction. All compounds will be sent to collaborators for high-throughput screening to screen for biological activity.

CHED 307
Variance of caffeine in different brews of coffee

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Have you ever wondered how much caffeine is in your daily cup of coffee? Consumers with this question sparked interest in analyzing the caffeine content of locally roasted and brewed Blackbird coffee. Specifically, the owners of the coffee shop wanted to know how caffeine varies among their different roasting processes. According to the literature, numerous components of coffee change across roasts, and caffeine should as well. Previous work within our research group has developed a reproducible method to determine the caffeine content of coffee through liquid-liquid extractions followed by analysis with ¹H-NMR spectroscopy. Two types of Blackbird coffee (one caffeinated,
one decaffeinated) have already been analyzed using this method. In this work, a third type of coffee will be analyzed, and the data will then be compared with previous data to look for trends. This work will determine which brews have higher caffeine content than others, so that it can be reported to Blackbird coffee and their customers.

CHED 308

Method development towards quantifying marijuana consumption using sewage based drug epidemiology: Preliminary results for Treatment Plant #1

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With the implementation of Initiative 502, which legalized recreational retail marijuana in Washington, there was a unique opportunity to estimate marijuana consumption before and after legal dispensaries opened. Marijuana consumption is typically based on survey data, however recently sewage-based drug epidemiology has emerged as a complimentary technique to estimate drug use. This study focused largely on method development to quantify the main metabolite of marijuana, 11-nor-delta-9-carboxy-tetrahydrocannabinol (THC-COOH) in raw wastewater influent to a Wastewater Treatment Plant (WWTP). A method was developed that employs Solid Phase Extraction (SPE) and LC-MS/MS for analyte extraction and quantification. Raw influent 24-hour composite samples were obtained from a city Central WWTP (Treatment Plant #1) before and after legal retail stores opened. The optimized method quantifies both THC-COOH and an anthropogenic population biomarker (PB). The PB chosen for this study is the metabolite of serotonin, 5-hydroxyinoleacidic acid (5-HIAA). The PB allows for better consumption estimates by allowing for the normalization of the contributing population. This paper will specifically focus on method development for THC-COOH, and the optimized method, as well as preliminary concentration results of THC-COOH, will be presented.

CHED 309

Study of the impact of ionization conditions on ion formation in electrospray mass spectrometry

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Mass spectrometry can provide a wide range of analytical information on compounds that produce either ions during electrospray ionization (ESI). This project centers on the study of a range of target compounds and the impact of ESI conditions on the observed data. For negative ion mode this research focused on the analysis of the pain relieving drugs. Optimal ionization conditions were determined over a wide range of solution and instrument conditions. For positive ion mode the research focus on the analysis of Polyethylene glycol (PEG) and polypropyleneglycol (PPG) solutions. Samples for each
polymer where studied with different complexing cations added (Li⁺, Na⁺, K⁺, Rb⁺, Cs⁺, NH₄⁺ and Ag⁺). Analytes were run at a range of cone voltages to study the impact of each complexing cation on the observed polymer distribution.

CHED 310

Optimization of the voltammetric analysis of heavy metals

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Analytical measurements of certain heavy metals implicated developmental disorders are important in order to prevent and diagnose exposure. While the experimental conditions of many electrochemical methods have been optimized for large sample volumes using conventional macroelectrodes, this work addresses the challenges associated with scaling down the analysis to smaller volumes and replacing large electrodes with microelectrodes. While the bulk analyte concentration is not expected to change dramatically during conventional voltammetry analyses, we measured a significant depletion of metal ions when milliliter volumes were used. We showed that ion depletion from a solution of small enough volume and low enough concentration was possible, and from preliminary tests the optimum deposition step for a Pb²⁺ ion was around 400 seconds for the electrode and cell geometry that we were using. In addition, we have explored the use extraction techniques that can be readily scaled down to small volumes. Preliminary results suggest that when iodide is used to form a neutral complex with several heavy metals, including cadmium, this complex can be effectively extracted into a nonpolar phase. Unlike many other extraction methods which are often incompatible with voltammetry, we hope to show that this particular extraction technique does not interfere with our ability to pre-concentrate heavy metals on a small electrode.

CHED 311

Synthesis of variable size nanoprisms for application in signal enhancement using Raman spectroscopy

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Silver nanoparticles encompass conductive, thermal, optical, and antibacterial properties that can be used in many applications. Examples of these applications include the following: inks, paints, footwear, wound dressings, cosmetics, and biosensors. The nanoparticle properties depend highly on their size. Thus the way of synthesis and characterization of these particles is very important. Sizes of those particles can be estimated based on their absorbance wavelengths and can be verified by using electron and probe microscopy. In our research we aim to synthesize different size silver nanoprisms and apply those to the enhancement of analyte signal using surface enhanced Raman Spectroscopy (SERS). While most nanoparticles are
spherical in shape, the prismatic shapes of nanoprisms provide more surface area and edges that could aid in analyte signal enhancement using SERS. Once the nanoprisms are prepared, their size and shape can be estimated using UV-visible spectroscopy and Transmission Electron Microscopy (TEM). The different size nanoprisms will be used to show signal enhancement using Raman Spectroscopy.

CHED 312

Optical evaluation of fluorescent nanoparticles embedded into silica aerogel hosts

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Investigation of the behavior of fluorescent nanoparticles in suspended in aerogel hosts was performed. Changes in fluorescent properties during the curing and solvent exchange steps of an aerogel matrix were measured. Specifically, optical properties of the fluorescent nanoparticles such as excitation and emission wavelength shifts, peak width and profile, and relative fluorescent intensity were used to investigate the changes the aerogel matrix and solvent environment have on the fluorescent nanoparticles. These properties will ultimately be used to assess the validity of nanoparticles suspended in aerogel solutions as useful chemical sensing platforms.

CHED 313

Direct and indirect detection of FMN and FAD released upon target binding

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The overall goal of this research project focuses on developing biosensors that are responsible for the detection of clinically relevant biomarkers. Sensors in general consist of target detection and signaling components. Once a target molecule is detected, it must then signal the binding event via a transducer. We are working towards building an accurate and efficient biosensor for relevant small molecules such as tryptophan, ATP and serotonin. Aptamer probes are used for detecting specific targets in combination with indirect signaling from a reactivated Glucose oxidase (GOx). The signaling mechanism of this experiment is to interpret the signal of flavin adenine dinucleotide (FAD) based reactivation of apo-GOx (enzyme without co-factor), which is released upon target binding. A direct signaling method is to detect FAD or FMN that is released via square wave stripping voltammetry or fluorescence spectroscopy. The current studies compare the different methods of detection of the released co-factors and aim to establish limits of detection for each method.
Preparation of FAD conjugates to signal target binding events

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The overall goal of this project is to develop a widely adaptable biosensor for the detection of small molecules and nucleic acids. The current work focuses on the conjugation of iron protoporphyrin (hemin) to N^6-(2-aminoethyl)-FAD (flavin adenine dinucleotide) in order to develop a sensor for hemin. The design for this strategy is dependent on using an aptamer selective for hemin to bind a suboptimal target consisting of a heme-FAD conjugate. Via a displacement reaction the presence of heme will result in an unbound heme-FAD conjugate that can be detected indirectly via a flavoenzyme reactivation or directly via cyclic voltammetry. The displaced conjugate can be used to quantitate the level of heme present in a sample. FAD was selected to serve as the signaling agent for this detection strategy since it is redox active and is an enzyme co-factor necessary for the reactivation of an apo-flavoenzyme. Towards this end N^6-(2-aminoethyl)-FAD was prepared by reaction between FAD and aziridine. Subsequently the conjugation of hemin to N^6-(2-aminoethyl)-FAD was optimized via changes in reaction conditions to increase purity. The N^6-(2-aminoethyl)-FAD precursor and the heme-FAD conjugate reaction crude were purified via HPLC and characterized via MALDI-Tof. The heme-FAD conjugate was used within enzyme assays to validate the signaling system for the displacement strategy. Additional work exploring the affinity of the heme-FAD conjugates to the aptamer was carried out. These preliminary data provide a suitable system to explore target binding events leading to co-factor release.

CHED 315

Synthesis and photophysical and photochemical characterization of osmium complexes for luminescence-based sensing

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Photochemical stability, long excited state lifetimes, and reasonable quantum yields of luminescent transition metal complexes make them especially well-suited for use in luminescence-based sensors, which typically require a support matrix such as the hydrogels or metal-organic frameworks used in the current work. Osmium complexes are of particular interest because of their longer wavelength absorptions and emissions that allow for inexpensive excitation and minimize interferences from autofluorescence when the luminescence-based sensor is used in clinical samples. Specifically, water-soluble osmium complexes including [Os(bpy)$_2$(sulf-dpp)]Cl$_2$, [Os(phen)$_2$(sulf-dpp)]Cl$_2$, [Os(dpp)$_2$(sulf-dpp)]Cl$_2$, [Os(CO)$_2$Cl$_2$(sulf-dpp)] and [Os(phen)$_3$]Cl$_2$ where bpy is 2,2'-bipyridine, phen is 1,10-phenanthroline, dpp is 4,7-diphenyl-1,10-phenanthroline, and sulf-dpp is sulfonated 4,7-diphenyl-1,10-phenanthroline, were synthesized and characterized in order to evaluate their potential as luminescent reporter molecules with environment-sensitive luminescence anisotropies, excited state lifetimes, emission
wavelengths, and emission intensities. The osmium complexes showed minimal oxygen quenching, making them particularly well-suited in sensor applications of variable oxygen concentration. As determined from measurement of osmium complexes in solutions of varying viscosity, the series of complexes shows potential for use in lifetime-based sensors, and \([\text{Os(bpy)}_2(\text{sulf-dpp})\text{Cl}_2]\) and \([\text{Os(CO)}_2\text{Cl}_2(\text{sulf-dpp})]\) exhibit greatest promise as luminescence anisotropy-based probes. Progress toward inclusion of these complexes for use in metal-organic framework and hydrogel-supported sensors will be highlighted, and recommendations for the rational design of improved sensors will be made.

CHED 316

Effects of cinnamon components on glycogenesis by anion exchange-high performance liquid chromatography coupled to conductimetric detection

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The antioxidant properties of cinnamon components have been shown to interfere with the traditional method of measuring glucose with the glucose oxidase-peroxidase test. Interactions of cinnamon components with the first step of glycogenesis, the conversion of glucose to glucose-6-phosphate (G6P), could also be possible. Understanding the possible effects cinnamon components have on this reaction may be important for diabetes research. A chromatographic method has been developed using the Obelisc N anion exchange column with high performance liquid chromatography coupled to conductimetric detection. G6P was monitored when the reaction was carried out in the absence and presence of the following cinnamon components: cinnamyl alcohol, transcinnamic acid, trans cinnamaldehyde, and tannic acid. Interactions between cinnamon and the first step in the glycogenesis pathway will be shown.

CHED 317

Qualitative and quantitative analysis of fluorine containing synthetic cannabinoids

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Fluorine-19 nuclear magnetic resonance (NMR) was used to analyze synthetic cannabinoid street samples of XLR-11 and AM-2201 that were obtained from the Cumberland County Forensic Laboratory. A standard curve was created using solutions of known concentrations of XLR-11 and AM-2201. The concentrations of street samples were then determined from the standard curve. Gas chromatography-mass spectroscopy (GC-MS) was used to verify the results.
Study of an alternative method for quantitative Ni(III) determination

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Determining the capacity of nickel cathodes can be useful in characterizing and determining failure in Nickel-Hydrogen and Nickel-Cadmium batteries. From this lab, a new procedure has been developed that can determine this capacity more accurately than the current NASA method, even with the complications of the reaction matrix. The NASA procedure utilizes Fe(II) and KMnO$_4$ to determine the Ni(III) content, while our new method uses $\text{N}_2\text{H}_4$ and IO$_3$. While this new method is faster and more precise, there is evidence that having Ni$^0$ present in the matrix affects the titrations in an unexpected manner. The extent to which this Ni$^0$ affects the titration has been quantified and titration conditions have been explored to mitigate all matrix effects. Results from this and the NASA procedures are compared.

CHED 319

Analysis of pharmaceuticals in water samples by gas chromatography-mass spectrometry (GC-MS)

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Pharmaceutical drugs play an important role in modern society’s health industry. There is an estimated amount of 3000 diverse compounds that are distributed in both human and animal therapeutics. The increasing consumption of pharmaceutical medicine shows some concern because they may have a negative ecological impact. This is largely due to the fact that a percentage of these drugs are not completely metabolized by the human or animal body. These unprocessed drugs are excreted and eventually end up into many water systems including lakes, ponds, and wastewaters. There is also some speculation that trace amounts of pharmaceutical products could be in our drinking water. Therefore it would be beneficial to optimize techniques in detecting drug concentrations in water samples. In this study, four drugs (ibuprofen, naproxen, sulfamethoxazole, and carbamazepine) are analyzed in trace quantities using gas chromatography-mass spectrometry. A derivatizing agent known as bis(trimethylsilyl)trifluoroacetamide (BSTFA) paired with a trimethylchlorosilane (TMCS) catalyst is used in this study. Following a series of parameter optimization studies to establish the analytical method, the method will be applied to real-world samples. The overall goal of this study is to detect these drugs in samples taken from natural water sources and drinking water in the Danbury, CT region. This detection would allow future studies in pharmaceutical impacts on the environment as well as improvements for water treatment.

CHED 320
Comparison of solid phase extraction and solid phase microextraction for the quantitative analysis of trans-resveratrol in red wine samples by HPLC

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Moderate consumption of red wine has been associated with reduced risk of heart disease and extended lifespan. These benefits are often attributed to trans-resveratrol, a polyphenol found in red grapes. Novel quantitative methods were developed for measuring trans-resveratrol in red wine samples using solid phase extraction (SPE) and solid phase microextraction (SPME). Each method employed an octadecylsilyl stationary phase. The extracts were analyzed by HPLC. Particular focus will be given to the SPME method, as these octadecylsilyl fibers are relatively new and have not been previously used for trans-resveratrol analysis. Additionally, it has been determined through preliminary testing that the SPME fibers can be used more often than the manufacturer’s recommendation. If proven true, the multiple use of these fibers can result in a significant cost reduction for the analysis. This new SPME method will be compared to the more conventional SPE method for ease of use, accuracy, and limit of detection.

CHED 321

Automated reaction monitoring using liquid chromatography-mass spectrometry

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Forced degradation studies are widely used in the pharmaceutical industry to investigate the degradation pathways of drugs. Forced degradation reactions are often monitored by liquid chromatography-mass spectrometry (LC-MS), which enables the quantitation of reactants, intermediates, and degradation products and aids in the identification of unknown species. Because degradation reactions may proceed for many hours, and because frequent sampling allows more precise determination of reaction time course, the investigations would benefit from automated analysis. Traditionally, aliquots of a degradation reaction are sampled into vials and are analyzed later by LC-MS. Disadvantages of this approach include the need for manual sampling from the reaction vessel and the delay in analysis of several hours or longer that sensitizes reaction quenching and could result in further degradation in the autosampler vials. We have developed a simple instrument for online monitoring of forced degradation reactions which can be adapted to any commercial LC-MS equipment. The system allows automated, continuous sampling of reaction mixtures by low flow rate vacuum aspiration followed by continuous, computer-controlled injections for online LC-MS analysis. The stability of the automated sampling and injection system was excellent, with 3% relative standard deviation in peak area over a 24-h period. The
A system was used to examine the forced degradation of a common antiseptic, chlorhexidine, for 24 h with 15-min temporal resolution. Additionally, the effect of low pH and high temperature on a mixture of drugs found in over-the-counter cold medicine was also investigated for over 12 h. The system is versatile and can be used for any application in which continuous sampling, automated injections, and liquid chromatography-mass spectrometry analysis are desired.

CHED 322

GC-MS characterization of cell culture media: Optimizing sample preparation using automation and design of experiments (DOE)

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Cell culturing technologies are prevalent across a wide range of applications, including biotechnology, pharmaceuticals, and the food and beverage industries. Therefore, the development of analytical characterization methods for cell culture media (the complex aqueous solutions that provide nutrients for the growth of cells) is crucial so that changes in the constituents can be monitored to better understand and improve upon the culturing process. Applying multiple reliable media characterization methods allows for the most complete metabolic profile and helps ensure consistency and reproducibility of cell culture. Common methods used to characterize cell culture media include liquid chromatography – mass spectrometry (LC-MS) and spectroscopic techniques, such as infrared and Raman spectroscopy. The work described here utilizes gas chromatography – mass spectrometry (GC-MS), for characterization of model media solutions containing amino acid constituents. In order to increase volatility and thermal stability prior to GC-MS analysis, chemical derivatization is necessary, which introduces complex sample preparation methods. Our work focuses on the development of completely automated sample preparation methods using a liquid handling robot. Specifically, we aim to optimize the sample preparation – including a two-step chloroformate derivatization and extraction – in terms of both reproducibility and GC peak area. Hardware settings (e.g., robot probe position), and chemical variables (e.g., pH) were determined to be major players in sample-to-sample reproducibility. Because of the high number of variables in the chemical derivatization process, design of experiments (DOE) is used in the optimization. Mixing parameters (number of cycles, flow rate, and volume) and interactions between these parameters have a significant effect on GC peak area. This poster will present our work identifying the major factors contributing to reproducibility and peak area, and how they affect optimization.

CHED 323

Evaluating graphene oxide electrochemically reduced on Pt-black as a support for H₂S detection
Selective in vivo detection of H$_2$S over CO and NO has gained a lot of recent attention due to its particular importance in the cardiovascular and central nervous systems. Previous attempts at electrochemical detection of H$_2$S showed a cyanide-coordinated ferriprotoporphyrin (FePP) electrocatalyst supported on Pt is an attractive electrocatalyst for selective H$_2$S detection over CO and NO interferences. However due to the elemental sulfur, produced as a product of the oxidation, adsorbing to any exposed Pt areas, a decrease in sensitivity and selectivity was observed. The focus of this research was on using Pt-black as a supporting layer to the FePP in order to inhibit this fouling process. We have learned that the likely first step in the FePP polymerization is for the FePP to adsorb to the electrode surface. However Pt-black was determined to be resilient to FePP adsorption, which makes polymerizing FePP directly on a Pt-black surface extremely difficult. To counteract this problem, a layer of electrochemically reduced graphene oxide (ERGO) was deposited on top of the Pt-black surface. This was chosen as a supporting layer because previous research has shown that FePP adsorbs to carbon layers very well. This presentation will focus on our attempts to polymerize FePP on an ERGO/Pt-black surface. This will include microscopic characterization as well as characterizing its electrochemical response towards H$_2$S, CO, and NO.

**CHED 324**

**Method of collection and detection for airbourne organo-arsenic compounds**

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Organo-arsenic compounds, specifically roxarsone and p-arsanilic acid, are common ingredients in both swine and poultry feed. The workers that package the feed are exposed to these organo-arsenic compounds, which can cause irritation to the skin, eyes, and respiratory tract. To protect the health of the feed workers, methods of detection for these compounds are needed. High Performance Liquid Chromatography (HPLC) has proven to be a successful method. The current research is focused on determining a sampling media/device that will accurately collect both roxarsone and p-arsanilic acid. Two different types of filters, spiked with the compounds, have been tested for their percent recoveries; polyvinyl chloride (PVC) and glass fiber filters. The two types of filters were spiked with various amounts of these organo-arsenic compounds, ranging in concentration from 0.1 x the Permissible Exposure Limit (PEL) to 2 x PEL. Test results show that the filters have produced percent recoveries between 83.31 and 99.33%. Preliminary work shows that the PVC filters generally produce higher percent recoveries compared to the glass fiber filters. Linear absorbance trends and the instrumental limit of detection (LOD) have been determined for both roxarsone and p-arsanilic acid. Storage and stability tests will be run for both filters and both
compounds. If time allows, other sampling devices, such as sorbent tubes, will be tested for their percent recoveries with both roxarsone and p-arsanilic acid.

CHED 325

Selection of protein-binding DNA aptamers for bacterial detection

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This study describes ongoing efforts to identify and isolate specific DNA aptamers that bind to p57 also known as Major Soluble Antigen (MSA), the principal antigenic protein found on the cell surface of the Rs bacterium, responsible for causing bacterial kidney disease (BKD) in salmonids. Two different templates, a 80-mer with a 40 bp random region and a 100-mer with a 60 bp random region, were used. Six sub constructs were constructed from the full length MSA protein based on three selected regions. Aptamers were identified from a very large, random pool through a process called Systematic Evolution of Ligands by EXponential amplification (SELEX). SELEX was performed on the R2c sub construct from region 2 which contains a putative DNA-binding domain and therefore is believed to be a good binding site for aptamers. Prior to each round of SELEX, ssDNA was isolated by reacting the biotin-labeled dsDNA with streptavidin coated sepharose beads. The separation is made possible by the fact that biotin binds strongly to streptavidin. The ssDNA was recovered by denaturing the biotinylated dsDNA with sodium hydroxide. Once isolated and characterized by DNA sequencing, aptamers will be used in binding assays to identify those with the highest affinity to R2c binding site with the purpose of developing a biosensor for Rs detection in water.

CHED 326

Development of a DNA biosensor for rapid detection of Renibacterium salmoninarum

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Current tools for environmental assessment of fish pathogens have low sensitivity and require involved protocols. In the case of Renibacterium salmoninarum (Rs), the pathogen responsible for causing bacterial kidney disease (BKD) in salmonids, methods for its detection (ELISA, FAT and PCR) have focused primarily on tissues such as kidney or ovarian fluid, thus requiring that fish be sacrificed. Attempts to use ELISA or PCR to detect Rs in water samples have not been successful. In this study we report ongoing efforts to develop a sensor for detection of Rs in water based on DNA
aptamers that show high binding affinity to p57 or Major Soluble Antigen (MSA), the principal antigenic protein found on the bacterium cell surface. Aptamers are currently being identified through SELEX (Systematic Evolution of Ligands by EXponential amplification) and will eventually be immobilized to gold nanoparticles to construct a colorimetric sensor.

CHED 327

Analysis and quantification of D-aspartic acid in marine bivalve mollusks

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For centuries marine bivalves (particularly oysters) have been thought to possess aphrodisiacal properties. Recently researchers have shown that the unnatural amino acid D-aspartic acid (D-Asp) occurs endogenously in several species of bivalve mollusks. D-Asp has also been found in the nervous and endocrine systems of many vertebrates and invertebrates where D-Asp has physiological importance as a neurotransmitter and as a hormone regulator. We have analyzed and quantified D-Asp in some marine bivalves such as oysters, clams and mussels. D- and L-Asp were isolated from homogenized tissues and separated from other amino acids by anion exchange chromatography. The D- and L-Asp were then derivatized with o-phthalaldehyde (OPA) and N-acetyl-L-cysteine (NAC) to form a pair of fluorescent diastereomers which can be separated and quantified by high performance liquid chromatography (HPLC) on a reversed phase C-18 column, eluted isocratically with sodium citrate-methanol (NaCit-MeOH) buffer, and fluorescence detection. The results and significance of these analyses will be reported.

CHED 328

Triarylmethane and xanthene dye synthesis and characterization of their photophysical properties

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Photodynamic therapy (PDT) has been used to treat cancer and skin diseases with a photosensitizer (dye), light, and molecular oxygen. The dyes chosen had triarylmethane and xanthene chromogens. Three triarylmethane dyes were prepared with a two-step synthetic route and one xanthene dye was prepared using a one-step synthetic route. The dyes were analyzed using NMR to obtain their structural information. Ultraviolet-visible spectroscopy (UV-vis) was used to identify the wavelength of maximum absorption ($\lambda_{\text{max}}$). Fluorescein was used as a standard to calculate the fluorescence ($\Phi_f$) and singlet oxygen ($\Phi_\Delta$) quantum yields using fluorescence and absorbance,
respectively. The octanol-water partition coefficient was measured to determine if the
dyes have greater solubility in the aqueous region (water) of the body or the lipophilic
tissues (octanol). The photophysical properties of dyes helped determine their potential
use in PDT.

CHED 329

Analysis of analgesics in the Quittapahilla Creek watershed

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Today, the widespread use of medications, especially various types of analgesics, is
resulting in increased levels of these drugs in the wastewater streams entering septic
systems and wastewater treatment plants. It is important, therefore, to determine the
efficacy of these means of sewage treatment in removing therapeutic drugs before they
reach streams, lakes, and groundwater. We have therefore embarked on a project to
measure the levels of three commonly-used analgesics, ibuprofen, naproxen, and
salicylate, in both influent and effluent streams of one municipal wastewater treatment
plant on the Quittapahilla Creek in Lebanon County, Pennsylvania. The project involves
concentrating the analytes using solid phase extraction (SPE), derivatizing the acidic
drugs as methyl esters, and analysis by gas chromatography/mass spectrometry. We
have successfully derivatized the analgesics using boron trifluoride/methanol, and have
developed a SIM program to separate and quantitate the derivatives. We are now
involved in perfecting the SPE method for use in analyzing the water samples for the
analgesics that they contain.

CHED 330

Cross-linker effect on metal ion detection using molecularly imprinted polymers

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Molecularly imprinted polymers coupled with spiropyran dyes can be used as chemical
sensors for metal ion detection. The imprinted polymer must maintain its structure in
order to be an effective sensor for a given metal ion. The cross-linker used in the
polymerization process connects polymer chains together, increasing the polymer
rigidity, and plays an important role in the resulting polymer structure and sensor
characteristics. This study has focused on determining how varying the cross-linker
molecular structure influences the resulting polymer sensor response features/
selectivity for divalent metal cations. Three different cross-linkers were investigated,
having two, three or four polymer cross-linkage points. The hypothesis was that having
more linkage sites would increase the rigidity of the polymer and lead to increased
selectivity and sensitivity for the imprinted metal ion relative to a control polymer.
Trimethylolpropane trimethacrylate with three cross-linking sites resulted in the greatest
sensitivity and improved selectivity for a zinc imprinted polymer. Future work will continue to investigate the effect of the rigidity in combination with polarity changes in the cross-linker structure to determine optimal polymers for enhancing selectivity and sensitivity for different metals of interest, such as cobalt, zinc and nickel.

CHED 331

Analysis of trace metals in tattoo inks using Agilent ICP MP-AES

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The art of skin tattooing has been practiced since medieval times, but has increased significantly in popularity since the 1970s. This is problematic as tattoo inks are not currently regulated by the Food and Drug Administration (FDA), and manufacturers are not required by law to inform users of the contents of their products. The minimal information provided, which is solely in the form of material safety data sheets, is often vague and inaccurate. The purpose of this research was to quantify the concentration of metals, particularly heavy metals, in tattoo inks. Using CEM MARS 6 microwave, we were able to digest the tattoo inks using concentrated nitric acid. Analysis of unknown concentrations was conducted with ICP MP-AES using a calibration curve. Results of this market analysis of 50+ inks are reported, and directions for future research are discussed.

CHED 332

Paper-based device for colorimetric detection of malondialdehyde in biological samples

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Oxidative stress in biological systems is known to be involved in the development of many diseases such as Alzheimer’s disease, Parkinson’s disease, many cancers, among numerous other disorders and diseases in patients. Oxidative stress in a biological sample is caused by the accumulation of Reactive Oxygen Species, which results in the formation of free radicals and peroxides which can damage and/or have adverse effects on cell function. Our research primarily involves the oxidative stress biomarker Malondialdehyde (MDA), one of the major products of lipid peroxidation in a cell. The goal of our research is to develop a paper-based microfluidic device that is able to colorimetrically determine levels of MDA in a biological sample, specifically in saliva. This will provide a portable and affordable way to easily and accurately determine ones level of oxidative stress without the use of invasive or expensive equipment.
Optimization of solid phase extraction of petroleum residues implementing green chemistry principles

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Previously, compound determination of petroleum residues from water accommodated fractions (WAF-water fraction of an oil/water mixture) was accomplished by liquid-liquid extraction requiring large volumes of several organic solvents. This solid-phase extraction method serves as a greener option where the smaller volumes of extraction solvents significantly reduce waste, improve safety and reduce environmental and human exposure to harmful chemicals. 3-aminopropyl silica gel (APS) columns were used to separate acid and neutral species while Phenomenex silica columns separated bases. It was found that for a 500 mL WAF sample, one APS and two Phenomenex columns yielded optimal species separation. Qualitative testing was performed by fluorescence-HPLC to determine method efficacy. Separately, it was noted (by comparison of chromatograph signal) that an increased number of aliquots for each wash may result in improved ionic return for each column. Further quantitative/qualitative testing will be performed by high resolution FT-ICR/MS.

Using solvent parameters for increased precision in chemical shifts

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The chemical shifts of small molecules such as methane and ethane have been previously reported, but in the intervening years there have been advancements in knowledge of solvents and how they affect a spectrum. This work determines the chemical shift of a few molecules, such as methane and ethane, to a greater degree of precision than these initial reports, and correlates these shifts with various solvent parameters.

Lab curriculum development involving the synthesis and characterization of molecularly imprinted polymers in the detection of aspirin

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MIP synthesis is relatively novel but increasingly important in trace-analysis characterization. Typically used for the detection of chemical warfare agents as a security measure, recent studies have broadened the application of MIPs to dyes, environmental toxins, and various drug compounds including common over-the-counter analgesics such as aspirin. The high selectivity of MIPs makes them extremely useful in the determination of the presence of trace amounts of compounds in a sample. Detection of the target in sample matrices is via molecular recognition and goodness of fit with respect to the molecular cavities. In the analytical curriculum, students synthesize an aspirin templated MIP along with a nontemplated (blank) MIP. Students determine the useful working range (expressed as mass of template or breakthrough volume), and specificity with respect to caffeine, acetaminophen and salicylic acid then determine the aspirin content in an over-the-counter medication. The experiment requires approximately two four-hour lab periods to complete. The experiment incorporates and reinforces several analytical techniques/skills and can be combined with alternative aspirin detection methods for statistical comparison.

CHED 336

Quantitative analysis of alcohol using nuclear magnetic resonance

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The Nuclear Magnetic Resonance (NMR) is introduced to students during Organic Chemistry. The NMR is typically used for qualitative and conformational analysis of a compound to determine the structure. The Instrumental Analysis lab uses the PerkinElmer FT-IR Spectrometer to quantify ethanol found in a sample of Skyy Vodka. For this study, an experiment was developed to use quantitative functions of the NMR to similarly quantify ethanol samples. The concentration of alcohol in Skyy Vodka was quantitatively analyzed by using a program called Eretic found in the Bruker NMR software. Eretic is used to quantitatively analyze a proton NMR to define the concentration of ethanol in the reference sample to be compared to the unknown concentration of ethanol in the sample. The analyzed data from the NMR will be compared to the analyzed data from the IR to see how accurate the NMR method is in quantifying ethanol found in the sample.

CHED 337

Conformational kinetics study of microperoxidase-11 using TIMS-MS and molecular dynamics

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Cytochrome C, a large globular protein in the body may go through many conformational changes, yet to this day remains unstructured. In the present work, the conformational kinetics of microperoxidase 11 (MP-11), a digest fragment of cytochrome C that contains 11 amino acids with a covalently attached heme group was studied. MP-11 like Cytochrome C go through many conformational changes when in solution. In particular, a novel technique recently developed at FIU in collaboration with Bruker Daltonics Inc. combined with theoretical calculation was used for the characterization of MP-11 conformational space [1-3]. Accurate ion-neutral collision cross sections were measured for all MP-11 generated charge states. Since MP-11 (like cytochrome C) undergoes conformational changes as a function of the solvent state, MP-11 ions were produced by electrospray ionization (ESI) in order to preserve the initial solution state structure and analyzed on the basis of size-to-charge, inside the Trapped Ion Mobility Spectrometer (TIMS) followed by mass identification using a time-of-flight mass analyzer (MS) [4-5]. TIMS-MS has the advantage that molecular ions can be trapped for several seconds which allow us to study the kinetics and stability of various isomers as a function of time, initial pH value (6.1, 4.5, 3.1), and molecular ion temperature. Results showed that MP-11 conformations vary with pH levels and trapping time, and multiple interconversion pathways were observed for [M+2H]+2 and [M+3H]+3 charge states. Candidate structures were proposed for each conformation observed and main molecular interactions responsible for the conformational changes are discussed.

CHED 338

Surface modification of photopolymerized sol-gel monoliths using thiol-ene click chemistry

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Photo-initiated thiol-ene click reaction with 1-octadecanethiol in the presence of free radical initiator, 2,2-dimethoxy-2-phenylacetophenone, has been applied for pore surface modification of photopolymerized sol-gel monoliths prepared from 3-(trimethoxysilyl)propyl methacrylate. This functionalization was carried out to increase the hydrophobicity of the parent monolith with an aim to enhance the suitability of the material for separations in reversed-phase liquid chromatography. Initially, the effects of the monomer concentration in the reaction mixture and the type of initiator including 2,2-dimethoxy-2-phenylacetophenone and benzophenone were examined. The chromatographic performance of the modified columns was tested in terms of column efficiency and retention of alkylbenzenes. In addition to 1-octadecanethiol, the click reaction was carried out with two more alkylthiols, 1-hexanethiol and 1-dodecanethiol. An increase in the length of alkyl group of thiol resulted in increased retention of alkylbenzenes, confirming an increase in surface hydrophobicity of the monolith. The
performance of monoliths functionalized using the thiol-ene click chemistry was found superior to performance of monolithic column prepared via photografting with octadecyl methacrylate.

CHED 339

Solid phase extraction (SPE) of urine in postmortem toxicology testing

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Coroners often perform postmortem toxicology screenings to measure the amounts of toxins, prescription medications, and drugs of abuse. This involves taking blood, urine, and tissue samples and preparing them for analysis. This project compared three urine sample preparation methods, solid phase extraction (SPE), liquid-liquid extraction (LLE), and un-extracted urine, for a toxicology screen for 58 drugs of abuse. The validation was a qualitative confirmation/identification plan that measured and analyzed percent recovery, carryover, limit of detection, and case comparison using a gas chromatography/mass spectrometry (GC/MS). Percent recovery compared SPE, LLE, and un-extracted analytes to see how well the extraction methods recovered the desired analytes. For most of the analytes, the percent recoveries were found to be better using the SPE columns. In the carryover step, SPE columns were used and the negative quality control (QC) was analyzed after the highest calibrator level to make sure no analyte remained in the GC/MS between samples. The limit of detection was examined to determine the lowest level the analytes can be detected using the SPE columns. The case comparison looked at 10 cases originally tested using the LLE tubes and compared the original results to the results found when the SPE columns were used.

CHED 340

Obtaining electricity from solar energy utilizing household products

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Solar energy is the electromagnetic radiation produced by the sun, and it can be used in a variety of ways to produce electricity. One way electromagnetic radiation can produce electricity is through a photovoltaic system that converts photons directly to a voltage difference. The objective of our research is to use only household items to produce an economical electrical potential with the use of solar cells. A Grätzel cell can be easily produced with household items with the exception of creating electrodes, which are usually transparent indium-doped-tin-oxide. To replace this expensive electrode, galvanized zinc steel that is woven was used, which allows photons to travel through
the electrical system and create the electrical potential. Initially, the native oxide on the zinc steel metal was too thin, which caused shorting of the system. To prevent the system from shorting, a thicker oxide was applied from a zinc acetate solution as an alternative. Once the zinc acetate solution was placed in a furnace it turned into zinc oxide. This prevented the metal from acting as a battery and allowed the electrons to travel through the whole cycle of a normal Grätzel cell. These Grätzel cells, recreated using only household products, displayed 21.2 mV, which is 1/3 of the electrical potential of a standard Grätzel cell. To optimize the efficiency of the Grätzel cells, different lengths of woven galvanized zinc steel were tested. The results indicated that a piece of galvanized mesh of two inches by one inch produced the most electric potential, a voltage of 64.9 mV. This small system is promising to the community because it indicates that creating an efficient solar cell at home is feasible.

CHED 341

Stabilities of mephedrone in biological and non-biological matrices

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Cathinone, an alkaloid found in the shrub Catha edulis (khat), causes the release of dopamine and is chemically similar to amphetamines and ephedrine. It is a Schedule I drug due to its ability to cause severe psychological or physical dependence. Many derivatives of cathinone have been synthesized to produce so called “bath salts” and LSD-type recreational drugs, such as NBOMes. These drugs appear frequently in forensic casework and it is critical that the stability of these substances is understood so that the best storage conditions may be used but also so that the results of unstable drugs can be interpreted. This research focuses on the stability of the cathinone derivative mephedrone in biological and non-biological matrices. Samples of matrix (human blood and urine, methanol, acetonitrile, carbonated soda and water) were spiked at 1 mg/L of drug and stored in the dark at room temperature, 4 °C (fridge) or -20 °C (freezer). Samples from each batch were extracted on day 0, 3, 7, 14 and 30 to determine how stable the drugs were in each matrix under each storage condition. The analyses were carried out by GC/MS. Results of this research have shown that mephedrone is more stable in acetonitrile than in methanol at all three storage temperatures, and more stable in human urine samples than in blood. The human urine samples have similar stability at 4 °C and -20 °C, and human whole blood samples show an increase in stability with decreasing storage temperature. Results from spiking water and Coca Cola have shown that mephedrone is more stable in the water samples and is more stable overall at -20 °C.

CHED 342
Development of paper analytical devices for the detection of substandard azithromycin and erythromycin

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The World Health Organization defines a counterfeit medicine as a pharmaceutical whose active ingredient is either under-dosed or completely absent. The worldwide counterfeit business was able to sell more than 200 billion dollars in counterfeit pharmaceuticals in the last few years. Communities which are particularly affected are those in which analytical resources, such as trained pharmacists or analytical instruments, are scarce. In these areas, Paper Analytical Devices (PADs), which involve simple colorimetric chemical tests on a paper-based device, can provide a screening method for the pharmaceuticals available. These PADs have been designed to provide an inexpensive and practical method for this front line drug screening. The PADs yield a quick identification of ingredients found in genuine and/or counterfeit drugs. For pharmaceuticals that are commonly under-dosed the PADs will offer a semi-quantitative analysis of the active ingredients. Macrolide antibiotics such as azithromycin and erythromycin are often found to be under-dosed or expired. Preliminary laboratory tests have yielded qualitative colorimetric tests which react with various functional groups on these antibiotics. In addition, both azithromycin and erythromycin have been found to react semi-quantitatively with sulfuric acid. Progress has been made towards finding instrumental methods using UPLC-UV and UPLC-MS analyses to quantify samples of azithromycin and erythromycin. These methods are being used to validate results obtained from tests carried out using PADs.

CHED 343

Raman probes as a rapid identification and detection tool for *E.coli* in fresh parsley

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Food pathogens are mostly bacteria that typically comprise among others *Escherichia coli*, *Salmonella* spp., and *Shigella*. Pathogens have long been recognized as one of the most important sources causing food poisoning worldwide. This and the fact that almost 98% of microbes found in food are non-pathogenic demands for the development of diagnostic tests that can specifically detect the target pathogen. Development of rapid methods for the detection and characterization of foodborne pathogens is vital not only to food industries but also to safeguard public health. Plasmonic Raman biosensors have the potential to shorten the time span between sample collection and results, by providing a relatively simple, low cost, and highly sensitive trace analytical tool for the analysis of bioactive agents. The work presented here uses Raman methods to provide
rich structural information of microorganisms through their sharp and distinguishable vibrational fingerprint. The study will focus on *L. casei* as an anthropogenic microbe model and *E. coli* as a target pathogen. Testing of the validated metal/PDMS substrates as a surveying tool is reported. An analysis of the characteristic fingerprints for DNA (1578, and 781 cm\(^{-1}\)), polysaccharides (1580, and 1290-1030 cm\(^{-1}\)), lipids (1730, 1490-1470 cm\(^{-1}\)), and proteins (1650-1600 cm\(^{-1}\)) bands on labs scale standards and spiked parsley samples is presented. The Raman based methods and multi-variate analysis for the effective and routine detection of *E. coli* in fresh crops is discussed.

![Graph](image)

Figure 3.1 SERS acquisition of *E. coli* (petri dishes/ plants), using excitation line 632 nm. Acquisition time 10.00s with 10X objective.

**CHED 344**

**Comparing the amount of caffeine in store-bought vs. locally roasted Blackbird Coffee**

*Belinda C. Schaafsma*, belinda.schaafsma@bobcats.gcsu.edu, Kimberly Cossey. (1) Georgia College, Momence, Illinois, United States (2) Georgia College and State University, Milledgeville, Georgia, United States

Are you trying to maximize (or minimize) your daily caffeine consumption through coffee? This can be difficult, since the amount of caffeine in a serving of coffee is surprisingly hard to find. The goal of this project is to determine the amount of caffeine
in coffee from a local distributor, Blackbird Coffee, and compare it to a store-bought alternative. It is important to the local distributor to inform their customers about the caffeine content because coffee is a popular stimulant and its effects depend on how much caffeine each cup contains. Blackbird Coffee roasts coffee beans in-house, and since roasting can affect the caffeine content, the final amount of caffeine in the brewed beverage for each type of roast was unknown. In previous work, a procedure utilizing liquid-liquid extraction was developed and found to be reproducible for quantifying the caffeine in store-bought Starbucks Dark Sumatra coffee. In this work, it was found that “old” and “new” batches of Starbucks Dark Sumatra coffee varied in the amount of caffeine and impurities isolated. This data will be compared with amounts of caffeine in a popular type of brewed coffee from Blackbird Coffee. Multiple trials will be analyzed, and then the caffeine content in Blackbird Coffee will be reported to the distributors and delivered to consumers.

CHED 345

**Studying the binding interactions of the chemokines CXCL12 and CXCL14 to heparin and heparan sulfate using affinity capillary electrophoresis**

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Chemokines are a group of small molecules that regulate cell migration and behavior in diverse contexts. The chemokine CXCL12 binds with the receptor CXCR4 and has been found to be closely related to the malignant growth of more than twenty different human neoplasms. Recent studies have shown that the chemokine CXCL14 also binds to CXCR4 with high affinity and inhibits the CXCL12-mediated chemotaxis of leukemia-derived cells. The functions of these chemokines are mediated by glycosaminoglycans (GAGs) such as heparin which are critical regulators of cell migration during organogenesis and immunosurveillance. This study will investigate the binding of CXCL12 and CXCL14 to heparin and heparan sulfate oligosaccharides using Affinity Capillary Electrophoresis (ACE). ACE has many benefits for determining binding constants for chemokine-GAG interaction including low sample consumption and easy automation. Knowledge of the binding constants is useful in identifying high affinity binding GAG oligosaccharides responsible for mediating chemokine function.

CHED 346

**Best spinach that Popeye ever ate**

*Kirsten Weishaar, knweishaar@gmail.com, Jeff Potratz. Chemistry, St. Edward’s University, Austin, Texas, United States*

Iron is essential for all life because of its need for the production of red blood cells. All the iron the body uses comes from the food consumed, which is why there is estimated to be in excess of one billion people who suffer from iron-deficient anemia. This
research attempts to increase the level of iron in spinach leaves, by spiking the soil with varying concentrations of ferric nitrate. The spinach plants are grown from seeds and then harvested at maturity. The leaves are then ashed in a furnace and acid digested. The solution is then analyzed using the Atomic Absorbance Spectrometer. The research so far has been concerned with testing the method described above using store bought spinach. The literature shows that 30g of store bought spinach contains 0.81mg of iron or 27 µg/g. Preliminary testing of store bought spinach, using the method above, showed an highest average of 118 µg/g and the lowest average of 99 µg/g. The standard deviation is 7.71 µg/g and 1.13 µg/g respectively. Currently work is focused on testing more samples of store bought spinach and testing spiked spinach samples to observe if their iron content can be increased.

CHED 347

Cyclic voltammetry of tris-dithiocarbamates in room temperature ionic liquids

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Research was conducted on 1-butyl-3-methylimidizolium hexafluorophosphate [bmim][PF₆], which is an ionic liquid at room temperature. This makes [bmim][PF₆] a potential candidate for electrochemistry. The only negative characteristic of [bmim][PF₆] is that it is very viscous, which leads to lower conductivity levels. [bmim][PF₆] is miscible in some organic solvents like dichloromethane. These solvents will be used to lower the viscosity and increase the ionic conductivity. Once the right combination is discovered, the new combination of [bmim][PF₆] will be used to study the electrochemical process of several new metal dithiocarbamates synthesized last year. If successful the [bmim] will potentially be used to synthesize iron dithiocarbamates with iron in the +2 or +4 states.

CHED 348

Development of analytical methods for detection of pharmaceutical pollution of surface water in Georgia using purge-n-trap GC/MS

Katherine Hachat, katiehachat@gmail.com, Nathan Potter, Catrena H. Lisse. Chemistry, Physics and Astronomy, Georgia College & State University, Milledgeville, Georgia, United States

Numerous literature sources state evidence of pharmaceuticals in drinking water systems across the nation. The pharmaceuticals have yet to be connected with harming humans but signs of distress to aquatic life are reported. The two main classes of pharmaceuticals present are hormones and antidepressants. These compounds can be present in human waste after the consumption of pharmaceuticals, which leads to the contamination of sewage. Although wastewater is treated by sewage treatment facilities
there are minimal methods for removing pharmaceutical byproducts, which increase the potential for contamination of surface water areas such as lakes and rivers. A collaborative group of undergraduates from various disciplines at Georgia College are monitoring and analyzing surface water in middle Georgia for xenoestrogens. Currently, the main focus of the project is to develop analytical procedures for GC/MS analysis to compare with previously obtained HPLC results. The presentation summarizes the experimental design and results of the GC/MS analysis.

CHED 349

**Novel application of low-field $^1$H-NMR for the quantitative analysis of ethanol at low concentrations**

*Erin Littleton, elittlet@heidelberg.edu, Bryan D. Smith. Chemistry, Heidelberg University, Tiffin, Ohio, United States*

This study investigated the feasibility of utilizing a low-field 45 MHz NMR spectrometer for quantitatively analyzing aqueous ethanol concentrations in the 0.00-0.350% (v/v) range. To accomplish this goal, the $^1$H-NMR spectrum was collected in triplicate for sixteen standard aqueous ethanolic solutions ranging in concentration from 0.025 to 0.400% (v/v). The data collected was used to construct a calibration curve. The concentration of ethanol in blind samples was experimentally determined using a standard curve of the ratio of -OH to -CH$_3$ (obtained via integration of the respective spectral peaks) versus the theoretical concentration of the standards measured. The goal is to extend this technique to ovine blood serum and ultimately to rat blood samples collected post-ethanol consumption. This technique has the advantages of minimal sample preparation, no intermediate chemistry required, and the ethanol concentration is measured directly.

CHED 350

**Investigation of toxic metals in over-the-counter eye shadow makeup**

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Eye shadow cosmetic products are used daily by millions of individuals around the world. Because heavy metals are naturally occurring and present in the environment, they can work their way into raw materials and thus show up in extremely small quantities in cosmetic products such as eye shadow. Exposure to heavy metals has been linked to various health concerns; therefore, if eye shadows contain significant amount of heavy metals consumers must be informed. Since eye shadow products vary in price, it could be assumed that the more expensive the eye shadow the more pure it is from heavy metals. Within this study, two different priced eye shadows will be tested for chromium, lead, and nickel. In order to test for the heavy metals, the eye shadows
will be digested in strong acid and then analyzed through the Inductively coupled plasma atomic emission spectroscopy (ICP-AES).

CHED 351

Assessing the reproducibility and applicability of a miniature gas chromatograph

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We describe efforts to further investigate the suitability of a commercial miniature gas chromatograph for field studies of vapor phase volatile organic compounds. The Vernier (Beaverton, OR) Mini GC is small (1.3 kg, 2.7 L) and power-efficient (24 VDC, 60 W). Although intended for the educational market, we are evaluating it as a portable instrument for field screening of volatile organic compounds (VOCs). The Mini GC contains an 11 meter capillary column (polydimethylsiloxane, inner diameter 0.53 mm, 30 °C-160 °C) with the capability of temperature programming. The mobile phase is ambient air, pulled through the column by a small pump (1.4 to 10.8 mL/min). Sample introduction by on-column injection of either liquid (< 0.8 microliters) or air containing organic vapors (< 1 mL) is possible. We replaced the AC/DC wall adapter with a home-made battery pack of sixteen 1.5V D cells which allowed operation for more than 40 ten-minute chromatographic runs. To assess reproducibility, mixtures containing ethyl acetate, propyl acetate, butyl acetate and iso-amyl acetate were analyzed at 40 °C. Variability in retention time, peak area, and peak shape will be described as a function of sample composition and injection size. Calibration curves, including statistically-based limits of detection will be presented. Gas injections of saturated of ethyl acetate vapor (100 torr) have been successfully performed; head space analysis of other compounds and everyday items such as magic markers and model cement will be described.

CHED 352

Synthesis of 1-butyl-3-methylimidizolium hexafluorophosphate: Investigation of its use as an electrochemical solvent for electroanalytical studies of metal dithiocarbamate complexes

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1-Butyl-3-methylimidizolium hexafluorophosphate [bmim][PF₆] is a viscous, colorless, hydrophobic, ionic liquid at room temperature. The negligible vapor pressure and low melting point of [bmim][PF₆] provide electrochemical stability for the molecule, therefore it can be useful as a solvent for electrochemistry and in industrial solvent applications. The high viscosity of [bmim][PF₆] results in much lower conductivity than inorganic molten salts; however, [bmim][PF₆] is totally miscible with several organic solvents such as acetonitrile and dichloromethane. Addition of these solvents to [bmim][PF₆] reduces
the viscosity, thereby significantly increasing the conductivity. This research focuses on the synthesis of \([\text{bmim}]\text{[PF}_6\text{]}\) and characterization of the properties of various \([\text{bmim}]\text{[PF}_6\text{]}\)/dichloromethane mixtures including conductivity, density, and viscosity, as well as cyclic voltammetry and coulometry of metal dithiocarbamate complexes in \([\text{bmim}]\text{[PF}_6\text{]}\)/dichloromethane mixtures. This research also investigates the exchange of ligands between iron and nickel dithiocarbamate complexes in \([\text{bmim}]\text{[PF}_6\text{]}\)/dichloromethane mixed solvents using electroanalytical techniques.

CHED 353

Influence of the cis/trans ratio of hop iso-alpha-acids on beer bitterness

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Understanding the effect isomerized alpha acids and their ratios have on the final product of beer is a hot area of research in the brewing industry. Hops are an important constituent of beer flavoring. Specifically, isomerized-alpha-acids derived from hops are soluble in water and are responsible for the bitterness needed for balance in beer. A variety of hop products are in use today and often have different cis/trans ratios. Observation of the cis/trans ratio throughout the brewing process will provide an insight into the kinetics of thermal isomerization and will allow an estimation of the cis/trans ratio in the finished product. A High Pressure Liquid Chromatography (HPLC) method coupled with a solid-phase extraction was used to quantitatively determine both the total concentration of iso-alpha-acids and the cis/trans ratio in raw hops, a wort matrix (pre-fermented beer), and finished beer products. These observations will inform brewers how the iso-alpha-acids ratio impacts the bitterness in their final product.

CHED 354

Separation of cations for waste reduction

Caitlyn Cookenmaster, ccookenmaster@adrian.edu, Michael Claus. Chemistry and Biochemistry, Adrian College, Adrian, Michigan, United States

Every year the students in the General Chemistry course at Adrian College perform a laboratory experiment that tests the solubility rules by combining solutions of anions and cations. They record their observations and dispose of their experimental materials in waste containers. This means that all of the metal ions are mixed together, creating a large volume of liquid waste and very little solid waste. As liquid waste is expensive to dispose of, it is ideal to reduce as much as possible into a solid state in order to dump the remaining liquid down the drain. The purpose of this experiment was to develop a method to precipitate as many heavy metal cations as possible out of the liquid waste so the rest could be discarded without having to pay a professional company. By following a cation separation flow chart, different reagents were used to form the
appropriate precipitates of heavy metal ions. These were separated from the liquid to be disposed of professionally, allowing the remaining material to be discarded efficiently and inexpensively.

CHED 355

**Identification of volatile organic compounds present in cigarette smoke via purge-n-trap coupled with GC/MS**

**Preston Skersick**, preston.skersick@bobcats.gcsu.edu, Elaine Smith, Catrena H. Lisse. Chemistry, Physics and Astronomy, Georgia College and State University, Milledgeville, Georgia, United States

Recreational use of tobacco products has been proven to directly correlate to health issues identified within the users. There are seventy known carcinogens present in tobacco smoke and those carcinogens are responsible for 30% of all cancer deaths in the United States. Environmental Tobacco Smoke (ETS), which is when harmful chemicals from tobacco smoke are absorbed into cloth, is another way. Qualitative analysis of acrolein and benzene are determined by analyzing the headspace of cloth samples exposed to cigarette smoke via purge-n-trap coupled with gas chromatography/mass spectrometry (GC/MS). This presentation summarizes the experimental design and preliminary results.

CHED 356

**In vivo expression of antimicrobial peptides in Escherichia coli**

**Susan A. White**, saw@wayne.edu, Nisansala S. Muthunayake, **Christine S. Chow**, cchow@wayne.edu. Chemistry, Wayne State University, Windsor, Ontario, Canada

Antibiotic resistance in pathogenic bacteria is a growing threat to human health. The development of new drugs to combat bacterial infection is critical. Small peptide drugs that target the bacterial ribosome are a possible alternative to the existing antibiotic agents. A novel set of small peptides, shown to have *in vitro* ribosome binding activity, were chosen for this study. The goal of this project is to measure each peptide’s antimicrobial effectiveness using an *in vivo* peptide expression plasmid system. Electrocompetent *Escherichia coli* cells were created and the plasmid vector was prepared. This approach required the cloning of each peptide into the plasmid system and measuring the effects of peptide expression on bacterial growth. The results will provide insight into the potential of peptide molecules as antibacterial drugs.

CHED 357

**Role of copper in the oxidative stress response of Chlamydomonas reinhardtii to heat shock**
In response to stress, cells produce reactive oxygen species (ROS) such as superoxide \( \text{O}_2^- \), peroxide \( \text{H}_2\text{O}_2 \) and hydroxyl radical \( \text{HO}^- \) which cause molecular damage in the form of DNA breaks, lipid peroxidation and protein carbonylation. ROS are also important in cell signaling and to induce differential gene expression, metabolic changes and thus adaptation to different environmental conditions. The hypothesis of this project is that the ROS response is a common denominator of different environmental challenges, including radiation and microgravity, during spaceflight. Algae, such as the unicellular green alga \textit{Chlamydomonas reinhardtii}, grown in spaceflight are exposed to stress. The goal of this work was to characterize the response of \textit{C. reinhardtii} to stress by examining biochemical and gene expression changes using heat shock. The heat shocked (42°C) \textit{C. reinhardtii} exhibited a selective regulation of ion transporters, and an increase in ROS in cells and supernatant. Such results provide new insights about the intracellular response to stress and its possible mediation during spaceflight.

CHED 358

Effect of antidiabetic agents on the \textit{in vitro} glycation of bovine serum albumin

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In addition to the antihyperglycemic effects, metformin has shown to inhibit glycation of proteins, protecting their structure and function in diabetes-associated complications. Formation of nonenzymatic advanced glycation end products was studied in the presence of antidiabetic agent metformin and its structural analogs, phenformin, buformin, and guanidinobutyric acid. Methylglyoxal was used as the glycating agent while aminoguanidine was used as the known standard antiglycation agent. The rate and extent of fluorescence generated upon formation of the \textit{in vitro} cross-linked bovine serum albumin (BSA) by methylglyoxal was studied using the excitation wavelength of 330 nm. The fluorescence emission spectra of cross-linked BSA gave maximum values at 410 – 430 nm, regardless of the antidiabetic agents used. The fluorescence generation was measured at 410 nm over 40 hours at two concentrations of antidiabetic agents. Buformin at 0.8 mM showed 48% inhibition at 37°C. Phenformin and metformin at 0.8 mM gave 11% and 16% inhibition respectively at 30°C. Guanidinobutyric acid did not show inhibition at the tested concentrations and temperatures. Regardless of temperature, 0.8 mM yielded greater inhibitory effects than 2 mM concentration. The molecular weights of the cross-linked products determined by SDS PAGE indicated the formation of intramolecular and intermolecular cross-linked proteins in the presence of antidiabetic agents. SDS PAGE also confirmed that the antidiabetic agents studied here were not potent antiglycation agents \textit{in vitro}. 
Ion-pair reverse-phase liquid chromatography analysis for separating and quantifying RNA generated via in vitro transcription reactions

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Run-off RNA transcripts of in vitro transcription reactions have traditionally been analyzed using denaturing polyacrylamide gel electrophoresis (PAGE) and detection of labeled-UTP incorporated into the transcripts. Although multiple products from in vitro transcription reactions can be detected, quantitative analysis of RNA transcripts by denaturing PAGE is difficult. Ion-pair reverse-phase high performance liquid chromatography (IP RP HPLC) is a high-resolution technique that can separate nucleic acids based on size. Using denaturing conditions, RNA run-off transcript samples of mixed sizes can be separated and quantified. Several in vitro transcription systems using different RNA polymerases and various linear DNA templates with multiple promoters were assessed. IP RP HPLC improves the ability in detecting run-off transcription products, and establishes a better quantitative method for comparing transcripts of different length.

Inhibition of the bacterial fatty acid biosynthetic enzyme FabI by secondary metabolites isolated from Artemisia californica

P. M. Joyner, matt.joyner@pepperdine.edu, Shane Bryant, Shane.Bryant@Pepperdine.edu. Natural Science, Pepperdine University, Malibu, California, United States

The Chumash Native Americans of Southern California have well-documented traditions of using plants for medicinal purposes. One of these medicinal plants is Artemisia californica (common name coastal sage), which is widely distributed along the coastal regions of Southern and Central California. Previous work in our lab resulted in the isolation of several flavonoids from extracts of A. californica that demonstrated in vitro antibacterial activity. In this study we tested these flavonoid compounds for their ability to inhibit the bacterial fatty acid biosynthesis enzyme FabI, which is the biological drug target for the antibiotic triclosan. The FabI enzyme catalyzes the NADH or NADPH-dependent reduction of enoyl-ACP in the biosynthesis of fatty acids. In this experiment, the enzymatic reduction of a butenyl-CoA by FabI was followed by measuring the change in absorbance of NADH at 340 nm. The flavonoid jaceosidin significantly inhibited FabI activity while other flavonoids from A. californica showed reduced inhibitory activity. These results demonstrate that further investigation of Chumash medicinal plants may yield compounds with medicinally relevant biological activities.

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Increased growth and mutagenesis in bacteria exposed to titanium dioxide nanoparticles

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Titanium dioxide (TiO$_2$) nanoparticles (NP) are a common additive in many industrial products such as paints and coatings, and in consumer products such as toothpaste, sunscreen, and cosmetics. Though presumed safe, the increased incorporation of these particles into every day personal care products has raised concerns over the effects of long-term exposure to these particles. We are investigating the possible mutagenic effects of TiO$_2$ NP by conducting bacterial growth rate studies, mutagenicity tests, and by examining the morphology and behavior of bacteria exposed to various levels of the nanoparticles. Building on previous work in our laboratory that indicates that TiO$_2$ NP are cytotoxic to lab strains of *S. typhimurium* at high levels and mutagenic at low, we are conducting studies to determine how nanoparticles affect the growth rates of those same strains. Prospective research includes confocal and electron microscopy to investigate the mechanism of nanoparticle-induced damage, as well as similar studies of *E. coli* and algae. This work is supported by a grant from the Defense Threat Research Agency.

CHED 362

Investigation of the effects of titanium dioxide nanoparticles on phospholipid bilayers using differential scanning calorimetry

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Metal-oxide nanoparticles have become increasingly common in consumer products to produce desired physical properties and visual effects. While assumed to be safe, relatively little research has been done into the long term effects of nanoparticles on eukaryotic cells. My research focuses on titanium dioxide (TiO$_2$) nanoparticles, because of their presence in personal care products, such as toothpaste, cosmetics, and sunscreen, where they are often used to create a white, lustrous appearance. These products are not only applied directly to skin or ingested, but are used on a daily basis, leading to chronic exposure. Using synthetic liposomes as a model for the eukaryotic plasma membrane, we have investigated the effects of TiO$_2$ nanoparticles on the thermal stability of phospholipid bilayers. We have used differential scanning calorimetry (DSC) to determine the transition temperature ($T_m$) of the phospholipid bilayers of a series of liposomes made of purified lipids, mixtures of lipids, and cellular extracts in the presence and absence of micromolar levels of TiO$_2$ nanoparticles. Lipids tested include phosphatidylethanolamine (PE), phosphatidylglycerol (PG), cardiolipin, and *E.coli* cellular extracts. It was found that the presence of the nanoparticles caused the $T_m$ to increase by between five and ten percent, suggesting interactions that stabilize the membrane rather than disrupt it. Working in collaboration with another member of the lab, I am...
currently determining the effects of TiO$_2$ nanoparticles at concentrations that have been shown to have mutagenic and cytotoxic effects on bacteria. This work is supported by a grant from the Defense Threat Research Agency.

CHED 363

Adsorption of snake venom by activated charcoal

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Over 7,000 people receive venomous snakebites in the United States each year. These envenomations produce severe symptoms such as necrosis and paralysis and may be fatal if not treated quickly. This study investigates the use of activated charcoal for the adsorption of rattlesnake venom proteins to reduce hydrolytic enzyme activity, specifically that of phosphodiesterase. The results will determine the efficacy of using activated charcoal as a potential treatment option for snakebites before emergency medical care is available.

CHED 364

Variation of protein components in successive regenerations of individual coralsnake venom

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Differences in specific enzyme components from one regeneration of venom in a given snake to the next has received little attention. This study involves the analysis and comparison of four successive venom collections from each of nine individual coralsnakes in order to detect these differences. Significant variation was found within the successive re-synthesis of both alkaline phosphomonoesterase and phosphodiesterase. Even greater differences were observed between the venoms from similar individual snakes.

CHED 365

Metal ion cofactor requirements of phosphomonoesterase

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Phosphomonoesterase is a major component of many snake venoms. The enzyme requires magnesium as a cofactor for activity. This study investigates the cofactor requirements of the enzyme by replacing the magnesium cofactor ion with other divalent cations and then comparing the enzymatic activity of the native phosphomonoesterase
with those in which the cofactor has been replaced with different metal ions. The results of this study will show the specific cofactor requirements of this enzyme for activity and the relative binding efficiencies of different metal ions.

CHED 366

Inhibition of lecithin-cholesterol acyltransferase by reactive aldehydes in electronic cigarettes

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Cigarette smokers have an increased risk of atherosclerosis, which is the hardening of the arteries due to the buildup of cholesterol. This premature hardening may be due to a variety of factors, one being altered lipoprotein metabolism, specifically, through the inhibition of Lecithin-Cholesterol Acyltransferase (LCAT). LCAT is the plasma enzyme that is responsible for removing cholesterol from artery walls. However, smoking appears to inhibit this enzyme. Previous work has shown that reactive aldehydes found in cigarette smoke might be one of the causes of this enzyme’s inhibition. The recent introduction of electronic cigarettes (e-cigs) to the market has brought about much debate over their safety. A recent study has shown that there are toxic substances in the vapor from e-cigs, including some of the reactive aldehydes in conventional cigarette smoke, although at lower levels. This research is designed to study the difference in inhibition of LCAT by formaldehyde, acetaldehyde, and acrolein in e-cigs and conventional cigarettes.

CHED 367

Phylogenetic analysis of the upstream region of the arcanolysin gene from smooth and rough biotypes of Arcanobacterium haemolyticum

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Arcanobacterium haemolyticum is a gram-positive, β-hemolytic, pleomorphic rod that causes pharyngitis, wound infections, and rare invasive diseases. There are two major colony biotypes of A. haemolyticum: smooth isolates associated with wound infections that have strong β-hemolysis, and rough isolates associated with pharyngitis that have weak β-hemolysis. The primary hemolysin is thought to be Arcanolysin (aln/ALN), which belongs to the cholesterol-dependent cytolysin (CDC) family. The PCR product of the aln open-reading frame is 2.0 kb in all smooth isolates. However, half of the rough isolates contain an insertion sequence (IS) element in the aln coding region, which results in a 3.2 kb PCR product. Additional PCR and sequence analysis of the upstream region of aln revealed nucleotide polymorphisms. These polymorphisms demonstrated
that ~90% of the smooth isolates phylogenetically cluster in a manner distinct from rough isolates. This differentiation was further confirmed by restriction enzyme analysis of the aln upstream region. None of the nine isolates from Germany/Denmark possess the IS element and all are of the smooth biotype. While the wild type strain had strong hemolysis, the aln mutant was markedly reduced. However, in some environmental conditions, the aln mutant still retained some hemolysis, suggesting presence of a second unknown hemolysin. Taken together, the data suggest aln can be used to distinguish smooth and rough biotypes of A. haemolyticum and that a second hemolysin exists.

CHED 368

Identification and characterization of a membrane-associated esterase from Propionibacterium acnes

Rachel Chapin, rchapin@drury.edu, Beth Harville, bharville@drury.edu. Chemistry, Drury University, Springfield, Missouri, United States

Propionibacterium acnes is best known as the cause of acnes vulgaris. In addition, P. acnes causes post-operative and device-related infections, sarcoidosis and synovitis, pustulosis, hyperostasis, and osteitis. P. acnes is an anaerobic bacteria that is resistant to phagocytosis. Several P.acnes virulence factors have been identified, but few have been isolated and characterized. This work describes isolation and characterization of a P. acnes membrane-associated esterase. P. acnes was grown, and the cells were collected and lysed. Cell components were separated using differential centrifugation, and the fractions were assayed for esterase activity. Esterase activity was found in the cytoplasmic and membrane fractions. Membrane esterase activity was further isolated using gel filtration chromatography. Fractions containing esterase activity were pooled and studied using esterase inhibitors.

CHED 369

Characterization of a Tannerella forsythia collagenase by SDS-PAGE and fluorescent spectroscopy

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The goal of this study is to characterize a collagenase produced by the periodontal pathogen, Tannerella forsythia. Data presented in this poster provides researchers with more information about the enzyme, hence furthering the development of a treatment for the disease. In this work, SDS-PAGE assays were used to show cleavage of native collagen by the T. forsythia collagenase. Collagenase activity was further studied by monitoring relief of fluorescent quenching of highly fluorescein-labeled collagen using a LS50 Luminescence Spectrophotometer. Enzyme activity was measured using collagen
I and collagen IV as the substrate. The isolated collagenase cleaved type I, but not type IV, collagen. Therefore further enzyme characterization assays were performed using type I collagen. A wide array of enzyme inhibitors were tested to determine their effect on the collagenase. Serine protease inhibitors antipain and phenylmethanesulfonyl fluoride were found to inhibit the collagenase activity in a dose-dependent manner. Inhibition by these compounds gives insight into the functioning of this collagenase and could have potential medicinal applications in the treatment of periodontal disease.

CHED 370

Porphyrin derivatives and photodynamic therapy effects on triple negative breast cancer

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Currently, there are limited effective options for treatment of triple negative breast cancer (TNBC) due to its lack of the three receptors typically used to target breast cancer. The use of photodynamic therapy (PDT) to kill cells that take up light-absorbing compounds (PDT agents) may be an effective option to treat TNBC. We tested the efficacy of modified porphyrins as PDT agents against cells from TNBC. We compared these to Foscan, which is similar in structure to porphyrins and has been approved for use in Europe. Our first goal was to measure which porphyrins were taken up best by TNBC cells. Directly measuring the uptake of some of our compounds had been problematic due to their hydrophobic nature. We optimized the uptake protocol and have shown that TNBC cells take up the compounds to different extents.

One of the primary side effects of PDT is skin toxicity for up to 4-6 weeks after treatment due to exposure to sunlight. Thus, our second goal was to compare the toxicity in the light and in the dark of PipOH, $H_2$TPPC, and Foscan at a range of concentrations. In previous experiments, Foscan showed dark toxicity at low concentrations, but in these experiments there was variability in our results with Foscan so no clear comparison could be drawn.

Our third goal was to find combinations of a PDT agent and a concentration that are effective on TNBC cells at high light energy but minimize killing cells with ambient light. We measured the effect on cell killing by varying both the light dose and the concentration of three compounds to find concentrations that are effective at high doses of light but minimize toxicity at moderate doses. All three tested compounds show promise, but the dose of the PDT agent must be carefully selected.

CHED 371
Expression of recombinant intimin and translocated intimin receptor proteins in E.coli cells

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Enteropathogenic and enterohermorrhagic E. coli (EPEC and EHEC) cells that attach to human intestinal epithelium result in the formation of effacing lesions, which is the precursor of intestinal cell membrane disruption and diarrhea in infected individuals. Two proteins, intimin and the translocated intimin receptor (TIR), play an essential role in attachment to intestinal epithelial cells. E. coli first expresses TIR, which is translocated to the host cell via a type-III secretion system. TIR then becomes immobilized in the intestinal epithelium with its intimin binding domain exposed on the intestinal cell surface. Intimin, from the E. coli surface, then binds TIR and attaches the E. coli cell to the intestinal epithelium, which leads to lesion formation. These types of infections can take up to 24 hours to diagnose and there has not yet been a small molecule developed to speed up this diagnostic process, prevent further infection, or allow sooner initiation of treatment. The initial expression of recombinant TIR and Intimin proteins and their purification will be discussed.

CHED 372

Influence of the second-sphere coordination on the nitrite reductase activity of globins

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Globins act as a nitrite reductase (NiR), converting nitrite (NO\textsubscript{2}) to nitric oxide (NO), and have recently become a system of important interest. NO plays many key roles in biological processes of most mammals, however, an imbalance of NO can lead to various health problems. Although the mechanism of nitrite reduction in globins is unknown, it is believed to follow a mechanism similar to cd\textsubscript{1} NiRs. In this work, we focus on myoglobin (Mb) as a model compound for globins. One facet that may control the NiR mechanism is the H-bonding second-sphere coordination between Mb and the heme. To study the effect of this network, heme b in wt Mb is replaced with a non-H-bonding heme, protoheme IX dimethyl ester (PPIX-DME). The electronic structures of the various forms of this reconstituted Mb sample (e.g. Fe(III), Fe(II), Fe(II)-NO, Fe(III)-NO, Fe(III)-NO\textsuperscript{2}, and Fe(II)-O\textsubscript{2}) were first investigated in order to analyze the contributions of one of these forms to the final product from the two-step NiR reaction. Slow kinetics reactions between PPIX-DME Mb and NO\textsubscript{2} were carried out using UV-vis spectroscopy, where the loss of the Fe(II) species was monitored at 432 nm as a function of time. Preliminary results indicate a pseudo-first order decay, with a bimolecular rate constant only slightly different from the reported value of wt Mb (~5.0 M\textsuperscript{-1} s\textsuperscript{-1} at 25 °C). Current studies on another reconstituted Mb sample containing a non-
H-bonding heme, octaethylporphyrin, are underway. Although neither porphyrin formed an H-bonding network with Mb, the unique presence of ethyl groups, as opposed to dimethyl ester at the 6,7-heme positions, present an interesting comparison. Implications of this change on their NiR activity will be presented.

CHED 373

Optimization of fragment inhibitors for the class D β-lactamase OXA-24

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Since the discovery of the penicillin, β-lactam antibiotics have emerged as the preferred and most widely used antimicrobial agents. However, due to the overuse of β-lactam antibiotics, bacteria have become resistant to therapeutics. The principle mechanism by which bacteria acquire resistance is through the expression of β-lactamase enzymes. Of the four known classes of β-lactamases (A-D), the class D enzymes are the most diverse and pose a threat to the carbapenems, which are considered to be “last resort” β-lactam antibiotics. Currently, all clinically-used inhibitors fail to effectively inhibit the class D β-lactamases. The ineffective inhibition occurs because the inhibitors contain the same β-lactam ring scaffold found in β-lactam antibiotics. In order to address this serious problem, molecular docking was used to identify novel inhibitors for the class D β-lactamase OXA-24. Two commercially-available chemical fragments with K\textsubscript{i} values of less than 5 mM were discovered, and their structures, in complex with OXA-24, were determined to 1.67 Å and 1.78 Å resolution. To optimize these fragment inhibitors, analogs were tested for inhibition of OXA-24. The insights gained from the fragment inhibitors and analogs will be used to develop a new series of novel β-lactamase inhibitors.

CHED 374

Fox-4 cephamycinase: Analysis of structure and function

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Beta-lactamases inactivate beta-lactam antibiotics, which target bacterial cell wall synthesis. Plasmid-encoded beta-lactamases have become a major public health
concern due to their transmissibility across species. The Fox1-10 family, a subset of plasmid-based enzymes, is unique in that their amino acid sequences are distinct from other class C members, and they are unusually active toward cefoxitin. To determine the molecular basis of resistance, the most active family member—Fox-4—was recombinantly expressed, purified, and tested in vitro against a panel of boronic acid transition state inhibitors (BATSI). The x-ray crystal structure of Fox-4 was determined to 1.9 Å in the presence of two of these inhibitors, as well as cefoxitin, providing insight into the catalytic mechanism through comparison of similar enzymes complexed with BATSI and cephamycins. Ultimately, this work will inform the design of more effective antibiotics against Class C beta-lactamases.

CHED 375

Denaturation resistance of polygalacturonase obtained from coffee mucilage

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The enzyme polygalacturonase (PGase) cleaves the α1-4 galactosidic bonds of polygalacturonic acid (PG), a major component of coffee mucilage, to produce galacturonic acid. PGase was found to be a very stable enzyme. It was stable to submersion in a boiling water bath for 1 hour or 10 minutes at 200 °C. When the PGase assay was conducted at a pH 3 or 14, no loss of PGase activity was noted. Guanidine HCl, a known protein denaturant, did not inhibit PGase at concentrations up to 162 mM. Addition of 0.3 M b-mercaptoethanol abolished PGase activity, so this concentration of b-mercaptoethanol was used as an assay control. Dithiothreitol was able to reduce PGase activity in a dose-dependent manner. A 38% reduction in enzyme activity was seen at 81 mM dithiothreitol and this increased to 95% inhibition at 162 mM dithiothreitol. Tris(2-carboxyethyl)phosphine hydrochloride (TCEP) inhibited PGase activity by 75% at 37.5 mM. b-Mercaptoethanol, dithiothreitol and TCEP reduced the disulfide bonds formed between the side chains of cysteine residues. This suggests that the resistance of PGase to denaturation by high temperature and acid or base is due to the stabilization of its tertiary structure by disulfide bonds. (We gratefully acknowledge Susan Jackels at Seattle University, the Department of Chemistry at Universidad Centroamericana Managua, Nicaragua for sharing coffee mucilage samples and the Department of Chemistry and Biochemistry, University of Detroit Mercy for support of this project.)

CHED 376

Hydrogen deuterium exchange used to study the interface of Plasmodium falciparum glutathione reductase and the antimalarial drug methylene blue
Plasmodium falciparum is the cause of human malaria and is one of two malaria parasites known to have drug resistance. Since there are no preventative vaccinations against malaria, the control of this disease is heavily dependent upon the use of antimalarial drugs. Antimalarial drugs, such as methylene blue, are effective therapies against human malaria. At a specific concentration, methylene blue has been shown to be a selective inhibitor of the parasite's glutathione reductase (PfGR). Glutathione reductase is an important target when studying malaria drug resistance because it is a flavoenzyme that regenerates glutathione, which is an essential protein for antioxidant defense against cell damage. Methylene blue is also a substrate that is reduced by glutathione reductase to produce leucoMB. This is then spontaneously oxidized by molecular oxygen to form methylene blue again. During this process, reactive oxygen species, such as hydrogen peroxide and superoxide, form. These act as recycling catalysts against infectious organisms. Due to PfGR's central position in redox control, it is ranked number one as an antimalarial drug target. The goal of this research is to study the interface between methylene blue and the putative protein target, glutathione reductase, in order to understand the drug action mechanism. PfGR was expressed and purified, and hydrogen-deuterium exchange (HDX) was used to map the drug-protein interface. We will present the mass spectrometry data for the solvent-exposed peptides after digestion with pepsin when PfGR is complexed with methylene blue, which will allow us to narrow down the active site.

CHED 377

Role of cytochrome c and its effects on the programmed cell death pathway of P. falciparum using yeast as a model organism

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Apoptosis is commonly seen in multicellular organisms as a method to regulate the development of said organism. A similar, programmed cell death pathway has been identified in the unicellular organisms, yeast and P. falciparum. In yeast, the cell death pathway is initiated once a target protein is activated, which causes a downstream proteolytic cascade to activate. The target protein is Apaf-1 (apoptosis promoting factor 1), which binds to cytochrome c. Apaf-1 then triggers the formation of an apoptosome, which, when induced by ATP, turns on the other proteases downstream of Apaf-1. Recent studies suggest that P. falciparum might contain a similar cell death pathway to yeast. Our aim is to identify the players of the putative apoptosis pathway in the malaria parasite. The activation of the cell death pathway was tested using a fluorogenic substrate (z-VAD-AMC). The assay aims to demonstrate that z-VAD-AMC is cleaved once the yeast is exposed to increasing concentrations of cytochrome c. This assay
was also used on *P. falciparum*, using the Pfcytochrome c as the initiator of the pathway. *Plasmodium falciparum* cytochrome c was expressed in electrocompetent *E. coli* C41 cells via electroporation of two plasmids, pMKL1 and pEC86, with the latter containing the cytochrome c maturation system. We will report on the expression and purification of the target protein, as well as the results of the assay.

CHED 378

Expression and purification of DPAP-1, a malaria protease, and its role in the putative apoptosis pathway of the parasite

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A large upregulation of the dipeptidyl aminopeptidase-1, DPAP-1, was detected in a quantitative proteomic study in which the parasite was subjected to treatment with antimalarial drugs. DPAPs are recognized to have a function in hemoglobin degradation in the erythrocytic stages of the malaria parasite, *Plasmodium falciparum*. DPAP-1 has been compared to the human ortholog cathepsin C in previous studies, concluding that both proteases belong to the same family of C-1 endo- and exopeptidases. An assay was developed using a fluorogenic substrate to test for the role of the upstream pathway initiator, cytochrome c, in the putative programmed cell death pathway. In order to test if DPAP-1 binds and is activated by cytochrome c, the expression and purification of DPAP-1 protease is needed. The inactive enzyme was expressed starting at residue 28, an aspartate that is part of the exclusion domain. The PCR product was cloned in the pMKL1 plasmid, which has a maltose binding protein and a TEV protease site. A his-tag was included to aid in purification and affinity studies with cytochrome c. The recombinant DPAP-1 protease will help expand the knowledge on its function and its role in *Plasmodium falciparum*'s apoptosis pathway.

CHED 379

Yeast cell survival in different concentrations of canavanine

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Drug resistance in microorganisms can occur when an organism acquires a mutation upon exposure to a selective pressure causing the cells to grow out of an arrested state, a process called adaptive mutagenesis. Using the yeast *Saccharomyces cerevisiae* as a model organism, we investigated the replicational mutation rates and adaptive mutation frequencies of wild type and 8-oxoguanine glycosylase-deficient (ogg1Δ) cell lines upon exposure to canavanine. The results show that both the replicational mutation rate and adaptive mutation frequency of ogg1Δ are higher (1.49E-06; 5.43E-07) compared to wild type (4.18E-07; 1.53E-07), due to an inability to repair oxidative
damage. Additionally, we assessed survival of cells in the presence of canavanine and are working to identify the optimal conditions for selective pressure that will yield the highest percent survival while the cells are under growth arrest, anticipating that longer survival would allow the cells more opportunity to generate an adaptive mutation.

CHED 380

Characterization of the non-native 1,2-naphthoquinone in vivo incorporation into the $A_1$ site in PS I complexes of *Synechocystis* sp PCC 6803

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Photosystem I (PSI) antenna chlorophyll absorbs a photon of light, which is channeled to the primary chlorophyll donor, P$_{700}$. An electron is ejected from P$_{700}$ through a series of redox active chlorophyll electron acceptors ($A_0$), a unique quinone ($A_1$), a series of [4Fe-4S] clusters, $F_x$, and the terminal acceptors $F_{A/B}$.

Phylloquinone (PhQ) acts as a secondary electron acceptor occupying the $A_1$ site between the $A_0$ site and the Fe-S clusters of photosystem I in higher plants and cyanobacteria. In the phylloquinone-less mutant (*menB*) of the cyanobacterium *Synechocystis* sp. PCC 6803, plastoquinone (PQ) occupies the $A_1$ site and functions in electron transport. Because of reduced electron transfer efficiency, plastoquinone-containing mutants are incapable of growing at high light intensities.

Previous work demonstrated that phylloquinone derivatives can replace the plastoquinone occupying the $A_1$ site upon supplementation of the growth media. A series of 1,4-naphthoquinone compounds are suitable analog replacements for PhQ and act as redox cofactor, restoring the mutant to the native wild type both physiologically and spectroscopically.

This research establishes for the first time *in vivo* incorporation of a 1,2-naphthoquinone (1,2-NQ) into the $A_1$ site of PSI. The significance is that the $A_1$ site is designed for a phytyleted 1,4-naphthoquinone. The 1,2-NQ will have considerably different protein binding interactions. This could involve changes in the quinone-protein H-bonding, with the 2-position carbonyl in the space normally occupied by the 2-methyl group of PhQ.

Growth experiments show that 1,2-NQ restores high light growth. Spectroscopic characterization of the *menB* cells that were incubated with 1,2-NQ *in vivo* for 15 minutes, followed by PS I trimers isolation, were made. Electron paramagnetic resonance and 808 nm kinetic back reaction data reveals at least a mixture of the mutant native PQ and the 1,2-NQ. HPLC quantifying the photosystem I PQ:NQ ratio will be discussed. Results suggest that this unusual 1,2-NQ is incorporated into PSI and is active in the $A_1$ site.

CHED 381

Characterization of highly reducing anthraquinones in the $A_1$ site of PS I complexes of *Synechocystis* sp. PCC 6803
Photosystem I (PSI) antenna chlorophyll absorbs a photon of light, which is channeled to the primary chlorophyll donor, P$_{700}$. An electron is ejected from P$_{700}$ through a series of redox active chlorophyll electron acceptors (A$_0$), a unique quinone (A$_1$), a series of [4Fe-4S] clusters, F$_x$ and the terminal acceptors F$_{A/B}$.

Phylloquinone (PhQ) acts as a secondary electron acceptor occupying the A$_1$ site between the A$_0$ site and the Fe-S clusters of photosystem I in higher plants and cyanobacteria. In the phylloquinone-less mutant (menB) of the cyanobacterium Synechocystis sp. PCC 6803, plastoquinone (PQ) occupies the A$_1$ site and functions in electron transport. Because of reduced electron transfer efficiency, plastoquinone-containing mutants are incapable of growing at high light intensities.

This poster will report on experiments in which the growth medium of the mutant cells was supplemented with highly reducing 9,10-anthraquinones (AQ). Interestingly, the supplements restored at least some capability to grow at high light, suggesting that the menB mutant utilizes anthraquinone. Quantitative HPLC of the extracted PS I complex pigments indicated that AQ was incorporated directly into PSI without modification. PQ content in the extracts dropped to less than 20% of non-supplemented native levels. The potentials of the supplemented AQ’s were significantly more reducing than either PhQ and PQ by as much as 400mV. These quinones may approach or exceed the potential of A$_0$ and lead to unusual electron transition behaviors.

The function of quinone in the A$_1$ site of the menB mutant was monitored by P$_{700}$ back reaction kinetics. The menB sample had a characteristic 3ms back reaction and the least reducing AQs (e.g. 1-NH$_2$-AQ and 2-NH$_2$-AQ) had lifetimes significantly slower. The most reducing AQs (e.g. 2,6-NH$_2$-AQ) had a 3 ms back reaction at reduced amplitude. Possibly these highly reducing AQ cannot participate in the back reaction process.

The results of spin-polarized transient X-band EPR at 80K were curious. In most cases, the samples indicated the A$_1$ site was occupied by only PQ. The AQ signal appeared to be absent, a marked contrast to the HPLC and kinetic back reaction data. Observing the quinone at room temperature by monitoring a nearby reporter molecule (carotenoid) at 480nm will hopefully yield definitive support for the active quinone in the A$_1$ site.

CHED 382

Effects of sphingosine 1-phosphate at the blood brain barrier

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Sphingosine 1-phosphate (S1P) is a biomolecule present in the body that has diverse cellular effects, including trafficking of lymphocytes, upregulation of gene expression, and cell proliferation. These effects are mediated through binding of S1P to specific G-
protein coupled receptors, which are expressed on both endothelial cells (EC) and astrocytes (AC), two important components of the blood brain barrier (BBB). The BBB is a highly selective cellular structure that monitors the homeostasis of the brain through regulation of exchange between the CNS and the periphery. However, when the AC and EC are unable to perform their key functions, the integrity of the BBB is compromised. Since S1P signaling plays a role in the egress of lymphocytes from the lymph nodes during an immune response, the modulation of the S1P receptors expressed on the AC and the EC was studied to determine if it would be beneficial for the integrity of the BBB. The effects of S1P were studied by using an in vitro model for the BBB, a transmigration assay. Experiments testing the effects of S1P on cell permeability and viability were also ran. The results showed that astrocytes release factors which improve structure and viability of endothelial cells. In addition, it appears S1P is an important factor in the signaling and transmigration of lymphocytes and may be a potential drug candidate for decreased lymphocyte trafficking across the BBB.

CHED 383

Characterization of a putative haloalkane dehalogenase from *Saccharomonospora azurea*

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Haloalkane dehalogenases (HLDs) catalyze the conversion of a halogenated alkane to an alcohol. HLDs have been studied for their potential use in bioremediation and chemical synthesis processes. Only a handful of HLDs have been identified and fully characterized, and the dehalogenase sequence-to-substrate specificity relationships are not fully elucidated. Studying new HLDs will provide information that will expand the current HLD toolkit, as well as provide greater understanding of the sequence-structure-function relationship within this enzyme family. A putative HLD from *Saccharomonospora azurea* (DsaA) was hypothesized to have dehalogenase activity based on sequence alignment comparisons and homology modeling with known HLDs. DsaA was synthesized, expressed and purified to homogeneity. A high-throughput colorimetric assay demonstrated that DsaA had dehalogenase activity on a range of halogenated substrates.

CHED 384

Expression and purification of farnesyl diphosphate synthase from *Thermoplasma volcanium*

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Farnesyl diphosphate synthase (FPPS) is an important enzyme for the formation of fifteen-carbon terpenes, also known as sesquiterpenes. Many FPPS structures are known, but the structure of the homolog from the thermophilic archeon *Thermoplasma volcanium* is not known. Studying the structural adaptations of this enzyme that allow it to thrive in high temperatures should yield insights into its activity. It is hoped that the expression, purification, and crystallization of FPPS will enable determination of the difference in this enzyme that allows for the thermophilic stability. The FPPS gene was cloned into the plasmid, pGEX2T, which provided a N-terminal GST tag. BL21DE3 cells were induced to produce the protein, and purification was attempted with reduced glutathione resin. Expression, however, was limited due to insolubility caused by the protein misfolding. The GST-FPPS plasmid was transformed into a new cell line, Lemo21DE3, and successfully expressed.

**CHED 385**

**Mutagenesis of a TfdA-like B. pertussis enzyme**

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TfdA is a Fe(II)-α-ketoglutarate hydroxylase enzyme that is commonly found in different species of bacteria, such as Ralstonia eutropha, Burkholderia pseudomallei, and Cupriavidus necator. The α-ketoglutarate-dependent hydroxylases catalyze a variety of reactions ranging from the production of collagen to scanning DNA for mutations. These bacteria contain a circular plasmid which holds DNA sequences that encode for amino acids. A certain area of the plasmid encodes for a Fe(II)-α-ketoglutarate hydroxylase. This enzyme metabolizes 2,4-dichlorophenyloxoacetate, otherwise known as 2,4-D, by hydroxylation. When metabolization of 2,4-D occurs, α-ketoglutarate chelates to the active site. The active site consists of an Fe(II) center, three waters bound to the iron, Histidine 114, Aspartate 116, and Histidine 263. After chelation of α-ketoglutarate, the 2,4-D is hydroxylated by multiple proposed steps which results in the products of 2,4-Dichlorophenol and glyoxylate.

**CHED 386**

**Quantifying *Escherichia coli* in recreational freshwater of the Saginaw Bay Watershed using Colilert and quantitative PCR**

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Tawas City, MI, is a popular area for water-based recreational activities. The Tawas River flows through the city and into the Saginaw Bay at a beach frequented by many people. Microbial contamination has been detected in the Tawas River and other sites within the Saginaw Bay Watershed, with high levels of *Escherichia coli* indicating unsafe conditions for fishing and other recreational activities. Water samples from the river and
a nearby Arenac County beach were collected over the course of eleven weeks, and the
*E. coli* levels were quantified and compared using the EPA-approved Colilert and a new
rapid quantitative PCR (qPCR) method. The Pearson correlation coefficient for the
comparison of the two was 0.592. Of the 33 total samples, fourteen were above the
minimal allowable level of 300 CFU/100mL as determined by Colilert. Further analysis is
underway to perfect the rapid method as well as determine the source(s) of
contamination.

CHED 387

Development of an LC-MS/MS-based assay for the quantification of trehalose

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The disaccharide trehalose has been found in many different organisms, including
bacteria, fungi, and plants. These organisms are able to survive extreme conditions,
such as dehydration and freezing temperatures, by using trehalose as a cellular
protectant. The exact mechanisms behind trehalose’s ability to act as a cellular
protectant remain unknown. Methods to accurately measure trehalose levels in different
organisms should provide a better understanding of these mechanisms. Although
techniques exist to quantify the concentrations of trehalose from biological sources,
these methods are either complex or not sensitive enough to accurately quantify low
levels of trehalose. Furthermore, many of these techniques lack the ability to
conclusively identify trehalose as the sugar being quantified. To overcome these
limitations, a liquid chromatography – tandem mass spectrometry (LC-MS/MS)-based
assay for the quantification of trehalose using sucrose as an internal standard was
developed. In this assay, single reaction monitoring (SRM) was used to quantify
trehalose concentrations with exceptional sensitivity and selectivity. The assay was
used to detect trehalose at picomolar concentrations, as well as to quantify trehalose
levels from bacterial cell extracts. This method enables efficient and reliable
quantification of trehalose concentrations from different biological sources.

CHED 388

Quantitative analysis of hydrocortisone levels in human saliva due to the effects
of positive and negative stressors

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Hydrocortisone, also known as cortisol, is a steroid hormone which is produced in the adrenal cortex. Cortisol is released in response to physical and psychological stress. This project was designed to use chemical techniques to determine cortisol levels present in an individual due to the effects of positive and negative stress. Cortisol was extracted from samples of human saliva that were collected during stress-related experiments, and the levels of each sample were quantified through the use of ELISA. Statistical analysis was used to determine changes in cortisol levels resulting from various types of stressors. The importance of this research lies in its ability to indicate whether a physiological difference exists between positive and negative stress. This information can be a useful asset in many situations to better motivate individuals and groups in the workplace.

CHED 389

**Determination of the signaling pathway leading to tight junction disassembly in diabetic retinopathy**

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Diabetes is a metabolic disease that is very common throughout the nation, presenting itself as either Type 1 or Type 2 diabetes. Both types of diabetes have several complications associated with them, one being diabetic retinopathy, in which people gradually lose their eyesight. Diabetic retinopathy occurs when tight junctions between retinal cells disassemble due to the activation of a specific signaling cascade. Disassembly results in leaky blood vessels and retinal damage. More specifically, the signaling cascade causes phosphorylation of several tight junction proteins, including zonula-occludin 1 (ZO-1). Phosphorylation causes a conformational shift of the protein complex leading to disassembly and increased permeability of the tight junctions. This research aims at elucidating the molecular mechanisms that lead to tight junction breakdown, specifically investigating the mitogen-activated protein kinase (MAPK) signaling cascade. Madin Darby canine kidney cells are being used as an accepted model for tight junctions. Cells were treated with a growth factor that is known to be elevated in diabetic patients, which initiates the signaling cascade that potentially leads directly to phosphorylation of ZO-1. Control cells were treated with an inhibitor of the MAPK signaling cascade. ZO-1 was extracted with immunoprecipitation and Western Blot analysis completed to determine the phosphorylation state of ZO-1. It is expected that with the treatment of the MAPK inhibitor the ZO-1 protein will not be phosphorylated when the growth factor is present. This would identify the MAPK signaling cascade as the pathway that leads to phosphorylation of ZO-1 and disassembly of tight junctions in diabetic retinopathy. This work supports further studies investigating the development of a drug that can prevent diabetic retinopathy.

CHED 390
Modified ELISA to determine levels of TTX and its links to the life history of the eastern newt, Notophthalmus viridescens

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Tetrodotoxin (TTX) is one of the most lethal non-protein neurotoxins. This neurotoxin is produced by many organisms, including the eastern newt (Notophthalmus viridescens). This ubiquitous eastern North America species secretes TTX from glands located throughout its skin. The TTX is lethal, or at least highly toxic, to many of the eastern newt’s predators, so it acts as an anti-predatory mechanism. To date, there is no reliable technique for quantifying this toxin, and little is known about its chemical levels in different stages of the eastern newt’s complex life cycle. A protocol for a competitive indirect ELISA was developed to quantify the amount of TTX secreted by eastern newts in the adult/reproductive stage of their lives. Once the TTX-specific ELISA was optimized, it was used on a population of eastern newts at Letterkenny Army Depot, in South Central Pennsylvania, to determine ontogenetic (egg, aquatic larvae, eft, adult), size (small, medium, large), and sexual (male, female) variation in toxicity levels. Ultimately, this research can unveil ontogenetic, morphometric, and sexual chemical distinctions that might explain the ecological and evolutionary significance of this interesting chemical adaptation of the eastern newt.

CHED 391

Toxicity of imidazolium room temperature ionic liquids towards biofilms

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Overuse of antibiotics has given rise to strains of antibiotic-resistant bacteria and a need for different antimicrobial agents. In recent years, room temperature ionic liquids (RTILs) have attracted attention as a possible solution to this growing problem. There are many possible combinations of cations and anions that have been used as RTILs. The structure of the cation can radically alter the physical properties of the RTIL. For this investigation, multiple imidazolium RTILs with carbon chains of varying lengths were synthesized; two such examples are 2-butyl-3-propyl-1-methylimidazolium bromide (BPMIM Br) and 2-pentyl-3-propyl-1-methylimidazolium bromide (PPMIM Br). Biofilms composed of bacteria that are commonly found infecting the human body were subjected to these RTILs to determine their toxicity. Additionally, the log $K_{OW}$ of the RTILs was measured. This poster reports on the findings of the toxicity and log $K_{OW}$ tests and makes suggestions for future research.

CHED 392
Toward inhibitors of cystathionine β-synthase (CBS): Examination of both the transsulfuration and hydrogen sulfide evolution reactions

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Pyridoxal phosphate (PLP)-dependent enzymes are found in all three kingdoms of life and make up two percent of all enzymatic activity. From controlling steady state concentration of neuroactive amines (dopamine, GABA) and amino acids (glutamate, glycine) to controlling the flux into important pathways involved in cell proliferation (polyamine pathways and the one-carbon shuttle for thymine biosynthesis), this enzymatic class continues to be of considerable interest for biomedical science.

Hydrogen sulfide (H₂S) is one of three identified gaseous signaling molecules in human metabolism, along with NO and CO. The PLP-dependent enzyme cystathionine-β-synthase (CBS) is a key enzyme in the transsulfuration pathway that ultimately takes the sulfur in dietary methionine into protective redox equivalents in the form of glutathione. It now appears that CBS is also the neuronal enzyme that is principally responsible for H₂S production by β-elimination from L-cysteine. In fact, during stroke-like conditions, H₂S released from L-cysteine in the brain through the action of CBS may contribute to neuronal cell death. Because of this, development of CBS inhibitors as lead compounds for the development of therapeutic agents to mitigate against neuronal damage pursuant to stroke has been an area of active research.

This presentation will discuss the design, synthesis, and enzyme kinetic evaluation of a set of potential CBS inhibitors. Three different reaction manifolds were examined kinetically in these studies to examine inhibitor efficacy: (i) the forward transsulfuration reaction, i.e. the formation of (L,L)-cystathionine (radioassay), (ii) the reverse transsulfuration reaction (UV/vis assay), and (iii) hydrogen sulfide evolution (spectroscopic assay, following Pb(OAc)₂ treatment).

CHED 393

Conformational variability of MTHFR characterized by hydrogen-deuterium exchange and mass spectrometry

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Mutations in the protein, methylenetetrahydrofolate reductase (MTHFR), disrupt function and have been associated with diseases such as cardiovascular disease, dementia,
neural tube defects, and Alzheimer’s. MTHFR typically binds flavin and catalyzes the reduction of 5,10-methylenetetrahydrofolate to 5-methyltetrahydrofolate. Two residues that are important to the binding and function of MTHFR in E. coli. are glutamate28 (Glu-28 or E28) and phenylalanine223 (Phe-223 or F223). In this study, the dynamics and conformational changes globally and locally for wild type (WT) and three mutants of MTHFR - E28Q, E28D, and the double mutant, E28Q/F223L, were investigated by hydrogen deuterium exchange coupled with liquid chromatography and mass spectrometry (HDX-LCMS). Replacement of Phe-223 with leucine (F223L) was particularly interesting because leucine is found in human form. Results will be presented for intact and pepsin digested MTHFR. Results showed increased flexibility for most peptides analyzed in E28Q and E28D mutants while E28Q/F223L showed rigidity in most regions. Differences in deuteration levels of peptides located near the mutation site and/or the site of bound flavin suggest that the mutations might be causing conformational changes in the protein.

CHED 394

Spectroscopic properties of the GFP chromophore containing substituted phenylalanine derivatives in place of tyrosine

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Multiple phenylalanine derivatives containing substitutions at the ortho and meta positions were incorporated at the Y66 position in the chromophore of superfolder green fluorescent protein (sfGFP) using a broadly permissive pyrrolysyl-tRNA synthetase mutant in conjunction with an orthogonal amber suppressor tRNA. Phenylalanine derivatives containing aldehyde, bromo-, chloro-, trifluoromethyl-, ketone, methyl-, methoxy-, and nitrile functional groups at the ortho or meta positions were substituted into the sfGFP chromophore in the current study. The mutated chromophores displayed absorbance maxima ranging from 311 to 423 nm and fluorescence maxima ranging from 386 to 476 nm for these mutant proteins, which is a significant shift in absorbance and emission maxima compared to the wildtype protein (λexc 485 nm λem 510 nm). Two of the phenylalanine derivatives resulted in chromophores that emitted in the visible region of the electromagnetic spectrum. The meta-methoxy (λexc 374 nm and λem 450 nm) chromophore emitted a blue light that could be seen with the naked eye when irradiated with UV light. The ortho-methoxy (λexc 423 nm and λem 476 nm) chromophore emitted a yellow light that could be seen by the naked eye under white light. The larger Stokes shift of these mutant proteins compared to wildtype sfGFP as well as the shift in absorbance and emission maxima will provide new tools for FRET and fluorescence imaging studies.

CHED 395
Investigation of IPTG and its products of oxidation in the induction of protein biosynthesis

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Isopropyl beta-D-1-thiogalactopyranoside (IPTG) is a common inducer for recombinant protein expression. In some contexts, as in the study of oxidative stress, it is useful to express proteins under oxidative conditions. As a thioglycoside, IPTG is susceptible to oxidation. In this study, the synthesis of these oxidation products--the IPTG sulfoxide and sulfone--is reported, along with an examination of each as an inducer in *E. coli*. Preliminary evidence suggests that both the sulfoxide and sulfone can serve as inducers. Using this discovery, implications for the study of oxidative stress and associated disease states are presented.

CHED 396

Lipid dynamics of cardiolipin/DMPC and cardiolipin/DOPC in nanodiscs

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Cardiolipin is a negatively charged phospholipid that comprises roughly 20% of the lipids in the inner mitochondrial membrane. The dynamics of this membrane can influence interactions between cytochrome c and cardiolipin, which have been shown to initiate the intrinsic pathway of apoptosis. This investigation studies how the dynamics of a model membrane system of varying composition will behave in the presence and absence of cardiolipin. Nanodiscs are composed of varying concentrations of 18:1 cardiolipin and DOPC or DMPC, doped with either NBD-PE or TMA-DPH. (18:1 cardiolipin: 1',3'-bis[1,2-dioleoyl-sn-glycero-3-phospho]-sn-glycerol DMPC: 1,2-dimyristoyl-sn-glycero-3-phosphocholine DOPC: (Δ9-Cis) PC 1,2-dioleoyl-sn-glycero-3-phosphocholine NBD-PE: 1,2-dimyristoyl-sn-glycero-3-phosphoethanolamine-N-(7-nitro-2-1,3-benzoazadiazol-4-yl) TMA-DPH: trimethylammonium diphenylhexatriene). Time-Resolved Emission Spectra (TRES) of NBD-PE doped nanodiscs are used to report on head group relaxation and Time-Resolved Fluorescence Anisotropy of TMA-DPH doped nanodiscs are used to report on acyl chain motions. These methods are combined to provide insight into how cardiolipin affects lipid membrane dynamics.

CHED 397

Biochemistry in the cosmetic industry: The effectiveness of synthetic and natural preservatives

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The use of natural ingredients in cosmetics has become increasingly prevalent; however, there are still synthetic preservatives used. Whether synthetic or natural, these preservatives are used as antimicrobials or antifungals. The goal of this experiment is to test the effects of more synthetic preservatives such as methylparaben, as well as naturally occurring preservatives such as benzyl alcohol. Benzyl alcohol is found in jasmine and ylang-ylang essential oils. Methylparabens are commonly synthetic and toxic at high concentrations, but are also commonly found in blueberries, which are used for their antioxidant properties in cosmetics. Two common kinds of bacteria, Serratia marcescens (gram-negative bacterium), found sometimes in damp conditions; and Staphylococcus epidermidis (gram-positive bacterium), which is part of the normal human skin flora, were exposed to these two preservatives by dose-response and dilution. Dilutions of up 1.0% benzyl alcohol and 25% methylparaben are allowed in skincare products. In this experiment, ten-fold dilutions from 99% benzyl alcohol and 25% methylparaben were performed. Dilutions of $10^{-3}$, $10^{-4}$, and $10^{-5}$ of each bacteria were used. Colonies were grown on standard agar plates in an incubator at 25C. Survivability rate was measured as a variable of time and frequency of exposure. The expected outcome of this experiment is that the gram-positive bacteria will have a lower percent survivability when exposed to these preservatives. A decline in survivability of gram-negative bacteria is anticipated due to the damp environments, such as bathrooms, where skincare products are often stored. Mutagenic effects on bacteria, as well as survivability will be measured, as to hopefully draw conclusions about the effects and safety of these preservatives in skincare products.

CHED 398

Binding kinetics and transition of structural components of RNA polymerase

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The mechanism of forming and stabilizing the open, transcriptionally competent E. coli RNA polymerase-promoter complex was studied through stopped-flow kinetics with fluorescence detection and fast-mixing with radioactivity detection. The intermediates generated from opening the enzyme using T7A1 promoters allowed for kinetic studies. Those results were compared to ones previously calculated using the $\lambda P_R$ promoter. The fluorescence experiments confirmed two kinetic phases, a fast followed by a slow. When compared to the T7A1 promoter, $\lambda P_R$ forms the open complex slower but it remains open for a longer time. The information gained from studying E. coli RNAP is of relevance for design of new antibiotics and for understanding how human RNAP works due to the enzyme’s highly conserved nature.

CHED 399

Amyloid-perturbing dyes inhibit adhesion of Cryptosporidium parvum to the human ileocecal adenocarcinoma HCT-8 cell line
Cryptosporidium parvum is a parasite that causes diarrhea for immunocompetent individuals. However for immunocompromised individuals, the symptoms are more severe and lethal. The waterborne disease is found worldwide and undergoes colonization in epithelial tissue. Bioinformatics data indicate that C. parvum has sixteen amyloid positive amino acids in its adhesion proteins. Activated amyloid nanodomains on the surface of Candida albicans cells were shown to mediate adhesion for cell-to-cell binding interactions (Lipke et al. 2014). Amyloid-perturbing dyes Thioflavin S and Congo Red were shown to decrease adhesion of Candida albicans to substrates (Chan, Lipke 2014). C. parvum sporozoites fluoresce when stained with 20 µM of Thioflavin S. Since adhesion is an essential first step to the infection of host cells, we studied whether amyloid-perturbing dyes would decrease adhesion of the parasite C. parvum to host ileocecal HCT-8 cells. We tested whether Thioflavin S, Congo Red, and Thioflavin T would inhibit adhesion of C. parvum to HCT-8 cells. We treated C. parvum sporozoites with 10 and 200 µM of Thioflavin S, 1 and 20 µM of Congo Red, and 0.1 and 2 µM of Thioflavin T. After a 15-hour infection of HCT-8 cells, we utilized the Merifluor reagent to measure the immunofluorescence of C. parvum oocysts and evaluate adhesion. The uninfected/non-treated HCT-8 cells’ fluorescence was measured at approximately onefold, while the infected but non-treated host cells’ fluorescence was at a near twofold increase. The most effective treatments for reducing adhesion were 20 µM of Congo Red (onefold) and 0.1 µM of Thioflavin T (onefold). These results show that these dyes lead to a decreased adhesion of C. parvum to the host HCT-8 cells. It is also demonstrated that the inclusion of these dyes can bring the infected host cells’ level of adhesion back down near the uninfected host cells’ level of adhesion, which denotes an inhibition of adhesion of C. parvum to the host HCT-8 cells.

CHED 400

Relationship between redox potential and light production in the mucus of the marine tubeworm Chaetopterus sp

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The bioluminescent parchment tubeworm Chaetopterus sp. produces light in a manner different from most bioluminescent organisms. The light produced occurs as a long lasting blue glow that is associated with mucus secreted from the worm epithelium. The mechanism behind the light production is unknown and unique in being independent from molecular oxygen, which is otherwise required in known luminous systems. The worm builds a U-shape tube that goes deep into the anoxic layers of the sediment and during its secretion from inside the tube, the mucus experiences a natural gradient of redox potential while diffusing out the tube, into the open seawater. Hence, we were
interested in identifying whether redox potential correlates with light production of the mucus. Chemical treatments with MgF$_2$, Al$_2$(SO$_4$)$_3$, CaCl$_2$, ZnCl$_2$, and guanine, which are known to alter redox potential in different ways, were used to investigate this particular question. Our data indicated that redox potential and light production were inversely related, with decreasing light intensity going with increasing redox potential over time. In all cases, the treatments resulted in an increase of redox potential and decrease in light production; the only exceptions were ZnCl$_2$ and guanine that showed a decrease in redox potential. For ZnCl$_2$, this went together with a decrease in light production, however it was an increase in light production for guanine. This data indicates that redox potential could possibly be a key factor affecting light production in the luminous mucus secreted by the worm *Chaetopterus* sp. in the field.

**CHED 401**

**Identification of acid/base residues important to the mechanism of Thil**

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Although named for a role in the production of thiamin, the enzyme Thil catalyzes the transfer of sulfur originating in cysteine to uridine-8 of tRNA to make 4-thiouridine, which acts as a photosensor for near-UV light in bacteria. Absorption of near-UV light triggers the crosslinking of 4-thiouridine and cytidine-13, which prevents an amino acid attachment to tRNA. The resulting stalled ribosomes activate the stringent response, which causes growth arrest, a protective mechanism to prevent mutation induced by UV light. This process is the basis of a UV screening method that allows assessment of Thil function (whether it can produce the photosensor). The two proposed mechanisms for s$^4$U generation both invoke persulfide formation on Cys-456 of Thil by transfer of sulfur by the enzyme IscS. Both mechanisms also include unspecified general acid and base residues, which this work seeks to identify. Sequence alignments suggest five candidate amino acid residues for the mechanistically important acid/base groups. The polymerase chain reaction (PCR) with primers mismatched at the codons of interest allows site-specific mutation within the plasmid encoding Thil. The mutagenesis has been completed for the five positions, as confirmed by DNA sequencing. After transformations into *thiI E coli*, UV screenings allow determination of a position’s significance in Thil function. Inactive variants do not make s$^4$U and lack near-UV sensitivity because no s$^4$U is made. After critical residues are identified, the altered Thil will be overexpressed. Structural integrity can be assessed using CD spectroscopy and *in vitro* activity assays that monitor the incorporation of $^{35}$S into RNA will be employed to measure the activity of the variants. Through the use of mutagenesis, UV screening, and protein overexpression, the mechanistically important acid/base residues will be found.

**CHED 402**
General method for analysis of RNA structures by deoxyribozyme sensors

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All cells use RNA to regulate cellular processes, induce gene expression, and control cellular functions. Correct RNA processing and folding is essential to performing its function. For instance, one proposed cause of Alzheimer’s disease is the mis-folding of RNA. Cellular processes can be distorted or completely halted if RNAs are folded improperly. Analyzing correct RNA folding at cellular conditions is essential to accurately determine their behavior; however, current methods require high RNA concentrations or chemical reagents, conditions far from those found in native environments. A method for fast, inexpensive, quantitative, and accurate analysis of RNA secondary structures at low concentrations is needed for the research community. Here we propose a new, general method for quantitatively determining the stability of RNA hairpin loop and potentially other structures under near physiological conditions. By taking advantage of recent developments in synthetic biology and DNA nanotechnology, we designed a highly selective and sensitive deoxyribozyme sensor to produce a fluorescent response even at low RNA concentrations. Here we adopted the sensors for analysis of RNA secondary structures. The proposed method compares signal output of the deoxyribozymes bound to the RNA of interest and a truncated version of RNA. The folded RNA would have nucleotides competing for hybridization with the probe, while the truncated version of the RNA would not. This will allow for a quantitative determination of the stability of the RNA secondary structure. This sensitive method allows for quick probing of a specific hairpin loop, easy sample preparation, and allows for a seamless, inexpensive transition for analyzing different RNA species.

CHED 403

Designing peptide-coated gold nanoparticles for the bottom-up assembly of amyloid nanocompartments

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Among the possible phase networks accessible by amyloid beta (Aβ), peptide nanotubes have generated considerable research interest because of their ability to self-assemble into robust nanostructures. The Aβ peptide nanotube wall is four nm thick and consists of a peptide bilayer of β sheets, which is a configuration similar to the lipid bilayers observed in cell membranes. To strengthen the correlation between biomembranes and peptide nanotubes, current efforts are directed towards blocking the peptide nanotube termini with Aβ-coated gold nanoparticles to design a nanocompartment that can accumulate substrates and segregate the internal environment from the surroundings, resulting in the development of peptide-derived protocells.
Therefore, devising a method for directing Aβ assembly to gold nanoparticle surfaces to form peptide nanotube-compatible capping agents was the primary goal of these studies. Circular dichroism and fourier transform infrared spectroscopy suggested that the kinetics of peptide self-assembly are greatly favored over conjugation of Aβ to the gold nanoparticle surfaces. However, conjugation of Aβ to the gold nanoparticles was observed in the most concentrated peptide solution that contained Aβ congeners altered to have a glycine spacer, providing evidence that gold nanoparticle coating kinetics exhibits a concentration threshold and is sensitive to the length of the putative peptide.

The formation of “peptide coronas” around the gold nanoparticles, visible via transmission electron microscopy, was used to confirm the successful coating of the gold nanoparticles. Electron microscopy was also used to evaluate the capping efficacy of the Aβ-coated gold nanoparticles. Preliminary attempts at nanocompartment formation demonstrated that the affinity of Aβ-coated gold nanoparticles for peptide nanotube termini is too low for a robust nanocapping event to occur passively. Future venues for optimizing these protocols involve maximizing the concentration of nanocapping agents or designing covalent cross-linking entities to actively guide the Aβ-coated gold nanoparticles to the peptide nanotube termini.

CHED 404

Chemical characterization of novel bacterial LOV-domain photoreceptors

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The Light-Oxygen-Voltage domain family of photoreceptors mediates blue-light regulation of diverse signaling pathways. One key aspect of LOV domain photoreceptors is a large variation in photo cycle kinetics that is believed to dictate sensitivity to the quantity of environmental light. In eukaryotes, these fluence-dependent responses enable detection of day-length and prediction of diurnal stress pathways. Although circadian clocks do not exist in most bacteria, blue-light induces similar stress responses that are mediated by LOV domain containing photoreceptors. We have identified several bacterial homologs of fungal circadian clock photoreceptors that share key regulatory elements. Chemical and structural characterization of these proteins indicate a potential evolutionarily conserved mechanism of detecting oxidative stress that may be an ancestral function of LOV domain containing photoreceptors. Herein, we outline chemical characterization of bacterial LOV proteins that reveal unique aspects of LOV function that may have implications to our understanding of stress response pathways in fungi and plants.

CHED 405

Initial steps toward antimicrobial photodynamic textiles
According to the CDC, 5-10% of all patients admitted into a hospital will acquire a new infection from exposure to local pathogens, resulting in approximately 1.7 million healthcare-associated infections in the United States each year. Such infections are the sixth leading cause of death in America, as well as a $30-45 billion burden on the healthcare system. In order to reduce the incidence rates of such nosocomial infections, we have envisioned employing textile products with antimicrobial properties to prevent pathogens from transmitting to immunocompromised patients in hospitals and in other high-risk environments. As our chosen method of sterilization, we have focused on antimicrobial photodynamic inactivation (aPDI), which employs a non-toxic photosensitizer, visible light, and ambient molecular oxygen to inactivate microbial pathogens. Upon illumination, the photosensitizer generates singlet oxygen (\( ^1O_2 \)), a highly reactive species that has been shown to cause non-specific cell damage, which is thought to prevent the evolution of drug resistance. In addition, singlet oxygen rapidly decays back to its triplet ground state if unreacted, so it is thought of as being environmentally benign. Our strategy is to first test a textile coated in a photosensitizer dye, and if successful prepare a covalently modified textile product. With this in mind, we have synthesized a porphyrin-based photosensitizer, zinc(II) 5,10,15,20-tetrakis(N-methylpyridinium-4-yl)porphyrin, and characterized it by NMR and UV-vis spectroscopies, and electrospray ionization mass spectrometry. After confirming its synthesis, we tested the photosensitizer’s antimicrobial properties against two model species of bacteria: a Gram-positive strain of Staphylococcus aureus and a Gram-negative strain of Escherichia coli, and demonstrated its ability to inactivate both strains under reasonable illumination conditions (400-700 nm, 30 min). In the future, we will continue to explore the antimicrobial activity of this photosensitizer against other strains while preparing our initial antimicrobial photodynamic textile.

CHED 406

Species differences in detoxification rates

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Cytochrome P450s (hereafter, CYPs) are a broad class of enzymes largely responsible for drug metabolism. Preclinical drug discovery programs monitor drug metabolism by CYP enzymes in a variety of model species to ensure that drugs are circulating at safe and therapeutic levels. Different species, however, possess CYPs with varying affinities for substrates and therefore metabolize drugs at different rates. This is a potential problem for the translation of preclinical data to predict the effect of drugs in humans and non-model systems. The aim of this study was to measure the activity of CYPs isolated from multiple species to metabolize standard CYP substrates and natural
products from plants being developed as potential drugs. We hypothesized that laboratory-bred species would have faster rates of metabolism for standard substrates than domestic or wild species and that wild species that naturally consume plants would have faster rates of metabolism of natural products from plants. Gas chromatography was used to measure metabolism of volatile natural products by nonspecific CYPs, and a bioluminescence assay was used to measure metabolism of standard substrates by two specific CYPs. The rate of substrate loss or formation of metabolites was compared among species using an ANOVA. Variation was observed among species for degradation of standard substrates and natural products, and rates for a specific substrate differed for different CYP enzymes. These in vitro data will be used to interpret in vivo studies to translate rates of metabolism of existing and newly developed drugs in model species to predict their metabolism in humans, domestic and wild species.

CHED 407

Effects of dia2 degradation on checkpoint recovery in Saccharomyces cerevisiae

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Accurate DNA replication is essential for cell viability. During this process, cell division can be blocked by replication stress. This occurs after DNA damage has been encountered by the replication complex, which initiates a fork stall that causes activation of a checkpoint kinases cascade. When this takes place, a higher probability of accumulating mutations exists, which may transmit defects to daughter cells. The S. cerevisiae F-box protein Dia2 is involved in the degradation of a checkpoint protein, Mrc1, after checkpoint activation during recovery. Since the Dia2 protein has multiple roles in the cell cycle, we needed an approach to remove Dia2 function specifically in checkpoint recovery. We hypothesized that a Dia2 degron strain would delay checkpoint recovery by failing to target Mrc1 for degradation after checkpoint activation. Studying this process would help achieve better understanding of the importance of an F-box protein during recovery. The generation of a Dia2 degron strain was done with the addition of a Myc9 tag and Auxin Inducible Degron to the DIA2 gene via PCR amplification. The purpose was to control protein expression of the Dia2 protein with the exposure of auxin. In the future, the insertion of our product will be done into dia2Δ strain to ensure the only copy of DIA2 in the genome is the degron-tagged version. After verifying that the strain functions correctly, cells can be tested during checkpoint recovery in order to observe the effects of the absence of Dia2 in the system.

CHED 408
Computational and experimental approaches to investigate substrate binding of the enzyme OGA

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Many proteins are functionally regulated by the O-GlcNAc post-translational modification, and O-GlcNAcase (OGA) is the only cytosolic enzyme known to remove this sugar. We are proposing a new method to identify the O-GlcNAc modification could be based on a mutant OGA enzyme that binds to O-GlcNAcylated proteins without cleaving the modification or releasing the substrate. Furthermore, studying mutations in the OGA active site can lead to a better understanding of the enzyme’s structure-function correlation. Two adjacent aspartic acids, D174 and D175, comprise OGA’s active site, while amino acids G67, K98, N280, D285, N313 are included in its binding site. An in silico model of the wild-type (WT) OGA was used to study the enzyme-substrate interaction and was represented by a homology model provided by de Alencar et al. UCSF Chimera visualization software and a molecular dynamics package were used to prepare WT and mutated OGA structures. AutoDock was used to run binding simulations on these structures with the substrate PUGNACa, a competitive inhibitor. These computational results directed the decision on which OGA mutations to experimentally investigate. OGA enzymes were expressed in E. coli bacteria and purified by metal-affinity chromatography. Enzyme assays using a para-nitrophenol-GlcNAc (pNP-GlcNAc) substrate were used to investigate OGA activity, with the extent of the enzymatic reaction quantified by spectroscopy. Isothermal titration calorimetry (ITC) was used to study the binding activity of OGA. These experimental results will be compared to the computational data in order to evaluate the accuracy of the homology model and docking studies. The goal is to identify OGA mutants that can bind substrate without cleaving or releasing it.

CHED 409

Characterization of xanthine dehydrogenase regulator protein of Ralstonia solanacearum, a tomato infecting bacterium

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Ranked as number two in the top ten plant pathogen list, research reveals that Ralstonia solanacearum is exposed to reactive oxygen species (ROS) during infection of tomato plants. It has evolved redundant and efficient oxidative stress response mechanisms to adapt to the host environment and cause disease. Expression of the R. solanacearum xanthine dehydrogenase (xdh) gene is increased during oxidative stress. Xanthine dehydrogenase participates in purine metabolism and is responsible for
production of the antioxidant urate. The gene encoding XdhR, a transcription factor, is divergently oriented to the xdh gene cluster. We have cloned xdhR from R. solanacearum and shown that XdhR binds to the intergenic region between the xdh gene cluster and xdhR. The ligands guanosine triphosphate (GTP) and guanosine monophosphate (GMP) effectively dissociate XdhR from the intergenic DNA. This study presently aims at identifying other ligands of XdhR and identifying the role of XdhR in regulating expression of the xdh gene cluster under oxidative stress conditions.

CHED 410

Dissociation constant (pKa), pH and related thermodynamic functions of TRIS buffer from 5 to 55°C

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Potentiometric measurement of the buffer TRIS have been made in the temperature range of 5 to 55°C, including 25 and 37°C. The Harned cell of the type: Pt, H₂ (g, 1 atm) | Tris (m₁) + Tris·HCl (m₂) | AgCl, Ag was used. The pKa values have been determined at 12 temperatures at intervals of 5°. The thermodynamic quantities ∆G°, ∆H°, ∆S°, and ∆Cp° have been calculated at 5, 25, 37, and 55°C. The values of pKa at 25 and 37°C are 8.0741 and 7.7528, respectively. The pH values of the buffer solutions composed of TRIS (0.05) and its hydrochloride (0.05) in a molar ratio of 1:3 at 25 and 37°C are 8.174 and 7.852, respectively. These values lie in the physiological pH range and would be discussed in terms of its usefulness in biomedical and clinical studies.

CHED 411

Application of the Pitzer Formalism for the aqueous solution of HCl + KCl, HCl + NiCl₂, HCl + PrCl₃, and HCl + ThCl₄ at 25 °C

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The binary interactions (θH, K, SθH, Ni, SθH, Pr, and SθH, Th) and the ternary interactions (ΨH, K, Cl) have been determined from published results, mostly from our laboratory. These results are compared with similar electrolyte mixtures containing bromide ion instead of chloride ion. It was found that Sθ values are in close agreements and Ψ values are different, as expected, from the Pitzer ion-interaction theory. For example θH, K (HCl + KCl) and θH, K (HBr and KBr) = 0.005 whereas ΨH, K, Cl = -0.006 and ΨH, K, Br = -0.014. These values will be interpreted in terms of the calculation of the mean molal activity coefficient γ±, of the component, (HCl) or KCl in mixtures of electrolyte solutions. The differences in γ± values from the simpler treatment (Harned empirical equations) and the comprehensive treatment of Pitzer formalism will be discussed.
CHED 412

Carbon nanotube separation beyond size-selective protein hydrogels

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Carbon nanotubes constitute a useful class of nanomaterials, the applicability of which is significantly expanded when tubes of only a single chirality are utilized. The functionalized hydrogel Sephacryl S200 has been demonstrated to achieve superior single-chirality separation in comparison when used as a site-selective chromatography medium. However, because Sephacryl S200 was not engineered for nanotube separation, there is opportunity for improvement upon the site selection separation technique. Utilizing the specific properties of Sephacryl S200, custom made functionalized hydrogels and surface modified silicon microspheres can be made, tending towards a less expensive and more efficient carbon nanotube separation process.

CHED 413

Combining metabolic inhibitors to preferentially target cancers with deregulated p27

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A primary goal of cancer research is to preferentially destroy tumors without harming normal cells. P27kip1 (p27) is a tumor suppressor protein commonly deregulated in aggressive cancers. Current models posit that p27 disruption leads to inappropriate cell cycle progression, so therapeutic intervention is geared towards the use of cell cycle inhibitors. However, our lab recently discovered that p27 deregulation provides cancer cells with a growth advantage by altering nutrient metabolic pathways. We compared nutrient use over time in immortalized cells with and without p27. As expected, wild type cells were completely dependent on glucose and grew until it was depleted. Cells lacking p27 also initially used glucose, but when its levels dropped modestly they abruptly switched to the amino acid glutamine. This switch could provide a growth advantage to cancers with deregulated p27 by allowing amino acid metabolism during early tumorigenesis (before blood vessel formation). As the tumor grows and develops blood vessels, p27 function could be re-established to utilize plentiful glucose. We sought to exploit this switch to target tumors with deregulated p27 by artificially decreasing glucose levels with 2-deoxy-D-glucose (2-DG). This should preferentially force p27(-/-) cells to use amino acids, and these pathways can be specifically targeted using drugs affecting amino acid metabolism. Preliminary results indicate that cells lacking p27 can be preferentially killed without affecting viability of wild type cells,
supporting further development of this drug treatment protocol for targeting aggressive cancers with deregulated p27.

CHED 414

Analogs of cisplatin: 4,4'-disubstituted-2,2'-bipyridine complexes of Pt(II) dichloride

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Cisplatin (CDDP) is used as a chemotherapy drug. Cisplatin has also many side effects including hair loss, weakness, renal toxicity, neurotoxicity and vomiting. The most important side effect is the kidney damage. The kidney accumulates cisplatin and this reduces renal perfusion. It is used against some types of cancers like carcinoma, head and neck cancers, breast cancer etc. It functions as a cytotoxin by interfering with replication and transcription, thus inducing necrosis or apoptosis. Structural work supports its activity as an alkylating agent which binds imine nitrogens of guanine and cytosine residues in single strand DNA and RNA. Passive diffusion is the main way Cisplatin enters the cell, because of the different concentrations of Cl- in and out the cell. A certain degree of cis-CDDP uptake seemed to be energy dependent and could be modulated by pharmacological agents like enzymes and membrane interactive agents like digitonin.

Modification of its activity is sought through generation of analogs with improved activity through the substitution of ammonia ligands with 2,2'-bipyridine. The complexes were synthesized through reaction of bipyridine with K2PtCl4 and characterized by NMR (1H, 19F, 13C). The activity of the complexes in cancer cell lines will be presented. In the many lines tested, the EC50s of the complexes are smaller than those of CDDP.

CHED 415

Identifying biocompatible redox mediators for electrochemical imaging of Dictyostelium discoideum
Dictyostelium discoideum is an amoeboid protozoan that serves as a model organism for the study of a variety of cellular processes including cell motility, phagocytosis and chemotaxis. Our interest is in developing protocols for imaging this organism using Scanning Electrochemical Microscopy (SECM). In a typical SECM experiment, the chemical reactivity and topography of a surface are probed by monitoring the diffusion of a redox-active mediator between the surface and an ultramicroelectrode (UME) positioned closely above (on the order of micrometers) the surface. Current measured at the UME can be used to discern the conductivity, roughness and chemical activity of the surface. In experiments involving living cells, it is critical that the redox mediator does not negatively affect the cells. Dose response assays for common redox mediators used in SECM studies will be presented. Mediators with sufficient biocompatibility will be used to image the topography of Dictyostelium discoideum cells on a planar substrate, and results will be compared to those obtained with an ultramicroelectrode biosensor utilizing glucose as a non-redox-active mediator. These results will be beneficial in providing a tool to measure the dynamics of glucose levels in the microenvironment surrounding individual cells.

CHED 416

Detection and Identification of biochemical molecules secreted by Entamoeba varieties for taxa discrimination based on aggregative behavior

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The Entamoeba lineage includes free living or parasitic cells which phylogenetic and behavioral characterization is unknown. Aggregation by different varieties of Entamoeba is a response to different environmental cues such as stress. We have shown that Entamoeba discriminate between one another depending on the relatedness of the taxa. Previous experiments have provided strong evidence to support the presence of kin recognition and cell signaling. Signaling and aggregative behavior could impact pathogenicity and virulence. The purpose of this study is to determine the presence of chemical molecules in different strains of Entamoeba. Based on preliminary data, we have proposed that analogous signaling pathways to single cell eukaryotes may exist in Entamoeba. The purpose of this study is to elucidate the chemical molecules involved in the signaling between individual and clustered cells. Methods were developed to help determine the structure and composition of the chemical signaling molecule, including the use of conditioned and unconditioned media to cause aggregation. The resulting chemical signaling molecule, if discovered, will help in future studies to help develop better strategies for the identification and phylogenetic classification of different varieties of Entamoeba. The strategies can be used to expand our scientific knowledge and medical applications.
Effect of retinoid receptor agonists on K562 cellular adhesion, proliferation, and α5β1 integrin cell surface expression

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Establishment and maintenance of proper immunity requires a precise balance between cellular adhesion and proliferation. A disruption in either event culminates in a variety of pathologies encompassing immunosuppression, auto immunity, and cancer. Retinoids, profoundly affect immune function by mediating cellular adhesion and proliferation in certain leukocytes. Retinoids, by binding to retinoid receptors (RARs or RXRs), modify the expression of a variety of signaling proteins involved in immune cell proliferation and adhesion including, integrins. Integrins are a family of transmembrane heterodimeric receptors consisting of non-covalently linked α and β subunits that are considered to be the principle receptors involved in attachment to the extracellular matrix and provide adhesive interactions that control cellular proliferation. Currently, the contributions by retinoids in immune cell adhesion and proliferation have been independently examined; however, in retinoid responsive immune cell lines there appears to be a potential synergism between cellular adhesion and proliferation, which may be mediated through integrins, specifically the α5β1 subset. In this study, the effect of all-trans-retinoic acid agonists on K562 cellular adhesion, proliferation, and α5β1 integrin cell surface expression was investigated. RARgamma agonist exposure increased K562 cellular adhesion to RGD containing extracellular matrix proteins fibronectin and FN-120. Cell surface expression of both the α5 and β1 integrin subunits was increased in the presence of a RARgamma agonist; however, RARgamma agonists decrease K562 cellular proliferation. In the presence of the RARbeta agonist, K562 cellular proliferation was increase, while α5β1 cell surface expression was decreased. The RARalpha agonist was comparable to the control in K562 cellular adhesion, proliferation, and α5β1 integrin cell surface expression. Our study is the first to demonstrate that specific RAR agonists alter cellular adhesion, proliferation, and intergrin cell surface expression.

Thiophene N-substituted tetrahydro pyridinium salts as functionally selective muscarinic partial agonists

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Several thiophene N-substituted tetrahydropyridinyl compounds were synthesized and found to inhibit the specific binding of the antagonist [3H]N-methylscopolamine in radioligand muscarinic assays. All compounds were found to be selective partial agonists. Compound 7A in particular was found to be an absolute M2 selective partial agonist in functional assays. This compound stimulated GTPγS binding that reached
about 76% $E_{\text{MAX}}$ of the full agonist carbachol and only activated $M_2$ receptors. Other compounds were found to be potent and efficacious $M_2$ partial agonists. Compound 7A and other analogs contain the NCCSC backbone which serves as a novel scaffold for the design and synthesis of agonists with absolute muscarinic functional selectivity.

**CHED 419**

**Lactate dehydrogenase: A study of kinetics and inhibition**

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Anaerobic glycolysis occurs when the concentration of oxygen is not sufficient for aerobic respiration. During anaerobic glycolysis, lactate dehydrogenase (LDH) converts pyruvate to lactate while oxidizing nicotinamide adenine dinucleotide (NADH). LDH exists as several isozymes in the body and is often used as a diagnostic test for tissue injury as a result. It is particularly useful to diagnose injury of heart, liver, kidney, muscle, brain, and lung tissue. This study involves the isolation of LDH from beef, mouse, and rat heart followed by its purification using various types of chromatography, including ion-exchange and affinity chromatography. A full kinetic study was performed on the purified LDH and was compared to a known LDH standard. Inhibition of LDH was studied through the synthesis and characterization of known inhibitors, such as oxamate. Kinetic studies of LDH are useful as it plays a major role in medical diagnostic tests.

**CHED 420**

**Effect of catalase overexpression on ethanol-induced hepatic mitochondrial DNA damage in mice**

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Ethanol administration induces oxidative stress, which is defined as a disturbance in the prooxidant-antioxidant balance in favor of the former, potentially leading to oxidative damage. The primary result of oxidative stress is the increase in the steady state concentration of oxidizing reactive oxygen species including hydrogen peroxide. In mammalian cells, mitochondrial DNA is a sensitive target for oxidative attack; it is more prone to damage than nuclear DNA because, unlike nuclear DNA, it does not contain introns or long sequences of noncoding bases and is not protected by histones, and its repair pathways are limited. Literature results show that ethanol treatment causes hepatic mitochondrial DNA damage and dysfunction. In this work, the specific role of hydrogen peroxide on ethanol-induced mitochondrial DNA damage was explored using transgenic mice that overexpress catalase, an enzyme that catalyzes the dismutation of hydrogen peroxide into molecular oxygen and water. Transgenic mice overexpressing...
catalase and wild-type controls were administered orally for four weeks an isocaloric liquid diet such that 0% or 36% of energy was contributed by ethanol. Oxidative damage to mitochondrial DNA was evaluated as lesions that block the progression of the thermostable DNA polymerase in long qPCR, which include strand breaks, bulky adducts, and oxidative base lesions. A long (8.9 kb) PCR mitochondrial fragment was generated using specific primers. In addition, a quantitative amplification of a small region of mitochondrial DNA (221 bp) was also performed to normalize copy number differences between samples. The PCR products were quantified using the Quant-iT PicoGreen dsDNA assay kit (Life Technologies, Grand Island, NY), and characterized by 0.8% agarose gel electrophoresis with ethidium bromide detection. Long PCR amplification of the mitochondrial DNA from the different groups was compared with that of the control group, and relative mitochondrial DNA integrity was calculated assuming that the control group mitochondrial DNA has 100% integrity. Mitochondrial DNA integrity was significantly lower in ethanol-treated wild-type mice than in control wild-type mice. Overexpression of catalase in transgenic mice prevented the effect of ethanol on mitochondrial DNA integrity. These results suggest that hydrogen peroxide plays a central role in the mechanism of ethanol-induced mitochondrial DNA damage.

CHED 421

Effect of oral chronic ethanol administration on hepatic mitochondrial biogenesis in mice

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Mitochondrial biogenesis is defined as the growth and division of pre-existing mitochondria. Mitochondrial biogenesis is triggered by environmental stresses that activate a transcriptional program that upregulates the expression of mitochondrial biogenesis genes. These genes include co-activators such as peroxisome proliferator-activated receptor gamma-coactivator-1 alpha (PGC1a, the master regulator of mitochondrial biogenesis) and DNA-binding transcription factors such as mitochondrial transcription factor A (TFAM). Ethanol administration to experimental animals can affect hepatic mitochondrial biogenesis, inducing mitochondrial depletion or proliferation, depending on experimental protocols. Key variables that determine the effect of ethanol on mitochondrial biogenesis are the concentration of ethanol, duration of exposure, ways of administration (oral of intragastric), and animal species. In this work we explored the effect of chronic (4 weeks) oral ethanol administration (at 36% of total calories) on hepatic mitochondrial biogenesis in mice. The expression of PGC1a and TFAM was evaluated at the protein level by western blotting, against beta actin as a loading control. Quantification of the bands by densitometry showed that the PGC1a and TFAM content did not change in mice exposed to oral ethanol for 4 weeks (with respect to the controls), in contrast with published results showing increased hepatic PGC1a and TFAM expression in mice exposed to ethanol intragastrically for 4 weeks. These results suggest that the effect of ethanol on hepatic mitochondrial biogenesis depend critically on the administration protocol.
Effect of ethanol and catalase overexpression on hepatic mitochondrial DNA content in mice

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Ethanol administration to experimental animals can affect hepatic mitochondrial DNA content by inducing mitochondrial DNA depletion or proliferation, according with experimental protocols. Key variables that determine the effect of ethanol on mitochondrial DNA content are the concentration of ethanol, duration of exposure, ways of administration (oral of intragastric), and animal species. Ethanol-induced oxidative stress may play a key role in the mechanism of both depletion and proliferation of hepatic mitochondrial DNA. The primary result of ethanol-induced oxidative stress is the increase in the steady state concentration of reactive oxygen species including hydrogen peroxide. In this work, the specific role of hydrogen peroxide on ethanol-induced changes in mitochondrial DNA content was explored using transgenic mice that overexpress catalase, an enzyme that catalyzes the dismutation of hydrogen peroxide into molecular oxygen and water. Transgenic mice overexpressing catalase and wild-type controls were administered orally for four weeks an isocaloric liquid diet such that 0% or 36% of energy was contributed by ethanol. The relative amount of mtDNA in mouse liver was determined using quantitative real time. For mtDNA quantification, 0.01-1 ng of genomic DNA was used as template, and real-time PCR analysis was done by amplifying a targeted mitochondrial gene (mitochondrial NADH dehydrogenase subunit 5 or ND5) using the QuantiTect SYBR Green PCR Kit (Qiagen, Valencia, CA). A nuclear DNA gene was used as the reference. The Ct was defined as cycles to the threshold for each amplification experiment (mitochondrial or nuclear). The fold-change relative to control animals was calculated using the following equation: $2^{-\Delta \Delta \text{Ct}(\text{mitochondrial/nuclear})}$, where

$\Delta \Delta \text{Ct}(\text{mitochondrial/nuclear})=\text{dCt}(\text{mitochondrial/nuclear})$ of animals from different treatments− $\text{dCt}(\text{mitochondrial/nuclear})$ of control animals, and

$d\text{Ct}(\text{mitochondrial/nuclear})$ is equal to $\text{Ct}(\text{mitochondrial})-\text{Ct}(\text{nuclear})$. Mitochondrial DNA content increased in ethanol-treated wild-type mice relative to control wild-type mice. Overexpression of catalase in transgenic mice prevented the effect of ethanol on mitochondrial DNA content. These results suggest that hydrogen peroxide plays a central role in triggering an increase in mitochondrial DNA content after chronic ethanol administration to mice.

Effect of catalase overexpression on ethanol-induced oxidative stress in mice

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Alcohol administration induces oxidative stress, which is defined as a disturbance in the prooxidant-antioxidant balance in favor of the former, leading to potential damage. The primary result of oxidative stress is the increase in the steady state concentration of reactive oxygen species including hydrogen peroxide. Many processes and factors are involved in causing alcohol-induced oxidative stress, including redox state changes as a result of ethanol and acetaldehyde oxidation, acetaldehyde generation and acetaldehyde adduct formation, mitochondrial damage and decreased ATP production, Kupffer cell activation via increases in endotoxin levels, and induction of cytochrome P450 2E1 (CYP2E1). In this work, the specific role of hydrogen peroxide on ethanol-induced oxidative stress was explored using transgenic mice that overexpress catalase, an enzyme that catalyzes the dismutation of hydrogen peroxide into molecular oxygen and water. Transgenic mice overexpressing catalase and wild-type controls were administered orally for four weeks an isocaloric liquid diet such that 0% or 36% of energy was contributed by ethanol. The redox state of the GSH/GSSG was used as an indicator of oxidative stress. The redox state of the GSH/GSSG pair was determined by measuring the concentrations and the ratios of the main interconvertible reduced (GSH) and oxidized (GSSG) forms of glutathione. The hepatic level of total glutathione and the GSH/GSSG ratio were significantly lower in ethanol-treated wild-type mice than in control wild-type mice, reflecting hepatic oxidative stress conditions induced by chronic ethanol. Overexpression of catalase in transgenic mice prevented the effect of ethanol on total glutathione and the GSH/GSSG ratio. These results suggest that hydrogen peroxide plays a central role in the development of hepatic alcohol-induced oxidative stress.

CHED 424

N-acetylcysteine inhibits the upregulation of mitochondrial biogenesis genes in livers from rats fed ethanol chronically

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Chronic ethanol administration to experimental animals induces hepatic oxidative stress and upregulates mitochondrial biogenesis. The mechanisms by which chronic ethanol upregulates mitochondrial biogenesis have not been fully explored. In this work, we hypothesized that oxidative stress is a factor that triggers mitochondrial biogenesis after chronic ethanol feeding. If our hypothesis is correct, co-administration of antioxidants should prevent upregulation of mitochondrial biogenesis genes. Rats were fed an ethanol-containing diet intragastrically by total enteral nutrition for 150 days, in the absence or presence of the antioxidant N-acetylcysteine (NAC) at 1.7 g/kg/day; control rats were administered isocaloric diets where carbohydrates substituted for ethanol calories. Ethanol administration significantly increased hepatic oxidative stress, evidenced as decreased liver total glutathione and GSH/GSSG ratio. These effects were inhibited by co-administration of ethanol and NAC. Chronic ethanol increased the expression of mitochondrial biogenesis genes including peroxisome proliferator activated receptor gamma-coactivator-1 alpha and mitochondrial transcription factor A,
and mitochondrial DNA; co-administration of ethanol and NAC prevented these effects. Chronic ethanol administration was associated with decreased mitochondrial mass, inactivation and depletion of mitochondrial complex I and complex IV, and increased hepatic mitochondrial oxidative damage, effects that were not prevented by NAC. These results suggest that oxidative stress caused by chronic ethanol triggered the upregulation of mitochondrial biogenesis genes in rat liver. Because NAC did not prevent liver mitochondrial oxidative damage, extra-mitochondrial effects of reactive oxygen species may regulate mitochondrial biogenesis. These results predict that the effectiveness of NAC as an antioxidant therapy for chronic alcoholism will be limited by its limited antioxidant effects in mitochondria, and its inhibitory effect on mitochondrial biogenesis.

CHED 425

Effect of chronic ethanol administration on hepatic genomic (nuclear and mitochondrial) DNA integrity in mice

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Chronic ethanol administration induces hepatic oxidative stress. Oxidative stress is defined as an increase in the steady state concentration of reactive oxygen species, caused by a disturbance in the prooxidant-antioxidant balance in favor of the former, potentially leading to oxidative damage. DNA is potentially a target for oxidative attack. Oxidatively generated damage to DNA generally starts with an initial abstraction of an electron or hydrogen atom producing DNA-centered radicals. These often react with oxygen, resulting in the formation of oxidized end products and fragmentation of the DNA molecules. In many oxidative stress models, it has been shown that mitochondrial DNA is more prone to damage than nuclear DNA because, unlike nuclear DNA, mitochondrial DNA does not contain introns or long sequences of noncoding bases and is not protected by histones, and its repair pathways are limited. Based on this previous knowledge, we hypothesized that chronic (4 weeks), oral ethanol administration in mice (at 36% of total calories) produces a higher level of mitochondrial DNA than nuclear DNA damage. Oxidative damage to mitochondrial DNA was evaluated as lesions that block the progression of the thermostable DNA polymerase in long qPCR, which include strand breaks and oxidized end products. A long (8.9 kb) PCR mitochondrial DNA fragment was generated using specific primers. In addition, a quantitative amplification of a small region of mitochondrial DNA (221 bp) was also performed to normalize copy number differences between samples. Nuclear DNA damage was evaluated by amplifying a long (10.1 kb) fragment of the beta-globin nuclear gene. The PCR products were quantified using the Quant-iT PicoGreen dsDNA assay kit (Life Technologies, Grand Island, NY), and characterized by 0.8% agarose gel electrophoresis with ethidium bromide detection. Long PCR amplification of the DNA from the different groups was compared with that of the control group, and relative mitochondrial DNA integrity was calculated assuming that the control group DNA has 100% integrity. Mitochondrial DNA integrity was significantly lower in ethanol-treated mice than in
control mice. In contrast, ethanol administration did not change hepatic nuclear DNA integrity with respect to the controls. These results suggest that chronic oral ethanol administration in mice selectively induces mitochondrial DNA damage.

CHED 426

Effect of polycystin-2 disruption on osmotic response of renal epithelial cells

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Renal epithelial cells exposed to hyperosmolality in the inner medulla withstand these conditions by activating the osmotic stress response. Primary cilia detect mechanical and chemical stimuli including osmolality. We have previously shown that renal epithelial cells with loss of cilia formation due to Kif3a deletion have an attenuated osmotic response, and that TRPM3 is involved in cilia-dependent osmosensation. It is unknown whether the osmotic response is compromised in cells that harbor functional, rather than structural, defects in cilia. We characterized the osmotic response of renal epithelial cells deficient in polycystin-2 (PC2), a protein expressed in primary cilia that is defective in some patients with autosomal dominant polycystic kidney disease (ADPKD).

Murine inner medullary collecting duct (mIMCD3) cells were transduced with an shRNA construct targeting Pkd2, or a non-target control sequence. PC2 expression was reduced by 90% by the Pkd2 shRNA construct as determined by immunoblotting, and cilia structure was normal in both cell lines as observed by immunofluorescence. Both cell lines were exposed to hyperosmolal culture conditions with NaCl (500 mOsm/kg), or maintained under isoosmolal conditions (300 mOsm/kg) in the presence of pregnenolone, an agonist for TRPM3, or DMSO vehicle. Western blotting for aldose reductase (AR), an osmotic response protein, was performed on whole cell lysates.

Induction of AR expression by hyperosmolality was markedly reduced in PC2 knockdown cells compared to non-target controls. Pregnenolone attenuated the AR induction in non-target control cells only.

We demonstrate a novel finding of diminished osmotic response in mIMCD3 cells with reduced PC2 expression, but intact cilia structure, suggesting that impaired osmoregulation may play a role in ADPKD pathogenesis. Further, the impaired osmotic response in PC2-deficient cells may result from altered TRPM3 activity.

CHED 427

Effect of transglutaminase on the deregulation of the p27 protein
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The tumor suppressor protein p27 is often deregulated in aggressive human cancers via post-transcriptional mechanisms. Identifying and understanding how this occurs is essential for developing effective therapies to treat these types of tumors. Because p27 is an unstructured and heat stable protein, we postulated its activity might be modulated by enzymes imparting structure to its polypeptide chain. Intriguingly, some cancers exhibit elevated levels of transglutaminase, a family of enzymes best known for cross linking proteins via formation of an isopeptide bond between glutamine and lysine residues on different protein monomers. To determine whether transglutaminase could alter p27 structure, we purified His tagged p27 from E coli by nickel affinity chromatography and incubated it with transglutaminase. Products were then analyzed by denaturing polyacrylamide gel electrophoresis. Surprisingly, p27 monomers were not crosslinked as expected. Instead, p27 migrated faster on the gel, suggesting a more compact form of the monomer. P27 structure was evaluated by limited protease digest and supported a change in p27 confirmation. Importantly, the related family member p21 was not modified, suggesting the reaction was specific to p27. To determine if altering p27 structure modified its function, we analyzed the effect on p27 binding partners. Results indicate that transglutaminase can alter p27 structure and function, which might represent a novel regulatory pathway involved in the development of cancerous tumors.

CHED 428

Analysis of p53 protein in hepatocellular carcinomas using 2D and 3D culture models

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Cancer research is driven by the focused and specific investigation of the development of the disease. One mechanism of interest is the widely documented TP53 gene. The gene is known to be a necessary proponent of healthy cells, and acts as a tumor-prevention measure on the cellular level. TP53 mutations are common among many cancers. It has been estimated, for example, that 60\% of primary breast tumors contain mutations in at least one form of the gene (Khoury, Bourdon, 2010). Nine isoforms of the protein have been documented, each presenting a structurally distinct and functional form of p53 protein. However, the specific function of each isoform, and whether it is related to tumor-suppression is not well known. Furthermore, it is still unclear the extent to which mutations must affect the gene to prevent its tumor-suppressive function. In this preliminary study, we investigated the full-length p53 isoform (FLp53) in five hepatocellular carcinomas using protein immunofluorescence (IF). The studied cell lines
were two p53 mutants (SNU-475, SNU-378), two lines with wild type p53 (C3A, HepG2), and one line that is p53 null (Hep3B). Cells processed with IF were cultured in two ways: Traditional two-dimensional (2D) culturing in flasks, as well as three-dimensional (3D) spheroid formation using Perfecta3D® Hanging Drop plates. 3D cultures were supplemented with methylcellulose to improve spheroid structure. The produced spheroids were also processed using lactate dehydrogenase (LDH) and alamarBlue® assays to study cell viability. Optimizing 3D culture will better emulate the structure and physiology of in-vivo tumors. In the future we plan to further investigate other documented p53 isoforms to determine their presence in various liver cancers. This knowledge will guide future understanding of the role isoform mutation has in tumorigenesis. Finally, an optimized technique for 3D culture of liver cancers will allow us to compare TP53 gene expression in both 2D and 3D models in the future, and thereby provide a clearer path for developing cancer treatments.

CHED 429

Turning off the lights: A novel luciferase inhibitor

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The naphthoquinone 12,13-dihydro-N-methyl-6,11,13-trioxo-5H-benzo[4,5]cycloheptal[1,2-b]naphthalene-5,12-imine (TU100) was originally synthesized as a potential chemotherapeutic agent. During its characterization, however, we discovered TU100 is a potent inhibitor of luciferases, the class of enzymes responsible for bioluminescence. Luciferases are evolutionarily distinct with different structures and substrates, so it is surprising that a single compound is able to inhibit multiple forms of the enzyme. TU100 inhibits firefly, Renilla, and NanoLuc luciferases to varying degrees and displays either competitive or mixed inhibition with respect to the luciferin substrate. Present studies have investigated the mechanism of inhibition and evaluated the ability of TU100 to inhibit luciferase inside cells. Results reveal that TU100 is not covalently bound to the enzyme, nor is it generating reactive oxygen species causing enzyme inactivation. Tissue culture cells were transiently transfected with a Renilla plasmid to determine if TU100 can inhibit a luciferase expressed inside cells. Data indicate TU100 is a novel luciferase inhibitor with broad specificity against this class of enzymes. Thus, it may have utility in biological assay systems where controlling luciferase activity is important. TU100 might also be useful in the study of bioluminescence in organisms.

CHED 430

Isolation of bioactive compounds from novel actinomyces strains

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Actinomyces are gram-positive bacteria of the order actinobacteria that play an important role in soil ecology. They secrete a wide and complex array of organic and biological compounds into their environment, which have proven to be a productive source for the discovery of numerous anti-cancer and anti-microbial drugs. In the present study, a large sample of novel actinomyces strains was collected from the Great Salt Plains of Oklahoma. Individual isolates were prepared and grown in liquid media, followed by centrifugation to remove the bacteria. The remaining supernatant was screened for potential bioactive compounds by evaluating the effect on viability of tissue culture cells using a resazurin fluorescence based assay. Two strains related to the species *Streptomyces tendae* were found to secret components into the supernatant that were highly toxic to cancer cells. The cytotoxic agents were further characterized and their mechanism of action investigated by evaluating heat stability, size, and molecular composition. Results suggest that these novel strains of actinomyces are secreting highly active compounds that dramatically compromise critical cellular processes required for viability. Thus, they represent viable candidates for further development into potential chemotherapeutic agents.

**CHED 431**

**Molecular docking studies of novel flavonoid derivatives as dual binding site acetylcholinesterase inhibitors**

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Studies show that one of the many factors contributing to Alzheimer's disease is the hydrolysis of Acetylcholine (ACh) from the enzyme Acetylcholinesterase (AChE). The resulting decrease of ACh concentration in the brain has been linked to complications including, but not limited to, memory loss and uncontrolled muscle movements. Research has also found that AChE inhibitors decrease the rate at which ACh is metabolized, therefore increasing the concentration of ACh in the brain. Furthermore, the recent identification of multiple binding sites within AChE presents the opportunity for the design of dual binding site inhibitors. Flavonoids, naturally occurring compounds, are known for their ability to inhibit AChE and can serve as potential dual binding site AChE inhibitors. In the current research study, Autodock 4.0 in addition to Autodock Vina were used to provide binding free energy values of several novel ligands of interest. Inhibitory concentration (IC$_{50}$) values were then calculated, and the results aided in the identification of promising novel flavonoid derivatives as dual binding site AChE inhibitors.

**CHED 432**

**Standard buffer POPSO for use in the physiological pH range**
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The second dissociation ($pK_2$) of the zwitterionic buffer POPSO and the pH of its buffer solutions have been studied in the temperature range 278.15 – 328.15 K. Experimental emf measurements have been made using the Harned cell without liquid junction of the type: Pt, H\textsubscript{2} (g, 1 atm) | Na\textsubscript{3}POPSO (m\textsubscript{1}) + Na\textsubscript{4}POPSO (m\textsubscript{2}) + NaCl (m\textsubscript{3}) | AgCl, Ag. The $pK_2$ values and the thermodynamic quantities ($\Delta G^\circ$, $\Delta H^\circ$, $\Delta S^\circ$, and $\Delta C_p^\circ$) will be reported at 278.15, 298.15, 310.15 and 328.15 K. The pH values for 4 buffer solutions at equimolar concentrations as well as at ionic strength ($I = 0.16$ mol\cdot kg\textsuperscript{-1}) matching those in physiological fluids have been determined from (278.15 – 328.15) K. The Bates – Guggenheim convention and the Pitzer equation have been used to calculated the single ion activity coefficient chloride ion, of $\gamma_{cl}$. The $pK_2$ of POPSO at 298.15 K and 310.15 K are 7.8029 and 7.6628, respectively. The pH values of buffer solutions ($I = 0.08$ mol\cdot kg\textsuperscript{-1}) at 298.15 K and 310.15 K are 8.0438 and 7.9281, respectively. This physiological buffer will be recommended to fulfill the need for a new physiological primary pH standard in the studies of biomedicine.

CHED 433

Mechanistic and kinetic studies of a new ROS-activated compound

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Some cancer cells, such as acute myeloid leukemia (AML) cells possess elevated levels of reactive oxygen species (ROS) compared to healthy cells. ROS are a product of cellular metabolism and they play an important role in cell signaling and homeostasis. There are two key forms of ROS: superoxide and hydrogen peroxide. Our lab uses this knowledge to synthesize new ROS-activated anti-cancer agents. Compounds display selectivity between target cancer cells over healthy cells. One of the compounds synthesized, named Michael Acceptor-14 (MA-14), is activated in the presence of the hydrogen peroxide. We hypothesize that upon oxidation, this new agent reacts with DNA to form adducts that ultimately results in cell death. I have examined the oxidation, hydrolysis, and DNA reactivity of MA-14. I have found that the oxidation can occur under ambient conditions with a half-life of 5hrs. In the presence of hydrogen peroxide the half-life is near instantaneous. Additionally, as expected there is a strong pH dependence with elevated pHs leading to faster oxidation. Next, I have found that MA-14 can potentially react with DNA via the study of reactions with a model nucleoside. Upon further investigation I found that dC and dA can also react with MA-14. These studies are paving the pathway towards an understanding of this compound’s reactivity, and potentially elucidating its mechanism.

CHED 434
Dietary sodium suppresses digestive efficiency: Role of the renin-angiotensin system

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Foods containing large amounts of fats and sodium chloride(NaCl) are highly palatable (e.g. - potato chips), and their consumption is associated with obesity. We therefore hypothesized that eating a diet with high fat and high NaCl content (HFHS) would increase weight gain over eating a diet with high fat, but low NaCl content (HFLS). Surprisingly, we found that nine week old male C57BL/6J mice fed HFLS gain more weight than mice fed HFHS. We determined that this increase was not due to increased food intake, reduced resting metabolism, or reduced physical activity. We then tested the hypothesis that increased dietary NaCl reduces digestive efficiency. Mice were fed chow (n=6), HFHS (n=7), or HFLS (n=8), and fat absorption by the intestine was determined by fecal acid steatocrit. HFHS significantly increased the fat loss to feces versus HFLS (Chow: 0.5±0.2, HFHS: 2.4±0.2, HFLS: 1.5±0.1 %, P<0.05), confirming our hypothesis. Further, dietary sodium is known to suppress circulating renin-angiotensin system activity. We found that replacement of angiotensin II in HFHS-fed mice normalized fecal acid steatocrit (1.4±0.3 %, n=7, P<0.05 vs HFHS). In contrast, blockade of angiotensin AT1 receptors by losartan in HFLS-fed mice had no effect (1.5±0.1 %, n=5). We conclude that dietary sodium suppresses weight gain with high fat diet feeding, and this is mediated through a suppression of the renin-angiotensin system – though not through the AT1 receptor. Mice with genetic deletion of the angiotensin AT2 receptor are currently under study to evaluate its role in digestive efficiency.

CHED 435

Pattern analysis of abnormal blood producing low velocity spatter

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Blood spatter is well established in providing crucial information in crime scene investigation. Over the years spatter has been thoroughly researched, allowing investigators to use it to help understand and reconstruct the events that occurred during the commission of a crime. This research looks to specify differences that may be seen in cases involving a victim with abnormalities in their blood, such as an iron deficiency, as seen in anemia, or a deficiency in the red blood cell count, resulting in less viscous, freer flowing blood. Porcine blood was utilized to simulate low velocity spatter dripping from a weapon. Spatter from blood with normal levels was compared to blood with both varied viscosities and iron levels. The diameter of the primary drop, the number of satellite drops, and the length of tails presents were analyzed at angles other than 90 degrees. Photos of the blood patterns were taken to show any other visible
differences. Blood with less viscosity is expected to flow faster, producing larger diameters with longer tails. As viscosity increases the spots should be smaller because the blood is more uniform. An individual with iron deficiency, such as anemia, reduces the flow of the blood, which means the blood will drip slower and produce shorter tails. Overall, both of these abnormalities affect spatter, which could cause changes to the analysis of a crime scene.

CHED 436

Alteration of the specificity of putrescine oxidase by mutations to the active site

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Putrescine oxidase is an enzyme that converts Putrescine into 4-aminobutanol and Hydrogen peroxide. The enzyme is known to be fairly specific for putrescine when activity with other biologicaldiamines such as cadaverine is examined. It has been proposed that the specificity of Putrescine oxidase can be manipulated by means of site directed mutagenesis in the active site to yield an enzyme that does not require a diamine for activity. Previous studies have suggested the role histidine 432 plays is in stabilizing the substrate. Current studies have attempted to investigate if the tyrosine at the 326 can be altered to adjust the interaction between glutamate 324 and the terminal amine of putrescine.

CHED 437

Identification of sulfopeptides as HIV entry inhibitors through phage display

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Given its complexity and high rate of mortality, Human Immunodeficiency Virus (HIV) has been one of the most studied topics by researchers and clinicians since it was identified as the causative agent for AIDS. The HIV envelope glycoprotein gp120 works as a detector and a binder that detects and binds CD4, the protein receptor in the cell membrane. Upon binding to CD4, gp120 undergoes a large conformational change and exposes the binding site for co-receptor CCR5 (or CXCR4). The binding of co-receptor causes membrane fusion of the virus and the target cell, which allows viral RNA genome to enter the target cell. Previous studies have shown that sulfoxytyrosine (sTyr) residues within the N-termini of CCR5 receptors are essential for the binding of gp120. Our goal is to synthesize and identify sTyr-containing peptides that can effectively disrupt the interactions between gp120 and CCR5 (or CXCR4). We synthesized sTyr
from tyrosine via organic synthesis, and tested genetic incorporation of sTyr into green fluorescent protein (GFP) in response to amber nonsense codon in Escherichia coli. We next examined phage display of sTyr-containing peptide by fusing its encoding gene to the pIII gene of the phage. After further optimization of phage display system, we will construct phage library and conduct selection against HIV gp120 protein.

CHED 438

Screening peptidomimetic ligands against patient-specific chronic lymphocytic leukemia monoclonal antibodies

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Chronic Lymphocytic Leukemia (CLL) is characterized by the uncontrolled proliferation of antigen experienced B lymphocytes. Auto antigen-stimulated B cell receptors fail to initiate an immune response, and the B lymphocytes to which they are attached proliferate in an uncontrolled, cancerous manner. The leukemic B lymphocytes soon overtake healthy B lymphocytes in the blood and cause the cancer disease state seen in CLL patients. The current method for treatment of CLL is a combination of immunosuppressant and chemotherapy agents which aim to kill all of the immune system’s B cells, including healthy B cells. Our ultimate aim of this project is to selectively target the cancerous B lymphocytes in CLL patients by way of binding to the CLL B cell receptors on those lymphocytes. Peptidomimetic ligands allow for the possibility of hijacking the body’s own natural protein-protein interactions. We are especially interested in hijacking protein-protein interactions seen in diseased states, such as CLL. Peptidomimetic compounds such as peptoids, chiral oligomers of pentenoic acids (COPAs), and peptide tertiary amines (PTAs) have previously proven to be valuable ligands to human proteins. The CLL B cell receptor antibody binding ligands utilized in the study were chosen from a library of synthesized peptidomimetic compounds. To determine whether or not the ligand selectively targets CLL B cell receptors, the ligand is covalently linked to a TentaGel bead and bound to an antibody of interest. The binding event is subsequently labeled using a red fluorescent Quantum Dot. We tested previously identified CLL antibody hit peptidomimetic ligands against the CLL antibodies of interest to revalidate the ligands’ strength at targeting patient specific CLL antibodies. Select peptidomimetic ligands show strong evidence for specificity in binding to CLL B cell receptors.

CHED 439

Oxidation of cytochrome C by guanine radicals

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Oxidative damage to DNA plays a role in the progression of many diseases, including cancer. This damage is observed primarily at guanine (G) because it is the most easily oxidized base. Base excision repair (BER) enzymes, like Endonuclease III, readily detect these DNA base lesions and contain [FeS] clusters that are active in electron transfer. In our experiment, we chose to use cytochrome c as a simpler and cheaper model for Endonuclease III. Cytochrome c is a heme protein found in mitochondrion that plays a crucial role in the electron transport chain. Here, we investigate if cytochrome c can use redox chemistry to repair guanine radicals generated by photooxidation. To create the most desirable conditions for the experiment, we artificially synthesized two complementary DNA strands (with 2-Aminopurine (AP) inserted near the 5' end of one strand). The AP-containing strand was designed to contain guanine sites that decrease in oxidative potential as the distance from AP increases, to facilitate charge transport and prevent back electron transfer. Then, AP was excited with the 325 nm output from a HeCd laser for 0 to 360 seconds, conditions known to induce guanine oxidation. Using uv-visible spectroscopy, our results showed that the 550 nm absorption characteristic of reduced cytochrome c was seen to decrease irradiation of the aminopurine. Since AP is known to oxidize guanine on a fast timescale, these results are consistent with protein to DNA electron transfer that repairs the guanine radical produced by the 2-aminopurine photooxidant, suggesting that this could be a possible route for repair of immediate oxidative DNA damage in vivo.

CHED 440

Effect of glutathione on DNA-protein crosslinking caused by guanine oxidation

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Oxidative damage to DNA plays a role in the progression of many diseases, including cancer. This damage is observed primarily at guanine (G) because it is the most easily oxidized base. The flash-quench technique is a method that is used for selective guanine oxidation in double-helical DNA and it can induce DNA-protein crosslinking. Glutathione is a small cysteine-containing peptide responsible for redox buffering in the cell. Here, we investigated whether it might be possible for glutathione, a strong reductant, to play a role in diminishing DNA damage (e.g. DNA-protein crosslinks) by engaging in redox repair of the 1-electron oxidized guanine base as formed by the flash-quench method. Samples containing Ru(phen)₂dppz²⁺ [phen = phenanthroline, dppz = dipyridophenazine], Co(NH₃)₅Cl²⁺, histone protein, salmon sperm DNA and glutathione (reduced form) were irradiated for 0-240 seconds with 442 nm light to effect guanine damage. The % crosslinked was determined by the chloroform extraction assay: NaCl and SDS were added to the samples to disrupt noncovalent interactions between DNA.
and protein, then the proteinaceous material was extracted into 24:1 chloroform:isoamyl alcohol. After centrifuging, the aqueous phase containing unreacted DNA was assayed at 260 nm by uv spectroscopy. Our results showed as the irradiation time increased, the absorption of free DNA decreased, consistent with crosslinking. Less DNA-protein crosslinking was observed when glutathione was present in the samples. We also used the gel shift assay: pBR322 plasmid was seen to migrate to the wells upon flash quench treatment in the presence of histone, but this behavior is strongly inhibited by glutathione. Lastly, we investigated whether or not glutathione interfered with the quenching process by doing emission spectroscopy experiments. We found that glutathione only slightly interfered with the quenching of Ru(phen)$_2$dp pz$^{2+}$, indicating that it most likely reacts with the guanine radical directly.

CHED 441

Expression and purification of homocysteine methyltransferase Sam4 recombinant in Escherichia coli

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It is well known that, in organisms, one of the functions of enzymes is to avoid the accumulation of bioorganic compounds that can inhibit biological processes indispensable for cell function. Recently, it has been found that organisms such as yeast, fruit flies, nematodes and plants use a methyltransferase enzymes to convert isomer R-Adenosyl-L-methionine to its bioactive form S-adenosyl-L-methionine (AdoMet). This metabolite is the second most widely used substrate in all phyla of life and is involved in reactions essential for cellular biochemistry. The diversity of functionalities present in the metabolite explain its consumption in processes as the recycling of methionine, peptide and tRNA modification, lipid metabolism, metalloprotein cluster formation, among others. Particularly, yeast employs two homocysteine methyltransferase Sam4 and Mht1 (EC 2.1.1.10) to deplete R-AdoMet accumulation. Even though no disease has been directly associate to the presence of R-AdoMet, its accumulation can be toxic to cellular processes, as its presence occupy valuable intracellular space. In humans, the pathways that carry out the conversion of R-AdoMet to S-Adomet still remain elusive. Therefore, the focus of the study is to express and purify recombinant Sam4 in Escherichia coli by immobilized metal affinity chromatography. These procedure would help to obtain large amounts of the recombinant protein in order to study its enzymatic capacity by using AdoMet derivatives, which will potentially the study of the catalytic mechanism. First, the method was applied to the recombinant human thiopurine methyltransferase proteins (TPMT, EC 2.1.1.67), and the method results effective since a high yield and reproducible purification was observed. TPMT catalysis shows that a methyl transfer to aromatic thiols occurs in a time and enzyme concentration dependent manner. Sam4 expression
was performed successfully, but the purification was partially effective. Consequently, the study of the enzymatic capacity of Sam4 shows a minimum activity at the condition employed. The results imply that the purification method should be refined. The affinity purification can be optimized in Sam4 studies to fully understand and decrypt the enzyme mechanism and functions in vivo, to detect substrates that are catalyzed by it, and to elucidate the physiological response of R-AdoMet bioaccumulation.

CHED 442

Analysis of the antibody binding of MUC1 peptides and substituted peptides by STD NMR

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The binding epitope PDTRP, found within the VNTR domain of MUC1 glycoprotein, is recognized by the immune system and binds mucin monoclonal antibody SM3. This study analyzes the binding ability of the peptide GVTSAPD, an upstream sequence preceding PDTRP, as well as six substituted peptides against specific mouse MUC1 mucin monoclonal antibody (IgG1, 6A4) by Saturation Transfer Difference NMR (STD NMR) to determine the specific residue critical for antibody binding and whether analogous side chain characteristics in the substituted sequences would enhance binding. Of the substituted sequences resembling epitope GVTSAPD, five had the Pro residue substituted for Asp, Leu, Tyr, Phe, and Trp and one had the Ser residue substituted for Asn. The STD NMR results indicated that Pro is a critical residue for binding as it displayed greater saturation transfer effects for its side chain protons than did any other residue. Substituting the Pro residue with single hydrophilic or hydrophobic aliphatic residue (Leu or Asp) eliminated all STD effects while substitution of the same residue with single hydrophobic aromatic residue (Phe or Trp) produced STD effects at the aromatic protons. Substitution at Ser position for Asn produced STD effects that were quite similar in pattern and intensity to those of the native sequence. As indicated by the results, the Pro residue on native sequence, GVTSAPD, is critical for antibody binding and substitution at this position for aromatic residues (Trp or Phe) conserves binding ability, which suggests that these substituted peptides may possess biological activity.

CHED 443

Investigation of the aqueous chemistry in the elimination of glutathione from the glutathione-3-methyleneoxindole conjugate: A potential therapeutic agent

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The basis of my research was to study whether “GSMOI”, the Glutathione (GSH) conjugate with 3-Methyleneoxindole (MOI) is a mechanism-based inhibitor of the anti-
cancer target enzyme Glyoxalase 1 (Gxl). To fully understand the chemical mechanism, my research question asks whether the elimination of GSH from GSMOI follows the E1, E2, or E1cb chemical mechanism. To determine which mechanism this elimination follows, GSMOI was synthesized by two different methods producing (1) a solid sample, and (2) a working aqueous stock solution in phosphate buffer. The synthesized products were characterized using NMR and UV-Vis spectroscopy. Using the UV-Vis spectrophotometer chemical kinetics assays were conducted at pH 7 to determine the rate at which GSMOI breaks down into MOI. Furthermore, C-3 proton exchange kinetics on GSMOI were determined by observing the rate of hydrogen to deuterium exchange by NMR. Taken together, these data strongly suggest an E1cb mechanism for GSMOI elimination. This research is significant because if GSMOI is a potential cancer therapeutic, understanding how it reacts under physiological conditions is key to using it for pharmaceutical purposes. This research was funded by a summer 2014 grant from the Bridgewater State University Office of Undergraduate Research.

CHED 444

Thermostabilization of water soluble variants of the human β2 adrenergic receptor

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G-protein coupled receptors (GPCR) comprise the largest family of cell-surface receptors, and their important role in physiology makes them the frequent target of therapeutic drugs. Due to a number of challenges involved in producing diffraction quality crystals of GPCR, the structural characterization of these molecules has been slow. The Parrill lab has been working on a strategy of introducing a transferable set of mutations that will render GPCR water-soluble with the aim of accelerating their structural characterization. Thus far, collecting data on the structure and function of the water soluble mutants has proved difficult, presumably due to lack of thermostability. This poster presents preliminary efforts to introduce previously published thermostability mutations into water soluble constructs of the human β2 adrenergic receptor (hβ2AR). Trial expressions of the thermostabilized mutants showed that they expressed at approximately equivalent levels to the original water soluble construct.

CHED 445

Evaluation of off-target effects through double-stranded RNA interference in C.elegans

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RNA interference (RNAi) is a process in which messenger RNA (mRNA) is destroyed, silencing the corresponding genes. This process is used to study and regulate gene expression. Occasionally, genes other than the target are silenced. This research examines the scientific principles that govern transitive RNA interference and off-target effects by targeting a sequence 3’ away from the hairpin (37a), 5’ from hairpin (37b) and the hairpin sequence itself (37hp). These plasmids were fed to C. elegans by E. coli to test for off-target effects. RNA expression levels were determined using qPCR. It was found that dsRNAi is effective in knocking out the desired genes but also causes off-target effects.

CHED 446

Designing an undergraduate lab procedure for the synthesis of [R,S]-Boc-Phenyglycyltryptophan methyl ester

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The overall goal of this research was to design an undergraduate lab experiment that uses amide-coupling reactions to synthesize [R,S]-Boc-Phenyglycyltryptophan methyl ester and to analyze the resulting peptide by $^1$H-NMR to determine the epimer formation ratio of the product. Proteins are formed when different amino acids are linked together by amide-coupling reactions. When two amino acids are linked a dipeptide is formed. In chemical synthesis of peptides, two epimers of the product may be formed. Analysis of the product by $^1$H-NMR was used to determine which epimer was synthesized. Epimers are compounds that have multiple chiral centers but ultimately differ from each other in conformation at only one of these chiral centers. One purpose of this research was to evaluate the protocol laid out by Fray and determine if it was appropriate for our students and facilities, which it was. We followed Fray's protocol but substituted Tryptophan methyl ester in place of Valine methyl ester as the main target compound. We found that the synthesis of [R,S]-Boc-Phenyglycyltryptophan methyl ester was a better choice of a target compound for us.

CHED 447

Arabidopsis MMD-like genes and their roles in chromosome biology during male reproduction

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Mutations in Arabidopsis Male Meiocyte Death1 (MMD1) exhibit cytoplasmic shrinkage and chromatin fragmentation, leading to male meiocyte apoptosis. MMD1 is expressed during meiosis and encodes a Plant Homeo Domain (PHD) protein. Arabidopsis contains three other MMD1-like proteins, MS1, which is essential for tapetal cell
development and MMDL1 and MMDL2, which are expressed at elevated levels in the endosperm and sperm cells, respectively. MS1 has been shown to play a role in controlling transcription during tapetal cell development, raising the possibility that MMD-like genes may also be transcriptional regulatory proteins. Plants homozygous for single mutations in MMDL1 and MMDL2 appear normal, while homozygous mutations in both genes are lethal. Interestingly, while mmdl1-/- mmdl2-/- plants are viable, but display a seed abortion phenotype, mmdl1-/- mmdl2-/- plants are not able to be isolated. Detailed cellular and molecular analyses including the generation and analysis of plants expressing RNAi constructs are underway and the results of these experiments will be presented. Likewise MMDL1- and MMDL2- promoter β-glucuronidase reporter fusions are being generated to better understand the transcriptional regulation of MMDL1 and MMDL2. The results of these experiments will also be presented.

CHED 448

Molecular recognition of diatomic gases in *Rhodopseudomonas Palustris*
Cytochrome *c’*

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Cytochromes *c’* are bacterial heme proteins with a vacant distal coordination site available for binding diatomic gases. Distal heme ligation is sterically hindered by a non-polar residue (typically Leu, Phe, or Met). In the case of *Alcaligenes xylosoxidans* cytochrome *c’* (AXCP), distal steric hindrance is proposed to cause the conversion of the six-coordinate heme-NO complex (6cNO) to a five-coordinate heme-NO complex (5cNO) on the opposite (proximal) heme face. By contrast, the NO complex of *Rhodopseudomonas Palustris* (RPCP) exists as a mixture of 6cNO and 5cNO species. Here, we have explored the role of steric hindrance in controlling RPCP reactivity with diatomic gases (NO, CO, O₂) using resonance Raman spectroscopy and time-resolved UV-vis absorption.

CHED 449

Natural antisense RNA plays a role in *Arabidopsis thaliana* growth and development

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Plant Homeo Domain (PHD) proteins have been shown to play important roles in controlling gene expression in a number of organisms. In particular they have been shown to encode proteins that can bind to modified histones and control chromatin structure and ultimately transcription. *Arabidopsis* contains four related PHD containing genes that appear to play important roles in plant reproduction. Mutations in the *Male*
meiocyte death1 (mmd1) gene result in male meiocytes that undergo apoptosis during prophase I. Mutations in MS1 (Male sterility 1) disrupt pollen development by causing tapetal cells to die. Mutations in MMD-L1 and MMD-L2 result in reduced fertility with plants showing alterations in pollen and female gametophyte development. As part of a study to understand the roles of the MMD-like proteins, in Arabidopsis, we have characterized the MMD-L1 and MMD-L2 loci. We found that the MMD-L1 locus contains a natural antisense RNA that overlaps with the 3’ end of MMD1-L1 gene, raising the possibility that the antisense RNA may help control MMD1 like expression. In this study we have investigated this possibility by obtaining and characterizing an Arabidopsis line that contains a T-DNA insertion in the MMD1L1 anti-sense gene. Preliminary results show that the AS gene plays an important and unexpected role in plant growth and development and that the AS gene plays a role in MMDL expression. Studies are underway to determine if in fact the antisense RNA is controlling MMD1L gene expression and if so how. We will also investigate the possibility that the AS RNA plays a more global role in controlling gene expression by identifying genes that show altered expression levels when AS RNA levels are either reduced or elevated.

CHED 450

Reaction of strained alkynes with cysteine proteases

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Cyclooctynes are used commonly as probes in chemical biology in the azide-alkyne cycloaddition. Despite their inherent strain, these molecules have been described in many contexts as “bioorthogonal;” that is, they are thought to not react with biological functional groups. In this presentation we describe several instances where cyclooctynes are not bioorthogonal. Specifically, we demonstrate that certain cyclooctynes react efficiently with cysteine proteases. In some cases, the reaction between the cyclooctyne and the cysteine protease is faster than the alkyne’s reaction with small molecule thiols and azides. We discuss the implications of these results for bioorthogonal chemistry and practical applications of this novel class of cysteine protease inhibitors.

CHED 451

Platinum(II) complexes with sulfur-containing peptide building blocks for use in RNA binding studies

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To increase our knowledge of RNA structure-function relationships, there is a need for new RNA probes. Novel compounds can be used to better understand ligand-RNA binding interactions with future medicinal and experimental applications. With that goal in mind, this project involved the synthesis and characterization of various platinum complexes with sulfur-containing amino acid ligands. These compounds will later be used in DNA and RNA binding studies. The compounds were synthesized with potassium tetrachloroplatinate and amino acids, Met or Cys, as starting materials. The conditions were varied such as the molar ratio of metal to ligand. The products were characterized by using NMR and IR spectroscopy. During the course of this project, certain challenges were met and overcome with alternative strategies, such as the ligand choice and experimental conditions.

CHED 452

Role of H57 in synchronizing ammonia transfer within E. coli CTP synthetase

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CTP synthetase (CTPS) hydrolyzes glutamine and shuttles the resultant ammonia through an intermolecular tunnel to the point of incorporation with substrate UTP. Within the crystallized tetramer, E. coli CTPS subunits were seen to exist in two equally populated conformers that varied in the position of the side chain of H57. In one conformation, H57 is poised to hydrogen bond with substrate UTP and, in doing so, points away from the tunnel constriction; in the other conformation, H57 is pointed toward and potentially obstructs the ammonia passage. Thus, the conserved residue H57 is proposed to act as a “swinging gate”, coordinating the passage of nascent ammonia with the availability of acceptor-substrate UTP. To assess the potential role of this residue, we used site-directed mutagenesis to engineer H57A, H57N, H57L, and H57F and characterized the kinetics of each protein variant. Glutaminase activities remained largely unaffected by the mutations, whereas kcat/Km values for glutamine-dependent CTP synthesis reactions were decreased by nearly 100-fold. Thus, ammonia tunneling efficiencies were reduced to under 3%, compared to the ability of wild-type enzyme to incorporate 100% of nascent ammonia into the synthesis of CTP. Ammonia tunneling efficiencies were unaffected by the V-type allosteric activator GTP. These results suggest that substitutions of the imidazole ring result in nascent ammonia being unproductively released into solvent, consistent with the role of H57 in directing ammonia to the synthetase domain. The synchronizing movement of H57 is hypothesized to result from its H-bonding interaction with substrate UTP; such a mechanism would suggest contributions by H57 to the binding affinity of UTP. However, UTP saturation profiles for all of the variants reveal Km values that are similar to or (in the case of H57A) less than that of wild-type CTPS.

CHED 453
Kinetics of the reaction of 6-aminohexanoic acid with chlorine(I): Evidence for a role for dichlorine monoxide

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Hypochlorous acid (HOCl) is a powerful oxidizing agent that is produced in the body by the action of the enzyme myeloperoxidase. Production of excess HOCl in the body can be damaging to cells, DNA and proteins. The compound, 6-aminohexanoic acid (6-AHA), is a model for a lysine residue in a protein. The mechanism of oxidation of this residue by HOCl is not well understood and is the subject of this presentation. The mechanism of the reaction between HOCl and 6-AHA appears to be pH dependent. Evidence that over part of the pH range dichlorine monoxide (Cl₂O) may be the important form of the oxidant will be presented.

CHED 454

Isolation of corticosterone and its effect on personality in convict cichlids (Amatitlania nigrofasciata)

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Linking personality to hormone expression can help bridge the gap between disease and neurological processes. Personality is the suite of characteristics of individuals that account for repeatable behaviors across time and sometimes across contexts. One of the more commonly studied personality traits is boldness (how individuals respond to changes in their environment). Levels of corticosterone (CORT; a primary stress hormone in many organisms) have been shown to correlate with the extent of boldness exhibited in other fish species ergo CORT represents one potential link between condition and expression of personality. In this study, we aimed to look at the physiological and chemical response of individual convict cichlid (Amatitlania nigrofasciata) in response to changes in environment. After exposing individuals to predatory Oscar cichlids (Astronotus ocellatus), corticosterone was extracted from the aqueous environment and isolated using high performance liquid chromatography and microfiltration. Corticosterone levels were then quantified using an enzyme linked immunosorbent assay during which CORT was reacted with an antibody; the resulting complex was immobilized and subject to multiple liquid reagents, incubated and washed. These steps induce a color change indicating strength of CORT concentration. Preliminary results indicate that, in the presence of a stressful predator, there is a direct correlation between the level of stress-responsiveness and CORT secretion.

CHED 455

Effect of brewed coffee from various sources on the formation of amyloid-beta fibrils in vitro
Coffee has been widely studied due to its high consumption rate throughout the world, especially for its caffeine and chlorogenic acid content. Recently, studies have been performed on the effects of caffeine and chlorogenic acid on the disruption of amyloid formation. The formation of amyloid fibrils is a common protein misfolding mechanism which is the basis for numerous diseases prevalent today. Previous research had found that caffeine and chlorogenic acid reduced amyloid formation related to Type II diabetes: the caffeine and chlorogenic acid content disrupted the amyloid formation of human islet amyloid polypeptide protein in the pancreas. My research focuses on the effects of brewed coffee on amyloid fibrils in vitro in relation to Alzheimer’s disease. The misfolding of amyloid-beta 1-40 polypeptide into amyloid fibrils disrupts normal neuronal function in the human brain, thus leading to the characteristic deterioration of memory, motor function, and human expression associated with Alzheimer’s disease. Amyloid-beta 1-40 human polypeptide was exposed to three brewed 100% Arabica brand-name coffees (Dunkin Donuts®, Great Value®, and Starbucks®) over one, two, and three week periods at an incubation temperature of 37°C. High-performance liquid chromatography (HPLC) was utilized to determine the caffeine and chlorogenic acid contents of each brand-name coffee at incubation points of zero, one, two, and three weeks. At the end of each incubation period, the coffee-exposed amyloid-beta samples were examined for fibril formation via Thioflavin-T based fluorescence emission.

CHED 456

**Identification of bovine pregnancy markers in urine samples**

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Dairy and cattle farmers rely on the reproductive schedules of their herds to attempt to increase the production of milk and, eventually, profitability. The current method of determining the pregnancy status of cows is either by rectal palpation, ultrasound or through assays performed on blood plasmid or milk. These tests can be expensive and have a degree of uncertainty, in addition to having a time delay. The goal of our research is to create a more convenient and less costly method of evaluating bovine pregnancy status. Samples of urine from pregnant and non-pregnant dairy cows were analyzed using both LC/MS and TLC in hopes of finding a potential marker(s) for pregnancy. Precipitation tests of urine alcohol mixtures were also performed to qualitatively assess the turbidity of the solutions as previous work indicated a possible correlation of precipitate formation with pregnancy status.

CHED 457
Interaction of anthrax toxin protective antigen protein with model cell membranes at the air-water interface

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Anthrax toxin is composed of three proteins: protective antigen (PA), oedema factor, and lethal factor. PA binds to cell membranes to form a heptameric complex which forms a pore in the membrane. The pore then allows oedema and lethal factors to travel into the host cell, ultimately leading to cell death. The details of the PA interaction with membranes is not completely understood. In an effort to better understand how PA interacts with host cells, Langmuir monolayers were constructed at the air-water interface. Phospholipid monolayers are model cell membranes, and present as the exterior of a cell membrane when proteins are incorporated into the aqueous sub phase below the monolayer. Proteins including the wild form of PA (PA83), the heptameric form (PA63) and a PA 83 mutant were studied by measuring changes in surface pressure after placing proteins beneath the model membrane in separate studies. Protein penetration of phospholipid monolayers is indicated by increases in surface pressure over time. It was found that monomeric PA83 did not penetrate the films, and was crowded out of the surface with increasing lipid density. Heptameric PA63 penetrated the monolayers and caused significant increases in surface pressure through a range of lipid packing. The mutant PA83 was not expected to interact with the films and was tried as a negative control. Interestingly, this mutant did have positive interactions with the film at a pH of 5; a recently published structure indicates a nascent pore which may have limited interactions with membranes.

CHED 458

In silico studies of MMP-1

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The matrix metalloproteinases (MMPs) and the ADAMs (A Disintegrin And Metalloproteinase domain) are zinc-containing proteolytic enzyme families implicated in a variety of physiological processes such as inflammation, wound healing and tissue development. The pathologies associated with either increased or decreased activities of these enzymes include, but are not limited to, conditions such as rheumatoid arthritis, diabetes osteopenia, Alzheimer’s disease and cancer. The roles of metalloproteinases in cancer are complicated by the fact that most tumor cells, and frequently the surrounding stromal cells, synthesize MMPs to facilitate invasion into surrounding connective tissue and promote metastasis. While the matrix metalloproteinase family has been a pharmaceutical target for the last two few drugs have made it to market to date. Reasons for the low success rate include
unwanted side-effects caused by lack of selectivity, poor oral bioavailability and decreased potency in vivo. We are using the rational drug design methodology to characterize and understand the conformational flexibility of the MMPs and ADAMs. By understanding the factors driving the conformational associated with ligand binding we hope to be able to provide guidance for the design of more selective metalloproteinase inhibitors.

CHED 459

Investigation of the apoptotic biochemical mechanism of ajulemic acid in Ewing’s sarcoma cell lines

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Ajulemic acid (AJA) is a synthetic derivative of THC-11-oic acid. Previous lab results have shown that AJA can induce apoptosis in various Ewing’s sarcoma cell lines. The goal of this study was to elucidate the unknown biochemical mechanism by which AJA induces apoptosis. Currently, X-ray crystallography has only revealed AJA bound to peroxisome proliferator-activated receptor gamma (PPAR-γ), but western-blots results from previous studies have demonstrated that this protein is not expressed in Ewing’s sarcoma cells. In a prior study, this prompted the use of SMAP, a functional site analysis program, to survey protein databases for proteins with ligand binding domains similar to that of PPAR-γ. Ultimately, this approach generated that retinoid x receptor alpha (RXR), retinoic acid receptor (RAR), and vitamin D₃ receptor (VDR) have similar LBDs to PPAR-γ. An observation was then made that PPAR-γ, RAR, and VDR all heterodimerize with RXR, which led to the investigation of the heterodimers as receptors to which AJA may bind. First, a docking suite within Sybyl-X, a computational program, was used to dock AJA into the ligand binding domains of the receptors, which showed that AJA bound strongly with the receptors of interest. Furthermore, a mammalian 2-hybrid test was performed to determine if AJA could bind to the receptors in order to cause conformational changes, leading to subsequent changes in transcriptional activity. In this assay, a positive interaction leads to expression of luciferase reporter gene. Magellan, a data analysis software, was used to measure relative luminescence units (RLU), which quantifies reporter gene expression.

CHED 460

Enhancing the bioavailability of RAGE inhibitors: Toward new anti-Alzheimer’s therapeutics

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Alzheimer's disease is a neurodegenerative disease characterized by the progressive loss of brain function. Over the past ten years there has been a 68 percent increase in the number of people dying with Alzheimer's, and there are currently more than five million Americans living with the disease. A hallmark of Alzheimer's disease is the presence of amyloid-β (Aβ) peptide, which has been directly linked to increased levels of apoptosis in neurons. The receptor for Advanced Glycation End products (RAGE) has been demonstrated to mediate Aβ peptide transport across the blood brain barrier. Previous research has resulted in the design of a lead molecule which inhibits RAGE mediated Aβ transport. In this investigation, we set out to optimize the bioavailability of the lead compound by enhancing its hydrophilic properties via the addition of hydrogen bonding groups. Several analogs of the lead compound were synthesized using two basic schemes. The effect of these modifications on solubility and RAGE inhibitors potency will be described and investigated.

CHED 461

Effects of apolipoprotein E on M2 microglia

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The primary genetic risk determinant for late-onset Alzheimer's disease (LOAD) is the apolipoprotein E gene (APOE). Variations in this gene produce three different isoforms of the apolipoprotein E protein (ApoE): ApoE2, ApoE3, and ApoE4. ApoE3 is the most common isoform, so rates of LOAD among other genotypes are indexed to this variant. ApoE2 is rather rare, but its carriers are less likely to get LOAD; when they do, they get it later. The second most common variant is ApoE4, and its carriers are significantly more likely to get LOAD. They also tend to succumb earlier. Once developed, LOAD is characterized by inflammation-related (M1) changes in microglia, non-neuronal cells that mediate innate immunity in the central nervous system (CNS). Microglia are also capable of expressing gene products associated with an alternative, non-inflammatory (M2) form of activation in the periphery, but the degree to which microglia recapitulate those peripheral phenomena and the influence of LOAD etiology on the M1-M2 spectrum remain to be determined. Thus, identifying the effects of ApoE3 and ApoE4 on activated microglia could be helpful in two important ways: 1) by elucidating the differences in activity between ApoE3 and ApoE4 during LOAD and 2) by characterizing the M1-M2 spectrum of activation in the CNS. To explore these areas, we cultured primary microglia harvested from neonatal rats and treated them with ApoE3, ApoE4, an M2 activator—interleukin-4—or combinations thereof. We then measured expression of M2 genes, phagocytic activity, and mitochondrial respiration. Preliminary results have shown substantial effects of ApoE and IL-4 on all these parameters, notably, expression
of CD33 and TREM2, modulators of phagocytic activity and other genetic determinants of LOAD risk. Ongoing experiments seek to further characterize these effects.

CHED 462

Use of enhanced chemically defined media to improve uptake of L-telluromethionine by Escherichia coli DL41(DE3)

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In determining the three-dimensional structure of a protein, hurdles of x-ray crystallography can be overcome by incorporating unnatural amino acids into the protein of study. Most naturally occurring atoms do not have sufficient mass to diffract electrons. Incorporating unnatural amino acids containing a metalloid provides a solution to this problem. Bioincorporation of L-Telluromethionine can provide atoms with sufficient mass for electron scattering when incorporated serendipitously. However telluromethionine has cytotoxic effects which reduce cell growth and hinder uptake during protein synthesis. A proteomic analysis of telluromethionyl Escherichia coli was carried out using the methionine auxotroph E. coli DL41(DE3) (pCock) expression system. Both telluromethionyl and methionyl exposed cultures were analyzed with the objective of identifying differentially expressed proteins. The biological roles of differentially expressed proteins was elucidated and have been applied to improving methods for the bioincorporation of telluromethionine via the supplementation of chemically defined media with metabolites that were negatively affected due to the exposure to L-Telluromethionine.

CHED 463

Role of apoptosis in modulating effects of 2-aminoanthracene in pancreatic tissue of Sprague Dawley rat dams

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Modulation of the toxic effects of 2-aminoanthracene (2AA) on pancreatic tissue by apoptosis will be investigated. 2AA, also called anthramine, is a polycyclic aromatic hydrocarbon that is used in the manufacturing of chemicals, dyes, and inks, and it is also found in tobacco smoke and cooked foods. It is known to cause gene dysregulation, particularly of several genes of the pancreas that mediate protein and lipid metabolism (Gato and Means, 2011). To help determine the role of apoptosis in modulating the effects of 2AA, pancreatic tissue of Sprague Dawley rat dams exposed
to various concentrations of 2AA for during gestation through postpartum will be analyzed for apoptotic activity using TUNEL apoptosis assay. This will be followed by total RNA extraction. The activity of Casp3, which plays a central role in the execution phase of apoptosis, will also be analyzed via assay, and relative gene expression of specific apoptotic genes will be quantified using qRT-PCR to test for significant differences in gene expression.

CHED 464

Hepatic gene expression in pups exposed to 2-aminoanthracene in utero indicative of susceptibility to metabolic syndrome

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This project will find the effects of 2-aminoanthracene on the in utero pups after being ingested by the dams. The goal of this project is to determine if the same systemic injuries caused by 2-aminoanthracene on adult rats will also occur in the in utero pups after ingestion by their dams. This information is useful to determine the effects of pregnant humans ingesting 2-aminoanthracene. This could have effects on both the pregnant mother as well as her unborn child. These effects could last into adulthood and encourage or even cause insulin resistance or Type-II diabetes. This project will explore the histology, fatty liver, lipids, and genes expressed in the liver: SOCS1, SREBP1C, CD36, AMPK, PCK1, FASN, HNF4a, and PPARa.

CHED 465

Aliphatic protein side chain density correlates with phosphate crowding and helical curvature in protein/DNA crystal structures

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Sequence-specific binding of proteins to their DNA targets involves a complex spectrum of processes that often induce DNA conformational variation in the bound complex. The forces imposed by protein binding that cause the helical deformations are intimately interrelated and difficult to parse or rank in importance. To investigate the role of aliphatic protein side chains in helical deformation, we quantified the relationship between protein aliphatic residue density (CpH) and DNA phosphate crowding (Cpp). The correlation between CpH/Cpp was then calculated for a subset of 58 high resolution protein-DNA crystal structures. Those structures were sorted by direction of DNA helical curvature. Preliminary data suggests distinct roles of aliphatic side chain clustering around phosphate oxygens. Protein/DNA complexes containing concave helical curvature tend to have aliphatic protein residues closely associated with the crowded
phosphates (corr = 0.50) while complexes with convex helical curvature tends to have these residues around phosphate that are not crowded (corr = -0.45) Interestingly, complexes containing unbent DNA show little correlation between phosphate crowding and aliphatic residue density. Together these findings suggest an important role for aliphatic side chains in protein-DNA complexes involving helical curvature.

CHED 466

Protein purification and expression for glycine complex with rat estrogen receptor beta

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Estrogen is a hormone that controls sexual development and growth in the human body. Molecules that have similar structures to estrogen interact with estrogen receptors in ways that are not fully understood. Glycine is a phytoestrogen that has been shown to interact with estrogen receptors and negatively influence human health. Here we describe the isolation and purification the rERβ ligand binding domain (LBD) with the intent of complexing it with glycine for molecular structure determination and the elucidation of the structural changes that occur upon binding.

CHED 467

4T1 Murine breast cancer cell cytotoxins in Rumex crispus (Yellow Dock)

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Rumex crispus (yellow dock), an herbal remedy used in Turkey and the Far East, has been shown to possess anti-microtubulin, anti-inflammatory and antimalarial activity. It is used to treat constipation, diarrhea and eczema, and it has been shown to be cytotoxic and/or induce apoptosis in T47D, MDA-MB-231 and MDA-MB-436 breast cancer cells and other cancer cell lines. Studies in our laboratory have shown that plant species (e.g., Ginger, Turmeric) with anti-inflammatory activity have cellular components cytotoxic for 4T1 murine breast cancer cells. To our knowledge, the cytotoxicity of yellow dock against 4T1 cells has not been investigated. Yellow dock root powder was subjected to dichloromethane reflux (1 hr), and the resulting extract was resolved by Sephadex LH20 chromatography (75% ethanol). Fractions were pooled based upon UV-visible spectroscopic analysis (280 nm), and pooled fractions were assayed for 4T1 cell cytotoxicity (MTS assay). Pooled cytotoxic fractions were further characterized via HPLC (C₁₈, 0-75% methanol gradient over 30 min). Six HPLC peaks were identified as cytotoxic to 4T1 cells (MTS assay). None of the six peaks co-migrated with emodin or chrysophanol, known bioactive components of yellow dock.
Mass spectroscopic analysis (MALDI TOF) of the six HPLC is in shown in Table 1. None of the six HPLC peaks contained species that corresponded to emodin (270.24), chrysophanol (254.21), nepodin (216.13) or known bioactive anthroquinones. Further studies are underway to characterize these 4T1 cytotoxins.

<table>
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<th>HPLC Peak</th>
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</table>

CHED 468

Investigation of a HAD phosphatase from *Mycobacterium tuberculosis*

*Catherine Barnier*, barnier001@connect.wcsu.edu, Anne Roberts. Chemistry, Western Connecticut State University, Danbury, Connecticut, United States

*Mycobacterium tuberculosis* is the causative agent of tuberculosis. This infection of the lungs is responsible for between one to two million deaths annually, with multi-drug resistant strains generating concern for future treatment options. Although the genomes of several strains of *M. tuberculosis* have been sequenced, there are still many genes with unknown functions. These include members of the haloacid dehalogenase (HAD) superfamily, which are seen throughout all domains of life. Some thirty members have been putatively identified in *M. tuberculosis*. Approximately half of those enzymes have been designated as phosphatases, however, their *in vivo* substrates are not known. Rv3376 (NCBI Reference Sequence: NP_217893.1) is one of these phosphatases. This gene appears to be conserved across several strains of *M. tuberculosis* and yet has low homology to phosphatases in other bacteria. We will investigate the function of this enzyme by cloning, expressing, and purifying it and subjecting it to kinetic analysis.
Establishing RNAi in *Tribolium castaneum* at MSU Denver

**Chanda M. Lowrance¹**, clowranc@msudenver.edu, Emily Ragan². (1) Chemistry, Metropolitan State University Denver, Denver, Colorado, United States (2) Chemistry, Metropolitan State University Denver, Denver, Colorado, United States

RNA interference (RNAi) is a mechanism by which double-stranded RNA can trigger the degradation of mRNA with a matching sequence, leading to silencing of the gene. The target of this research is to inject double-stranded RNA into a red flour beetle, *Tribolium castaneum*, to trigger a change in its eye color. This double-stranded RNA will be a positive control used to help establish the use of RNAi in *T. castaneum* at Metropolitan State University of Denver. The gene responsible for eye pigmentation in *T. castaneum* is *vermillion*. The central part of this research is to successfully synthesize double-stranded RNA for silencing the *vermillion* gene. The research group is currently using a buffer solution of sodium phosphate and blue dye to establish a baseline for the volume of injection material. Furthermore, the group is establishing injection techniques to decrease the mortality rate of the beetles. Once the group has ascertained the appropriate methods and quantitative values necessary for the experiment to be efficient as possible, the injections of double-stranded RNA will commence.

Measuring the stability of iso-1-cytochrome *c* variants using heme spectra

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Heme-thiolate proteins are important biological molecules with functions that range from gas sensing to circadian rhythm regulation. Heme-thiolate proteins are characterized by a charged sulfur atom attached to the iron atom in the center of the heme prosthetic group. Cysteine and histidine typically serve as the axial ligands to the iron atom in these proteins. Heme-thiolate proteins also vary in their coordination scheme and can be penta- or hexa-coordinated. Proteins that are hexa-coordinated can often switch the ligand in the sixth position in response to changes in the protein environment. This ligand switching appears to be a regulatory function. The ultimate goal of this research is to build models of heme-thiolate proteins using yeast iso-1-cytochrome *c* (cytc). So far, mutations have been made to cytc to change stability and possible ligation schemes. We are interested in measuring the stability of the variants using guanidine hydrochloride denaturation and optical spectra in order to create titration curves. By analyzing the titration curves relative protein stabilities can be determined. This allows us to compare our model proteins with other known heme-thiolate proteins and investigate what role protein stability plays in the ligand switch process.
CHED 471

**Effect of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) on estrogen receptor beta and aryl hydrocarbon receptor using RT-qPCR**

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2,3,7,8-Tetrachlorodibenzo-p-dioxin (TCDD) is a toxic chemical formed through the manufacture of chlorinated phenols, primarily as a by-product of paper chlorination. This toxin is highly resistant to degradation and therefore easily accumulates in soil and groundwater. Previous research has shown that an amount lower than the concentration allowed in drinking water by the EPA is capable of decreasing estrogen levels. Estrogens lead to gene expression by binding to nuclear receptors. Expression of two target receptors, estrogen receptor beta (ERβ) and aryl hydrocarbon receptor (AHR), in luteinizing human granulosa cells were analyzed by quantitative real-time polymerase chain reaction (RT-qPCR), to explore where TCDD effects the expression of ERβ or AHR when cells were exposed to a concentration of TCDD 1000 times lower than the maximum amount of toxin legally considered safe.

CHED 472

**Investigating the mechanism of furfural inhibition in *E. coli***

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A current challenge in the production of biofuels from cellulosic biomass is to develop strains of *E. coli* that can be grown in the presence of toxins that are found in the biomass. Furfural is a cellulosic breakdown product that is found in processed biomass that is known to inhibit growth of *E. coli*. It has been suggested that furfural causes single-stranded DNA breaks in *E. coli*, membrane disruption of the cell, as well as an intracellular pH drop that all lead to cell death. In this study, we describe the isolation of genes from metagenomic libraries that appear to give tolerance to furfural using an enrichment cycle and a plate selection method. In addition, furfural interaction with a model cell membrane system was examined using the Langmuir Blodgett technique. Genes isolated from the metagenomic libraries to this date all contained aminoglycoside 3'-phosphotransferase, an enzyme that provides kanamycin resistance in the plasmid and not to furfural. Early studies suggest furfural does not affect the properties of the model cell membrane. Both experiments help gain understanding of developing strains of *E. coli* for biofuel production.

CHED 473

**Bacterial screening in search of novel pharmaceuticals**
Many biologically active compounds used as drugs are isolated from natural sources like bacteria. Three hundred new species of bacteria were obtained from the Great Salt Plains of Oklahoma. In order to screen for potential drug candidates, individual isolates were prepared and grown in liquid media. The bacteria were then pelleted by centrifugation and the supernatant removed for evaluation of biological activity by accessing cytotoxicity against mammalian tissue culture cells. Cells were treated with a fixed concentration of the supernatant overnight, followed by determination of cell viability using a resazurin based fluorescent assay measured on a plate reader. An initial screen of all bacterial supernatants was performed followed by confirmation of potential positives and determination of IC$_{50}$ values. Characterization of cytotoxic agent composition was carried out by evaluating size and susceptibility to inactivation by protease or heat treatment. Preliminary results indicate the biologically active compound(s) secreted by the bacteria are probably small organic molecules rather than large structured polypeptides.

**CHED 474**

**Fluorination of DNA aptamers through “Click Chemistry” synthesis**

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We are developing a condensed step procedure capable of attaching a tri-fluorinated molecule to an internally modified DNA aptamer. Simple detectability of the DNA aptamer as it binds its target is achieved with $^{19}$F NMR. Synthesis of non-DNA products have successfully formed triazoles between fluorinated terminal trifluorinated alkynes and azides, as well as fluorinated azides and terminal alkynes, via the click reaction. We will also report on our synthesis of the aptamer containing a fluorinated triazole group.

**CHED 475**

**Evaluating the expression levels of putative biomarkers in a panel of pancreatic cancer cell lines by qPCR**

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Pancreatic Cancer (PC) is a highly lethal disease with no reliable clinical markers for early detection, when the tumor is most readily surgically resectable. Patients with PC
have a five year survival rate of less than 5%. Predictive cancer biomarkers could serve as an invaluable tool for early detection of PC. A meta-analysis of pancreatic cancer microarray datasets has identified four genes, EPPK1, AHNAK2, IGHG3, and CTHRC1, as putative biomarkers for PC. The expression level of EPPK1 in a panel of pancreatic cancer cell lines were tested by qPCR to evaluate whether this gene was up-regulated. The expression level of EPPK1 was found to be up-regulated in four of the five cancer cell lines tested by qPCR, and preliminary data suggests AHNAK2 may also be up-regulated. The level of expression at the mRNA level gives indication that EPPK1 may be a promising gene for early detection of PC.

**CHED 476**

Probing the identity of the distal heme ligand in Cys80 variants of iso-1-cytochrome c

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Thiolate-ligated heme proteins contain a heme cofactor that is bound to a cysteine residue. Certain thiolate-ligated heme proteins can switch ligands upon reduction of the heme and this switch appears to be a method of regulation. In this research, several models of these thiolate-ligated heme proteins were made using yeast iso-1-cytochrome c. When the ferric absorbance spectra of the models were overlapped, shifts in the Soret band were observed. These shifts indicated different heme environments for the different model proteins. A variety of chemical and spectroscopic tests were performed to investigate the heme environment of the model proteins and the results of these experiments will be discussed.

**CHED 477**

Investigation of macromolecular crowding on ferredoxin and ferredoxin-NADP⁺ reductase kinetics

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Macromolecular crowding refers to the phenomenon in which biomolecular properties are altered due to high concentrations of macromolecules in an environment. In order to examine the putative effects of macromolecular crowding on biological redox reactions, the iron-sulfur protein ferredoxin (Fdx) and the FAD-containing flavoprotein ferredoxin-NADP⁺ reductase (FNR) from spinach were selected as a model system. Purification of the proteins from Spinacea oleracea was implemented through tissue homogenization...
and sonication followed by a series of chromatographic steps. With NADPH as a reductant, FNR is capable of reducing the dye dichlorophenolindophenol (DCIP) directly, and is also capable of reducing mammalian cytochrome c in a Fdx-dependent reaction. Steady state kinetics of cytochrome c reduction and DCIP reduction were measured using an NADPH-generating system. The polymers Ficoll and Dextran were utilized as model macromolecular crowding species at concentrations ranging up to 8%. Ovalbumin as a model protein crowding agent was also examined at concentrations up to 4%. Whereas the molecular crowding agents showed mixed effects on the rate of DCIP reduction, significant inhibitory effects were observed for the rates of ferredoxin-dependent cytochrome c reduction kinetics. Extent of inhibition was also dependent on the molecular weight of the crowding species.

CHED 478

RNA phosphoramidite monomer synthesis: An examination of phosphite selectivity improvement

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With the explosion of new research in the field of RNA, a significant demand for synthesis of oligoribonucleotides has materialized thus allowing the phosphoramidite method for oligomer synthesis to become a very valuable tool in biochemical research. As a result, the demand for synthesis of phosphoramidite monomers has increased. However, there is a lack of selectivity between the 2'- and 3'-OH groups in RNA for phosphite addition, resulting in a reduction in efficiency of synthesis. Silyl protecting groups have been developed to improve selectivity for the 2'-OH; however, in order to obtain the greatest utility, RNA monomer synthesis still must be streamlined. To this end, we have developed a structural analog of the 5'-OH dimethoxytrityl (DMT) protecting group, which while conjugated to an imidazole, aims to improve selectivity for 3'-OH phosphorylation via neighboring group participation. Synthetic methods for assembly of the protecting groups as well as computational models will be presented.

CHED 479

Detection of catecholamines using a paper-based microfluidic device

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This project focuses on the feasibility of developing a microfluidic assay for catecholamines. While there are three major catecholamines - dopamine, epinephrine and norepinephrine - this project focuses on assaying dopamine. When dopamine is present in the body at abnormal levels, it can have profound negative effects on the
body. Abnormal levels of dopamine are seen in diseases such as Parkinson’s. Current methods to detect catecholamines are long and tedious; developing a rapid and accurate method to quantify catecholamines would be an important step in medical diagnostics. Chemiluminescence of dopamine will be achieved using a luminol complex, a buffer and the dopamine solution. Chemiluminescence will be measured both with a fluorimeter and by visual inspection of reactions. The goal is to see if this assay is capable of measuring “unknown concentrations” of dopamine in a microfluidic environment consisting of filter paper with a hydrophobic region.

CHED 480

Analysis for genetic polymorphism of eastern Pacific bluefin and yellowfin tuna with microsatellite sequence PCR primers developed for Atlantic and western Pacific bluefin and western Pacific yellowfin tuna

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Two microsatellite repeat sequence PCR primers developed from Atlantic bluefin tuna (Thunnus thynnus thynnus), two PCR primers developed from western Pacific bluefin tuna (Thunnus thynnus orientalis), and three PCR primers developed from western Pacific yellowfin tuna (Thunnus albacares) were used to determine if they could detect genetic polymorphism for three bluefin tuna (BFT) and five yellowfin tuna (YFT) caught in the eastern Pacific off the coast of Baja California August 2012. DNA was extracted from frozen blood samples, subjected to PCR, subsequent gel bands were excised, and the extracted/purified gel band DNA was sequenced by GENEWIZ, Inc. Two of the three microsatellite PCR primers developed from western Pacific YFT and two of the four microsatellite PCR primers developed from Atlantic BFT indicated polymorphism for individuals within both eastern Pacific species. The other tested primers showed either no microsatellite repeat sequences or no polymorphism within or between tuna species.

CHED 481

Purification and expression of modified calmodulin protein (N-Cam.Y)

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Calmodulin from Homo sapiens is a small, α-helical protein that can be easily expressed in E. coli using standard protocols. When calmodulin binds to four calcium ions, it undergoes a conformational change that results in the exposure of hydrophobic pockets. Because of this increase in hydrophobic surface area, the protein binds with greatly increased affinity to phenyl sepharose, a hydrophobic resin, when in the
presence of Ca\(^{2+}\). This affinity to phenyl sepharose that is not as strong in other proteins, and therefore calmodulin can be used as part of a fusion system for the purification of other proteins as well. After the cell lysate containing the protein fusion system has been run over the resin, EDTA is added, which chelates the Ca\(^{2+}\) ions and allows the protein to fold back to its original conformation where the hydrophobic pockets are not exposed. The purified protein will then elute off of the column in a high concentration. We have used a fusion system similar to this one in the past to express two proteins that proved difficult to express otherwise. For this project, the N-terminus of a mutated calmodulin protein was used as the N-terminus of the fusion system; this variant is called N-Cam.Y. A proteolytic site was added between the N-Cam.Y and the protein of interest so that the calmodulin system can be cleaved off and removed after purification. We would like to compare this protein purification system, fused to a zinc finger protein and containing the protease site, to the current popular method using Ion Metal Affinity Chromatography (IMAC) systems. This purification process requires the use of a non-removable six-histidine tag on the C-terminus of the protein of interest, which we have shown can affect the structure, and therefore function, of certain proteins. We hypothesize that our system will result in a higher expression level of fusion protein, an ease of purification that is comparable to the current IMAC protocols, and no affect on the final protein produced because of the lack of the histidine tag.

CHED 482

Purification and characterization of *Bdellovibrio* derived \(\alpha\)-glucosidase, malA

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*Bdellovibrio Bacteriovorus* is a highly motile gram negative bacterium which preys on many other gram negative bacteria found in a wide range of environments. Its genome indicates a wide and varied arsenal of hydrolytic enzymes, many with unknown form and function. One such enzyme, mal A, was identified by sequence homology as a putative maltase, but the exact metabolic function of this enzyme is still unknown. Through purification and characterization of this enzyme it may be possible to gain insight on the as yet unknown metabolic role, or specific catalytic functionality provided by malA which causes its production in the bacterium. The enzyme was successfully overexpressed in *E.coli* and purified using ion exchange chromatography followed by hydrophobic interaction column chromatography. The activity of the enzyme is conveniently characterized using a synthetic substrate, 4-nitrophenyl \(\beta\)-D-glucopyranoside (\(K_M = 1.0\) mM) which allows the activity of the enzyme to be monitored photometrically. Initial characterization confirmed that the enzyme cleaves maltose as well as longer chain maltose oligomers. The enzyme is inhibited by, but does not cleave many \(\alpha\)-linked disaccharides (including isomaltose, palatinose, and trehalose), but is not
inhibited by the β–linked disaccharide cellobiose. The enzymatic cleavage mechanism was confirmed as stereoclectronically retentive by following p-NPG and maltose cleavage by \(^{1}\)H-NMR. The enzyme’s catalytic efficiency for maltose (k\(_{\text{cat}}/K_{M}\)) was determined to be 8.3x10\(^{5}\) M\(^{-1}\) sec\(^{-1}\) using enzyme concentration determined by active site titration with acarbose, a tight binding inhibitor with a Ki of ~2.0 nM.

CHED 483

Effects of floodplain silt on plant cell biochemistry

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Flood plains are made by a meander eroding sideways as they travel downstream. When a river breaks its banks and floods, it leaves behind layers of alluvium (silt). These gradually build up to create the floor of the flood plain and can contain 100 or even 1,000 times as many species as a river. The production of nutrients peaks and falls away quickly; however the surge of new growth endures for some time. This makes floodplains particularly valuable for agriculture. Plants have a stiff, rigid structure thanks to the plant cell wall, which is made up of three layers; the middle lamella is rich in pectins, the primary cell wall which is a thin, flexible layer, and the secondary cell wall which is a thick layer formed of primary cell wall after the cell is fully grown. The major carbohydrates involved in primary plant growth are cellulose, hemicellulose and pectin. Cucumis sativus is commonly used as a model to display plant vascular systems because they are fast-growing and produce large leaves which gives a large amount of material. Vascular plants have vascular tissue that allows for the distribution of nutrients which allows the plants to evolve to a larger size than non-vascular plants. Plants used for testing were grown in regular potting soil, as well as potting soil that was overlaid with a layer of silt collected from the Red River Valley in Spring of 2013.

CHED 484

Potential effects of betulinic acid on the formation of the calmodulin/CaMKKII complex

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Calmodulin-dependent Protein Kinase Kinase II (CaMKKII) is an important enzyme in the CaMKK/AMPK/CREB signaling pathway that ultimately results in suppression of hepatic glucose production through gluconeogenesis. This pathway is regulated by AMP-activated protein kinase (AMPK). CaMKKII is the upstream kinase that activates AMPK, and AMPK phosphorylation results in a cascade of enzymatic activity that leads to suppression of gluconeogenesis. CaMKKII must first be activated by calmodulin, a protein that does not have enzymatic activity. Once four calcium ions bind to
calmodulin, a conformational change occurs and it can activate CaMKII. Previous research concluded that betulinic acid, a pentacyclic triterpenoid which originates from the bark of *Albizia Julibrissin*, improved hyperglycemia through modulation of the CaMKK/AMPK/CREB pathway. The goal of this research is to determine if betulinic acid affects the interactions among calmodulin and CaMKII, shifting the equilibrium in favor of complex formation. By performing size exclusion chromatography and gel electrophoresis of calmodulin and CaMKII, while varying the concentration of betulinic acid, it is possible to separate the proteins based on molecular weight. This will allow for separation of the calmodulin/CaMKII complex from the individual proteins that do not form a complex. It can then be determined if the extent of complex formation varies as a function of the betulinic acid concentration.

CHED 485

2,3,7,8-Tetrachlorodibenzo-p-dioxin (TCDD) induces cell death in human granulosa cells

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2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) is classified as a polyhalogenated aromatic hydrocarbon (PHAH), compounds shown to have detrimental effects on reproduction and development. TCDD, found in herbicides and waterways, is primarily generated in the production of paper products. TCDD has been shown to negatively effect estrogen levels, and high concentrations of TCDD cause cell death, though by which pathway is not known. Autophagy induces cell death under a pathway mediated by lysosomes, while apoptosis leads to cell death via nuclear and DNA fragmentation. Both could in turn decrease estrogen production, lead to infertility in females, and promote cancer. In this study we attempt to determine which pathway is dominant by using RT-qPCR to examine how fM, pM, and nM concentrations of TCDD effect the expression levels of mTOR (autophagy) and Caspase-3 (apoptosis) in human granulosa cells (hGC).

CHED 486

Identification of genes involved in RQ₉ biosynthesis in *C. elegans* using RNAi knockdowns

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Approximately one in four people globally, and countless domesticated animals, are infected by parasitic helminths. Although infection by parasitic helminths has been largely eradicated in developed countries, parasitic helminths still exist as a public health problem in many third world countries. Parasitic helminthic infections in marginalized populations have been recognized to impede socioeconomic development, exacerbate poverty, and make infected individuals more susceptible to
infection by malaria and HIV/AIDS. Although antihelminthic drugs currently exist, many of these drugs are nonspecific, and may harm the host. This, concurrent with the increased cases of antihelminthic drug resistance, has made the search for new antihelminthic drug targets vital. Rhodoquinone (RQ) has been identified to be an excellent candidate for selective anti-helminthic drug therapy because it is used by parasitic helminthes, but not mammalian hosts. This is due to differences in the metabolic pathways between the host and parasite: mammalian hosts use ubiquinone (Q) as the main electron carrier in aerobic respiration; inside the anaerobic environment of the host, parasitic helminthes use RQ as the main electron carrier as part of the fumarate reductase pathway. To understand the biosynthesis of RQ in parasitic helminthes, Caenorhabditis elegans will be used as the model organism. Genes potentially involved with RQ production have been identified using bioinformatics, and are as follows: asns-1, asns-2, coq-3, coq-4, coq-5, coq-7, and nkat-1. The candidate genes were knocked down via RNAi feeding experiments. RNAi clones were transformed into Escherichia coli, which were then fed to C. elegans in liquid cultures. The lipids from each transgenic line of C. elegans were extracted, and the RQ content was analyzed via liquid chromatography – mass spectroscopy. Changes in RQ content in a transgenic population would indicate the gene’s role in RQ production, and provide a gene target for future studies.

CHED 487

Investigation of Nocardioides sp. metabolic, structural, biochemical properties, and its potential role in the sulfur cycle

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Stagnant seawater has a distinct odor that is generated by the microbial degradation of dimethylsulfoniopropionate, DMSP, to dimethylsulfide, DMS. This investigation began from the isolation of bacteria grown on DMS enriched media, which resulted in the identification of a novel Nocardioides species. Herein we report on the organism’s ability to metabolize DMS and dimethyl sulfoxide, DMSO, and thus elucidate its role in the biogeochemical cycling of sulfur. Furthermore, the percent meso-2,6-diaminopimelic acid contained within the cell wall of this halotolerant marine organism will be reported.

CHED 488

Investigation of the interference of extracted cinnamon components on the glucose oxidase-peroxidase test

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Several water-soluble components of cinnamon have been shown to interfere with the glucose oxidase-peroxidase test for glucose analysis. Methylhydroxychalcones (MHCP)
are components of cinnamon that may interfere with this test. Extractions, partitions, and chromatography have been used to isolate and separate the MHCP’s and other cinnamon components from cinnamon. The interference of the fractions on the glucose-oxidase-peroxidase test was then measured. The aqueous fractions showed the greatest interference with the glucose test. The components in the aqueous layer were further separated and tested for interference with the test and analyzed with GC/MS.

CHED 489

Screening an enaminone library for histone deacetylase inhibitors

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Histone Deacetylase (HDAC) catalyzes the removal of acetyl groups from lysine amino acids in proteins. HDAC is a popular drug target because it regulates histone association with DNA, which in turn plays a key role regulating gene expression in normal and diseased states. An enaminone library was previously generated using a novel synthesis method to accelerate the Eschenmoser coupling reaction with sonication. Because some enaminones are biologically active and can be used as anti-inflammatory, antibiotic, antitumor, and/or anticonvulsive medications, we screened the library for HDAC inhibitors. This was accomplished using an HDAC Glo I/II assay, in which the enzymatic removal of an acetyl group by HDAC generates a substrate for luciferase, resulting in the emission of light that can be quantified. Mammalian tissue culture cells were utilized as the source of HDAC activity. Two possible inhibitors were found in the enaminone library. Current efforts are directed at characterizing these inhibitors and determining their mechanism of action.

CHED 490

Improved model to predict the free energy contribution of dinucleotide bulges to RNA duplex stability

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The ability to accurately predict the 3D structure of RNA relies upon an in-depth model that accounts for unique structural motifs in the secondary and tertiary structure. Current algorithms utilize the free energy of nearest neighbors to calculate the secondary structure based on sequence. Dinucleotide bulges in RNA are one structure that is commonly found in nature, yet there is little data concerning their thermodynamic parameters. Current models assign a free energy penalty of 2.8 kcal/mol for all
dinucleotide bulges, regardless of their sequence. Short RNA duplexes containing dinucleotide bulges of different sequences and with different nearest neighbor combinations were optically melted. From these melts their thermodynamic parameters (enthalpy, entropy, Gibb’s free energy, and melting temperature) were determined. This thermodynamic data was utilized to create an updated model to predict the free energy contribution of dinucleotide bulges. This sequence dependent model assigns free energy penalties based on the sequence composition of the bulging nucleotides (two purines, two pyrimidines, or one of each). The predictive model also includes a penalty for an A-U pair and a bonus for G-U pair adjacent to the bulge. The new sequent dependent model results in predicted values that are within 0.18 kcal/mol of the experimental values; a significant improvement over the sequence independent model. This new experimental data and updated sequence dependent model can be utilized by algorithms that predict RNA free energies as well as those that use free energy minimization to predict RNA secondary structure from sequence.

CHED 491

Challenges in visualizing RecA-DNA interaction in chemiluminescent electrophoretic mobility shift assays

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A high-end DSLR camera was employed for analysis of protein-DNA interaction using chemiluminescent electrophoretic mobility shift assays (EMSAs) in order to study binding affinity of DNA repair protein, RecA, and selected Mycobacterium tuberculosis oligomers. This alternative method for EMSA visualization offers a low-cost benefit over using a phosphorimager with radioactively labeled DNA. Mini-format chemiluminescent, fluorescent, and large-format chemiluminescent EMSAs were used to determine percent RecA binding. Decrease in free DNA signal indicates RecA did bind to DNA, though a bound DNA band was not resolved in any of the three types of EMSAs. Future research will involve further examination of this protein-DNA interaction in order to determine why the complex is not migrating into the EMSAs.

CHED 492

Analysis of rhodoquinone production in knockout strain candidates in Rhodospirillum rubrum

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Currently, the World Health Organization estimates over two billion people are afflicted with parasitic helminth infections. However, in recent years these parasites have become increasingly resistant to modern antibiotics, both in humans and in livestock. Therefore, the need to elucidate a novel drug target is of utmost importance. One such target that is currently under investigation involves an alternate metabolic pathway that is utilized by the parasitic helminths under anaerobic growth conditions. In the fumarate reductase pathway, the parasites use rhodoquinone (RQ) as an electron carrier to reduce fumarate to succinate for the production of ATP. Since RQ is required for this pathway to function, and mammalian hosts do not utilize this pathway, RQ biosynthesis is a novel drug target. Mammalian hosts use a similar molecule, ubiquinone (Q), for electron transport in the aerobic respiratory chain. To examine the RQ biosynthetic pathway, this study used Rhodospirillum rubrum as a model organism since it also requires RQ to survive under anaerobic growth conditions. From previous experiments, it was shown that RQ can be synthesized in R. rubrum from ubiquinone (Q) in vivo. It was also discovered that the biosynthesis of RQ utilizes rquA, a gene which encodes for a putative methyltransferase. Further studies have compared anaerobic/aerobic mRNA expression levels of rquA to identify additional gene targets, since the RQ biosynthetic pathway likely requires additional enzymes. Currently, Rru_A3231, Rru_A1274, and Rru_A1729 are being examined. This project involves the knockout of these genes from the R. rubrum genome through homologous recombination, followed by quantitative analysis of RQ production by LC-MS and comparison to wild-type R. rubrum.

CHED 493

Rhodium(II) metallopeptides as a structural platform for selective Abl tyrosine kinase inhibition

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An oncogenic variant of the Abl tyrosine kinase, Bcr-Abl, is strongly associated with chronic myelogenous leukemia (CML). For this reason, Abl tyrosine kinases are potentially important therapeutic targets. While inhibitors of Bcr-Abl already exist for treating CML, they are not effective in all cases. As a result, new methods of targeting Abl tyrosine kinases are needed. This study expanded upon a novel method of using rhodium(II) metallopeptides to gain molecular specificity for specific protein targets. In particular, rhodium(II) metallopeptides were explored as selective ligands for targeting the SH3 domain of Abl. The metallopeptides developed harness a combination of inorganic and non-covalent protein-peptide interactions to achieve highly specific affinity. Two metallopeptides were developed based on the sequence APTYSPPPP which was reported to have a $K_d$ of 400 nm for Abl SH3. One of the metallopeptides developed, $p40$-$A1E^{Rh}$ ($E^{Rh}$PTYSPPPP), was found to have a $K_d$ of less than 22 nM for Abl SH3 by isothermal titration calorimetry. This is a significant improvement in affinity compared to the parent peptide and could potentially be leveraged to develop
potent inhibitors for the oncoprotein Bcr-Abl. The general design employed in this study could also be translated to other important therapeutic targets as well.

CHED 494

Investigation of the change in expression of neuropeptides with gluten free based diets

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In recent years, proteomics has uncovered ways to link the expression of neuropeptides with a change in diet. However, gluten-free diets, which often results in a change in grain based diets, require additional investigation. A growing portion of the American population has been proven to suffer from celiac disease, representing a subsection of the growing health concern related to gluten sensitivities. The purpose of this study is to identify a possible relationship between the amount of gluten introduced into a mouse model, and the resulting effect on the expression of neuropeptides. The study conducted separated twelve mice into three groups of four, containing gluten free (n=4), standard (n=4), and mixed (n=4) diets. The mice were given ad libitum, the ability to eat as much as desired, access to chow and water, and weighed weekly for a six week period. At the end of the six week period the mice were sacrificed and a resulting analysis of brain tissue was conducted measuring the expression of neuropeptide Y using a HPLC as a means to quantify a general elution profile, and a resulting follow up with a GC mass spectrum to identify and isolate neuropeptide expression.

CHED 495

Role of aspartic acid 101 in E. coli alkaline phosphatase architectural activity and stability

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Alkaline phosphatase serves an important cellular and commercial role as a highly stable, phosphomonoesterase that cleaves a wide variety of substrates to yield inorganic phosphate. Interestingly, previous mutants of the active site residue aspartic acid 101 in E. Coli alkaline phosphatase have shown increased activity with no affect on substrate binding promiscuity. To test if the D101 mutation yields an increase in active site flexibility and, hence, greater product release, we introduced an alanine at this position in the E. Coli enzyme and tested phosphomonoesterase activity and tungstate inhibition at pH 8.0 and 5.5. At an optimal pH (8.0) for activity, D101A velocity was increased and inhibition was decreased; however at pH 5.5 all enzymatic activity was knocked out relative to wild type. These pH dependent changes in activity and inhibition
suggest that aspartic acid 101 plays an important role in enzyme stability and/or deprotonation of the active site serine 102 nucleophile.

CHED 496

Increasing the activity of E. coli alkaline phosphatase through a structurally destabilizing mutation

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Alkaline phosphatase is a ubiquitous, phosphomonoesterase that produces free inorganic phosphate required for cellular uptake and use. In addition to the E. coli alkaline phosphatase, there are four isozymes found in humans with variable activity and sequence homology to the bacterial phosphatase. The most significant sequence homology is found in the active site; however small variations in active site sequence do exist and are thought to be related to changes in structural stability, enzyme efficiency, and chemical mechanism. For example, in a variety of mammalian intestinal alkaline phosphatase, position 100 consists of a proline residue instead of the E. coli threonine. Interestingly, it has been demonstrated in past experiments that mammalian alkaline phosphatase has higher activity and a higher optimal pH for activity. These results are not surprising given the proximity of this residue to the active site nucleophile, serine 102. To test the effects of this evolved sequence change on both activity and structural stability, a single point mutation in E. coli alkaline phosphatase was made replacing threonine with proline (T100P). This mutant enzyme showed increased activity and, interestingly, a decrease in stability relative to wild type. These results suggest that the introduction of the hindered proline residue yields a change in active site architecture that results in improved release of product and a potential change in the rate-determining step for phosphomonoester cleavage.

CHED 497

Why taking your vitamins is essential: The importance of architecture in metabolite sensing by the B$_{12}$ riboswitch

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Recently discovered, RNA riboswitches are critical, ubiquitous regulators of cellular metabolism and, as such, are important, new targets in therapeutic design. Like many metabolite binding proteins, these riboswitches regulate gene expression through negative feedback loops that are sensitive to metabolite concentration. For example, the coenzyme B$_{12}$ riboswitch, in E. coli, binds excess coenzyme B$_{12}$ metabolite (adocobalamin) and then represses translation of the downstream, encoded cobalamin-
transport protein that is required for cellular uptake of the metabolite. Like many protein regulators, this RNA riboswitch undergoes large structural changes upon metabolite binding blocking ribosome binding and, thus, protein synthesis. Using the coenzyme B\textsubscript{12} riboswitch as a model system for understanding the architectural requirements for metabolite sensing and gene regulation, we have generated a suite of \textit{thermatoga maritima}, B\textsubscript{12} riboswitch RNAs. Using a variety of sequence and structural alignment tools we have identified thermophilic, B\textsubscript{12} riboswitch RNAs that vary in total length and sequence at both the 5' and 3' ends. Due to the thermal stability of these designed B\textsubscript{12} riboswitches, small changes in sequence should yield changes in architectural stability and metabolite binding, thus providing a clearer picture of structural binding requirements when compared to the previously studied \textit{E. coli}, B\textsubscript{12} riboswitch.

**CHED 498**

**Peptides designed to target G-quadruplexes for transcriptional and translational regulation**

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G-quadruplex structures occur in guanine-rich sequences in various DNA and RNA molecules. These G-quadruplexes are often found in telomeric and regulatory regions of oncogenes, and because of this, G-quadruplexes have become a target of study in anticancer therapeutics. G-quadruplexes are also involved in regulation of transcription and translation when present in certain regions. Small molecules or peptides synthesized to specifically recognize the G-quadruplex structure could display anticancer activity or may regulate transcription or translation. To explore these possibilities, peptides were designed and synthesized to mimic some small molecule inhibitors which were previously reported in the literature and have been demonstrated to inhibit RNA G-quadruplex translation. Binding affinities of the interactions between the peptides and various G-quadruplexes will be determined using Isothermal Titration Calorimetry (ITC). The secondary structures of the peptides will be determined using circular dichroism spectroscopy (CD). Progress toward these goals will be reported.

**CHED 499**

**Biobased composites produced from collagen and vegetable oil polymers**

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A bio-based composite will be produced utilizing collagen and a vegetable oil polymer. Because of collagen’s high tensile strength and its bio-availability, it is thought to be a good source in producing a high-strength composite. Collagen has been purified from bovine tendon following a standard purification protocol. Collagen-based peptides have also been synthesized via solid-phase peptide synthesis using sequences which mimic
those of type I collagen. Mimics of the collagen triple helix will be produced via common equilibration techniques. Circular dichroism spectroscopy (CD) will be utilized to determine the structure and thermal stability of the synthesized collagen mimics as well as the natural protein. The CD data will confirm that the synthesized collagen exhibits the known triple helical structure. Once all samples are characterized, they will be integrated into the vegetable oil polymer and will have their mechanical properties tested. Progress made toward these research endeavors will be reported.

CHED 500

Peptides designed as mimics of NF-κB for transcriptional regulation

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Nuclear factor-kappa B (NF-κB) is a common transcription factor that is highly regulated and has been implicated in several physiological processes. These include its role in development, inflammation, immune reaction, cell death, and other biological processes. NF-κB regulates the expression of various proteins by binding specific κB DNA sites. Studies have shown that overexpression of the brain derived neurotrophic factor (bdnf) gene can result in epilepsy. The aim of this project will be the synthesis of peptide inhibitors that mimic NF-κB and bind the κB DNA selectively. Development of an inhibitor may lead to modification in gene expression to prevent overexpression of BDNF. Peptides will be produced by solid phase peptide synthesis and then purified via HPLC. Fluorescence binding studies will be conducted to determine the peptide binding affinities for the DNA, and structural studies will be completed using circular dichroism. Progress towards these results will be reported.

CHED 501

Analyzing exonuclease-induced hyperchromicity by UV spectroscopy: An undergraduate biochemistry laboratory

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The hyperchromic effect is the increase in UV absorption seen in double-stranded DNA upon denaturation of the DNA strand. The effect can be seen by either heating the DNA, altering the pH, or adding a nuclease. A laboratory experiment based on the nuclease-induced hyperchromicity of DNA was developed. This experiment is primarily suitable for undergraduate biochemistry courses. The maximum wavelength of the DNA (λmax) is first determined by using a standard UV-vis spectrophotometer to analyze the DNA sample in buffer appropriate to the enzyme being used. A kinetic scan is then performed at this λmax, where the nuclease is added to the solution and the absorbance at the selected wavelength is followed. Because of the hyperchromicity of
the sample after nuclease activity is induced, an obvious, permanent increase in absorbance is expected. The conditions for the experiment are being adjusted to scale up the experiment for use in the undergraduate biochemistry lab, but preliminary results have shown that an increase in absorbance of anywhere between 10-100% can be seen. This lab is useful because it demonstrates the role of hydrogen bonding in DNA structure as well as the inaccuracy of DNA concentration measurements without considering hyperchromicity. The results can be tied in to discussions involving when accurate concentration measurements are important in research settings, such as in protein-DNA binding assays or PCR. Comparisons can be made to the lack of hyperchromicity upon digestion of a true single-stranded DNA (one that exhibits no intrastrand interactions); should the instructor wish, online software suites can be introduced that will allow the students to predict whether selected single-stranded DNA will have secondary structure and therefore whether they will exhibit hyperchromicity after nuclease activity.

CHED 502

Characterizing the aggregates of a mutant Alpha 1-Antitrypsin protein associated with Alpha 1-Antitrypsin Deficiency

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This project focuses on characterizing the aggregates of a mutant Alpha 1-Antitrypsin protein associated with the disease Alpha 1-Antitrypsin Deficiency. Alpha 1-antitrypsin is a serine protease inhibitor that is crucial in the normal functioning of both the liver and the lungs. It protects the lung tissue from being damaged by proteases that work in the lung tissues to break down foreign invaders that cause infection. The protein contains 4 beta sheets that are hypothesized to be involved in the aggregation process. My goal is to characterize the structure of the monomers that make up the aggregates associated with the disease. Alpha 1-antitrypsin is expressed as a GFP fusion protein in the model organism, \textit{C. elegans}. The proteins are extracted using a GFP affinity column; the GFP is cleaved after purification through the column. Size exclusion columns and native gels are being used to estimate the size of the mutant monomer; this will provide insight into whether the mutant forms a partially folded or completely unfolded protein that then forms aggregates.

CHED 503

Analysis of lipid membrane content in dynamic environments

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Abiogenesis is the process by which living organisms arise naturally from non-living matter. There is only evidence for a single occurrence of this, represented by all life on Earth. To determine the mechanism for abiogenesis, smaller steps need to be elucidated before understanding the whole. One such step is the compartmentalization of life from the environment.

One of the simplest membrane forming materials is a group of amphiphilic molecules called fatty acids. Changes in aqueous environments like dilution from precipitation, influx of metabolic components and ionic compounds, or acidity changes could all affect the membrane composition and protocell morphology. We examined the equilibrium between free monomers in solution and aggregates using equilibrium dialysis to separate the two phases and analyzed the phases with gas chromatography after methylation of the fatty acids. The results are similar to results from critical vesicle concentration measurements, but show directly the concentrations of solubilized monomer. The effects of changing the environment on this equilibrium were also tested. Increasing ionic strength shifted the equilibrium towards aggregates, while increasing the temperature shifted the equilibrium towards monomers. These results illustrate the importance of environment in generating stable structures for the origins of life.

CHED 504

Investigation of bi-substrate enzyme kinetics for the introductory biochemistry lab

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Glutathione S-Transferase (GST) is a bi-substrate enzyme that plays an important role in drug detoxification. The enzyme’s activity is measured by colorimetric methods using 1-chloro-2,4-dinitrobenzene (CDNB), which is well suited to quantitative monitoring in real time using visible absorbance spectrometry. The conditions of this assay as previously employed in the Introductory Biochemistry Lab at Sacred Heart University were poorly suited to large scale kinetic analysis. Here, we are developing a tractable and highly reproducible large scale kinetic assay that is based on the CDNB method. We are also optimizing the conditions of this assay so that it can be applied within the educational environment and we are determining the optimal conditions for kinetic analysis to investigate the kinetic mechanism of GST. As a transferase, GST adopts an enzymatic mechanism that is thought to require at least two substrates: glutathione, and the target compound to which it is transferred (various drugs, or other metabolites). Over the course of our project, we will seek to investigate the enzymatic mechanism by which GST transfers glutathione onto its conjugation target, which in our research is CDNB.
**CHED 505**

Determining the function of Coq4 in *S. cerevisiae* coenzyme Q₆ biosynthesis via biochemical and genetic screening of Coq4 suppressors

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Coenzyme Q (ubiquinone or Q) is a lipid electron carrier in the electron transport chain. *COQ4* is identified as one of the eleven yeast *Saccharomyces cerevisiae* genes essential for Q biosynthesis. Though its function is uncharacterized, the gene product of *COQ4* is a peripheral protein associated with the inner mitochondrial membrane on the matrix side. Coq4 is also required for the stability of the CoQ-synthome, a high molecular mass Coq polypeptide biosynthetic complex. Previous studies have characterized two *coq4-1* yeast point mutants unable to synthesize Q. This project aims to characterize the function of Coq4 by examining potential suppressor proteins that interact with the Coq4 polypeptide in vivo and correct the Q biosynthetic defect present in the *coq4-1* point mutant. Each of the revertants retain the original mutations present in the parent strain as confirmed by PCR, but can grow in medium containing nonfermentable carbon source and produce detectable amounts of Q₆ as assayed by LC/MS-MS. Identification of revertants may proceed by mapping and separating the genetic complementation groups of the revertant strains. We hope to identify via molecular genetic approaches the synthetic interaction between the suppressors and the Coq4 polypeptide.

**CHED 506**

Effects of deletion of the Rru_A3004 gene on rhodoquinone biosynthesis in *Rhodospirillum rubrum*

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Helminths are a class of parasitic worms that are the cause of debilitating infections of 1 in 4 people globally. They are especially prevalent, and thus a larger problem in developing countries. Medications that are being used to treat helminth infections do not specifically target the parasites, and cause undesirable side-effects to mammalian hosts. The need for new drug therapies for parasitic helminth infections is crucial, as resistance to existing medications has been observed in animal infections, and is predicted to soon be a major issue in human infection cases. The Shepherd Lab is investigating the biosynthesis of rhodoquinone (RQ), which is produced in parasitic helminths, but not in mammals (the hosts of parasitic infections). RQ is a required electron carrier in the fumarate reductase pathway in parasites that is utilized during
anaerobic growth while inside hosts. A novel drug therapy would target and inhibit the synthesis of RQ, thus specifically harming helminthes, but not their mammalian hosts. In order to inhibit RQ biosynthesis, the genes that are involved in RQ production must first be identified. To identify a potential gene target involved in RQ biosynthesis, gene candidate Rru_A3004 was selected in Rhodospirillum rubrum using RNAseq and bioinformatics. This gene was knocked out via homologous recombination to create a deletion mutant, and RQ levels in lipid extracts from the knockout were determined using LC-MS and compared with wild-type R. rubrum RQ levels. If gene Rru_A3004 is involved in RQ biosynthesis, significantly lower levels of RQ in the deletion mutant are expected when compared to wild-type, making Rru_A3004 a viable gene target for future potential drug therapies.

CHED 507

Characterization of a human orphan G-protein coupled receptor, GP133

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Of the approximately 900 human G-protein coupled receptors (GPCRs) that have been cloned, the agonists of only 300 have been identified, consequently the remaining 600 are termed "orphan receptors." The human orphan GPCR, GP133, is classified as an adhesion receptor due to conserved structural characteristics. It displays significant homology to four GPCRs from the slime mold, Dictyostelium discoideum that initiate and govern the developmental pathway of the organism. The D. discoideum GPCRs bind the extracellular agonist 3',5'-cyclic adenosine monophosphate (cAMP) initiating the signaling pathway that results in increased intracellular cAMP. Given GP133's homology to the D. discoideum GPCRs and its classification as an adhesion receptor, it is possible that GP133 is activated by extracellular cAMP, initiates the same intracellular pathway and may play a similar role in human development. Initial experiments suggest that GP133 may be activated by cAMP and adenosine but not 5'-AMP, resulting in the synthesis of intracellular cAMP.

CHED 508

Prefractionation of natural product extracts provides a value added resource for high-throughput anticancer screening applications

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Natural product extracts are known to be valuable for the discovery and production of potential pharmaceuticals. However, crude extracts present many challenges for biological testing, such as cytotoxicity, due to the extract containing a complex mixture
of compounds. Using solid phase extraction, solvents of varying polarity produce unique fractions. These fractions allow natural products components to be separated and screened more efficiently for their potential use as an anticancer agent. The Molecular Target Laboratory (MTL) has fractionized over 22,000 natural products consisting of over 120,000 fractions which comprise the Molecular Target Laboratory Screening Library of Prefractionated Samples. Fractionalized products are tested in high-throughput screening applications for their respective biologically activity. Following screening of fractions it has been found that 10-30% of the samples which showed no indication of biological activity in their crude state exhibited measurable activity in one of their respective fractions following prefractionation. Prefractionation has proven a beneficial technique for effective evaluation of natural product extracts used in high-throughput anticancer screening applications.

CHED 509

Engineering of metalloenzymes with stacked metalloporphyrin dimers

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The design of more efficient artificial catalysts for oxygen reduction is important in fuel cell technology. Nature uses multi-nuclear transition metal complexes to catalyze this four-electron redox reaction in cytochrome c oxidase, which functions in aerobic respiration. HmuT is a heme-binding protein that was recently discovered to transport up to two hemes for translocation into the cytoplasm of Yersinia pestis. The hemes are stacked in close proximity with a metal—metal distance of 4.2 Å, similar to synthetic dicobaltporphyrin complexes with stacked cobalt porphyrins that act as functional mimics of cytochrome c oxidase. The hemes in HmuT are bound via histidine and tyrosine side chains, which act as axial ligands to the heme. Due to its ability to bind two stacked hemes, HmuT is being used as a template for metalloprotein engineering, with the goal of designing a metalloenzyme with a dinuclear metalloporphyrin active site not found among naturally occurring enzymes. Metal substitution with manganese or cobalt and site-directed mutagenesis of the axial ligands were performed on the HmuT template, testing the metal and axial ligand dependence on metalloporphyrin binding stoichiometry, binding kinetics, and electrocatalytic activity of the reengineered multinuclear metalloprotein active sites.
The heme-binding site of HmuT from *Yersinia Pestis*, which is being reengineered via metal-substitution and site-directed mutagenesis of the histidine and tyrosine side-chains.

**CHED 510**

**Pedagogical innovation: Using 3D printer technology in an undergraduate biochemistry course**

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Additive manufacturing, commonly known as 3D printing, is an excellent method for fabricating 3D models of structures and is gaining popularity in undergraduate education. Undergraduate biochemistry students often struggle with visualizing three-dimensional proteins using two-dimensional structure models. Thus, biochemistry students can potentially benefit from the innovative pedagogy of 3D printing, which provides tangible three-dimensional models. The presented research investigates the use of 3D printing in an undergraduate biochemistry course as a mechanism to enhance the understanding of protein structures that could once only be taught in a two-dimensional view. Course activities have been designed and implemented to investigate the ability of students to more easily connect basic protein structure concepts. The results showed that 3D printing was able to facilitate biochemistry learning and students enjoyed the process of interacting with 3D protein models.

**CHED 511**

**Characterizing HIV-specific CD4 T cell targeting and proliferation among HIV controllers**

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The human immunodeficiency virus (HIV) has grown into a world-wide epidemic due to its effective attack on the human immune system, particularly CD4 T cells. As researchers better understand HIV and its interactions with the host, different host classes have emerged based on disease outcomes. The controller class, which tends to control infection to the point of delaying or completely avoiding the progression to AIDS in the absence of anti-retroviral therapy, can be further divided into elite controllers and viremic controllers (elite controllers having even better disease outcomes than viremic controllers). The differences in the CD4 T cells of these two controller classes are of particular interest in HIV vaccine development. In this experiment, the proliferation capacity and the peptide targets of ENV- and GAG-specific CD4 T cells taken from viremic and elite controllers were compared. While no differences in peptide targeting or proliferative capacity were detected between elite and viremic controllers, striking differences in response breadth and proliferation between GAG- and ENV-specific CD4 T cells were observed. When looking at proliferation, it was seen that 7.1% of ENV-specific CD4 T cells proliferated, a significantly higher percentage than the 1.6% seen for GAG-specific CD4 T cells (p=.0069). Also, the response breadth of GAG-specific CD4 T cells was significantly higher with an average of 4.8 responses compared to the 1.9 ENV responses (p=0.0128). While these results were surprising, they provide novel insights into the immune responses of HIV controllers.

CHED 512

Characterization of the haloalkane dehalogenase, DccA

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Haloalkane dehalogenases (HLDs) are enzymes that catalyze the cleavage of a carbon-halogen bond, which yields a proton, halide, and an alcohol. These family members tend to possess broad substrate specificities and have been demonstrated to have numerous industrial and environmental applications. Characterization of novel HLDs is of interest because the substrate specificity patterns depend more on the structure of the binding pocket, access tunnels, and position of catalytic residues, than on evolutionary patterns. A previously uncharacterized HLD, dehalogenase A from Caulobacter crescentus (DccA), had been identified. DccA demonstrates activity on a variety of halogenated substrates, with its best substrate being 1-bromobutane. The crystal structure of DccA was solved to a 1.5 Å. Characterization of DccA will expand the HLD enzymatic toolbox for the growing number of applications while improving understanding of the sequence-structure-substrate-specificity relationship within this enzyme family.

CHED 513

Determination of aggregation equilibrium of fatty acid vesicles using gas chromatography with flame ionization detection
In aggregation behaviors, there is an equilibrium between the solubilized monomers and the aggregated complexes, including self-assembled fatty acid vesicles. Previous experiments show that the concentration of fatty acid required to form vesicles is dependent on hydrophobicity of the fatty tail, ionic strength, and pH of the solution. Initially, fatty acids from 6 to 12 carbons were tested individually to determine the equilibrium between solubilized and aggregated fatty acid. Mixtures of chain lengths were then tested to determine effects of more complex and realistic systems. Aggregates were separated from the solubilized fatty acid using size dependent separations, such as equilibrium dialysis. After separation of aggregates from solubilized fatty acids, the fatty acids were derivatized in order for them to be sensed by gas chromatography with flame ionization detection (GC-FID). Fatty Acid Methyl Ester (FAME) derivatives were created using a Fischer esterification. Fisher esterification is a standard organic reaction, in which a fatty acid was heated in the presence of methanol and sulfuric acid to produce FAME. Fatty acids alone have too low of a vapor pressure to be characterized by GC, however the FAME is ideal for GC characterization. FID detection is quantitative and, in conjunction with an internal standard, gave reproducible concentration information for FAME. Generally FAMEs are made from biological lipids, which are longer and have some unsaturated hydrocarbon chains. The method used was developed for shorter chain fatty acids.

CHED 514

Designing small molecule autoinducers for investigation into the binding pocket of LasR

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Pseudomonas aeruginosa (P. aeruginosa) is a gram-negative nosocomial bacteria species that targets patients suffering from immune-compromising diseases, such as AIDS, cystic fibrosis, cancer, and severe burns. It utilizes density-dependent quorum sensing (QS) signaling pathways to produce virulence factors and biofilm, a major component of antibiotic resistance. While there are multiple QS pathways utilized by P. aeruginosa, the focus of this paper is on the las pathway, due to its importance in the regulation of other QS pathways and biofilm production. The LasR receptor binds with the natural autoinducer (AI), 3-oxo-dodecanoyl homoserine lactone (3O-C12-HSL), to initiate the production of virulence factors. The goal of this research is to use synthetic AIs to bind with LasR and regulate production of virulence factors. A synthetic tri-phenyl
molecule, TP-1, known as an effective AI, has been used to gather insight into the binding site of LasR. The TP-1 molecule is comprised of a brominated core phenyl ring with two adjacent phenyl rings containing electronegative R-groups NO\textsubscript{2} and Cl. The synthetic AIs in development are based on the TP-1 scaffolding, and contain electronegative R-groups on the adjacent phenyl rings. The five-step synthesis of the core molecule [(3,5-dibromo-2(methoxymethoxy)phenyl)methanimine] of TP-1 has been completed. Using the core molecule, development of the TP-1R molecule and a library of other synthetic autoinducers is underway. Regulation of QS activity in *Pseudomonas aeruginosa* will be analyzed using a LasR GFP reporter assay. As the library is developed, a structure-activity relationship study will be conducted, guiding the design for future analogs.

**CHED 515**

**Acute and chronic effects of somatostatin on fast and slow calcium oscillations in the pancreatic β-cell**

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It is known that insulin secretion oscillates in the presence of glucose. There have been two types of calcium oscillations observed: fast and slow. It is known that somatostatin (SST) inhibits insulin secretion, but it has been found to have differential effects on fast vs. slow oscillations. It was hypothesized that chronic SST would increase the glucose sensitivity of islets by inhibiting insulin release overnight and thus cause the internalization of K\textsubscript{ATP} channels from the plasma membrane of the beta cell. To test this, calcium imaging was used to compare the effects of SST treated vs. untreated cells while varying acute concentrations of glucose. When islets were acutely exposed to SST, it was found that slow oscillations and fast oscillations were differently effected. These results indicate that the mechanism of the fast and the slow oscillations is different. Understanding pancreatic oscillations is critical, because patients with type 2 diabetes show irregular Ca and insulin oscillations.

**CHED 516**

**Effects of creatine supplementation on serum testosterone response in *Mus musculus***

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Creatine is a nitrogenous organic acid compound produced within the liver that, in turn, supplies energy to a variety of cells in the body, specifically the muscles. A study has shown the consumption of creatine with exercise (swimming) had an increase in
testosterone serum levels, decrease in serum cortisol, and no response in growth hormones. The purpose of this study was to determine if creatine supplementation without exercise would give a similar response. Twenty-three CD1 male mice were used in this seven-week experiment. One group (n=5) consumed creatine monohydrate (CMH) but did not exercise; the second group (n=7) consumed CMH and exercised; the third group (n=5) did not consume CMH but did exercise while the fourth group (n=6) did not consume CMH and did not exercise. The exercised mice were on a workout schedule like that of a typical human, consisting of a five-day schedule of ten minutes of swimming each day. Serum was collected at three different points in time: week 0, week 3, and week 7. These sera were tested through ELISA for testosterone response and compared between groups and within group (by week) and over the seven-week treatment. Through ANOVA and post-hoc testing, significant differences were found in the levels of the testosterone throughout these 7 weeks.

CHED 517

Construction of a *Burkholderia cenocepacia*-specific gene replacement vector

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*Burkholderia cenocepacia* is a gram-negative bacteria that is a part of the *Burkholderia cepacia* complex. These bacteria are opportunistic pathogens, found most commonly in cystic fibrosis patients. One of the hallmarks of these bacteria is their broad antibiotic resistance due in part to the unique structure of the outer membrane of the cells. To understand these resistance mechanisms, a tool to perform gene replacement studies is being constructed. Beginning with the suicide vector pEX100T, a *B. cenocepacia* specific resistance cassette was added. The gene of interest is BCAL0894, a potential *B. cenocepacia* membrane protein.

CHED 518

Electron transfer reactions of cytochrome c oxidase: Isolation, characterization, and ligand binding studies

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Cytochrome c oxidase is the key terminal enzyme (complex IV) in the electron transport respiratory chain. Malfunction of mitochondria, including cytochrome c oxidase, may result in neurodegenerative diseases, such as Alzheimer's and Parkinson's. In 1995, the crystal structure of oxidized cytochrome c oxidase at 2.8 Å resolution was reported. The presence of two hemes (cytochrome a and a₃) and two coppers (Cuₐ and Cuₐ₃) provide unique spectral signatures for ligand binding studies.
With the ultimate goal of probing the active site with redox active ligands that are known inhibitors of mitochondrial respiration, cytochrome c oxidase was isolated, purified, and characterized from beef heart mitochondria. The isolation of the enzyme involved repeated ammonium sulfate fractionation. The integrity of the enzyme was ascertained from spectrophotometric heme-analysis (8.9 µM heme per gram of the enzyme), and molecular activity measurements were obtained by spectrophotometric and oxygen electrode assay. In addition, cyanide binding and isolation of a complex (cytochrome c oxidase: cytochrome c) at low ionic strength will be presented.

CHED 519

Detection of melatonin and cortisol in hair

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This research evaluates the viability for using hair samples for the detection of melatonin and cortisol and compares this sampling method to salivary analyses. The use of saliva or blood samples has disadvantages because only a single time-point is observed and multiple samples must be obtained over a 24-hour period for proper diagnostics. Overall, it is important to be able to quantify both the magnitude and the phase for these two diurnal hormones. Melatonin, which is produced in the pineal gland and in hair follicles, typically increases during the early sleep period, and thus multiple samplings may tend to interfere in the accuracy of its detection. In a similar manner, the measurement of cortisol, produced in adrenal gland and in hair follicles will typically show a peak value in the early morning, and its observation may also be disrupted through multiple sampling. Thus, the ratio of melatonin to cortisol in hair was evaluated and compared to that obtained from 24-hour salivary samples. By evaluating both hormones in hair, some of the limitations of the variability observed in hair analyses may be bypassed while providing for a stronger diagnostic marker.

CHED 520

Purification of components from *Inula hilinium* (elecampane) which are cytotoxic to the 4T1 murine breast cancer cell line

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The plant *Inula hilinium* (elecampane) is a medicinal plant that is found widely throughout England. It has been used as a diuretic, antiseptic, and skin cream, and has
also been used in treating pulmonary diseases. Previous studies have shown elecampane to be toxic to 4T1 murine breast cancer cells. Powdered elecampane root was refluxed in dichloromethane for 1 hour, the dichloromethane was distilled off, and the extract was resuspended in ethanol. The resulting ethanolic extract was size-fractionated on a Sephadex LH20 column with 75% ethanol as the mobile phase and analyzed through absorbance at 280nm. Fractions from the column were assayed for cytotoxic effects on 4T1 cells. Cytotoxic fractions were further characterized using HPLC (solid phase: C18, mobile phase: 0-75% methanol gradient over 30 minutes). One peak was identified through HPLC from the most cytotoxic fraction. This peak was collected and further characterized using mass spectroscopic analysis (MALDI TOF). Based on the mass spectroscopic analysis, the most likely size of the cytotoxic molecule isolated through this study was determined to be 440g/mol. Further research is ongoing to identify this cytotoxic component of elecampane.

CHED 521

Discovery of a potential Middle East respiratory syndrome (MERS) PLpro inhibitor for the development of anti-MERS-CoV drugs

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The Middle East respiratory syndrome coronavirus (MERS-CoV) is a novel type of coronavirus first reported in 2012. MERS-CoV has a higher case/fatality rate (30%) than severe acute respiratory syndrome coronavirus (SARS-CoV) (10%). Coronaviruses cause mild to moderate upper-respiratory tract illnesses, and the most deadly infections are from MERS-CoV and SARS-CoV. They encode multifunctional enzymes, known as papain-like proteases (PLpro), that process the viral replicase polyprotein, deubiquitinate (DUB), and deISGylate host cell proteins. There are currently no vaccines or therapeutics that could treat or prevent coronavirus infections. In this study, a promising MERS PLpro inhibitor was discovered that could lead to the development of an effective anti-MERS-CoV drug. A primary high-throughput screen of 25,000 compounds was performed to identify MERS-CoV PLpro inhibitors, and a subset of inhibitors was selected for further experimentation. A single compound (MRL-05-2014) that inhibits MERS-CoV PLpro with an IC₅₀ value of 20.6 ± 1.0 µM was identified. Future studies will be aimed at improving the inhibitory potency of MRL-05-2014.

CHED 522

Inhibition of Y-family DNA polymerases

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Present-day cancer treatment involves DNA-damaging anticancer drugs designed to prevent replication of the cancerous cells. However, Y-family DNA polymerases found in these cells have been shown to catalyze synthesis of DNA past a variety of lesions by a process termed translesion DNA synthesis (TLS). Inhibition of human Y-family polymerases in tumors would yield more effective DNA-damaging chemotherapeutics by preventing resistance. Although not needed to maintain survival, Y-family polymerases also help microorganisms evolve under stressful conditions and can contribute to antibiotic resistance. Inhibition of microorganisms’ Y-family polymerases, such as *Escherichia coli* DinB, would lessen mutagenesis. *Escherichia coli* DinB polymerase and its mammalian ortholog, polymerase kappa (pol κ), catalyze TLS past an array of DNA lesions, most proficiently bypassing $N^2$-dG lesions. In this study, the extension of DinB and pol κ past an $N^2$-furfuryl-dG damaged template was assayed in the presence of varied concentrations of potential polymerase inhibitors. Under the same conditions, ligand-protein interaction was further demonstrated by thermal shift assays. Results have identified potential inhibitors of DinB and pol κ, as well as probable stimulators of DinB.

**CHED 523**

**Purification and characterization of wild type nickel uptake regulator (NUR) from *Streptomyces coelicolor***

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The nickel uptake regulator (NUR) is a metalloregulatory protein found in the microorganism *Streptomyces coelicolor*. It is the first Ni(II)-sensing member of the FUR family of metalloregulatory proteins. NUR is responsible for regulation of a variety of genes involved in nickel uptake and oxidative stress. Interestingly, NUR is also responsible for regulation of the enzyme superoxide dismutase (SOD) within *S.coelicolor*; it regulates Fe-containing SOD through a direct mechanism and indirectly controls Ni-containing SOD. The goal of this research is to purify and characterize the metal and DNA binding affinities in wild type (WT) NUR. There are two metal binding sites within NUR that are believed to contribute to the function of this protein. The “M-site”, which corresponds to a well-conserved site within FUR proteins, contains Zn(II) in a square-planar geometry when purified from E. coli. The second site, denoted the "Ni-site", is a unique site in FUR proteins and has been suggested to be the sensory Ni(II)-binding site. The work presented in this poster will describe a series of biophysical experiments that aim to assess the role of each metal site in NUR function. This was approached using a complement of biophysical techniques including site-directed mutagenesis, competitive metal binding assays, fluorescence anisotropy, atomic absorbance spectroscopy, and quantitative chromatography. Together, the data suggests that the “M-site” plays a more profound role in the metal sensory function of NUR.
Inhibition of formation of blood clots by tetrapeptide inhibitors acet-LSPR-amide and acet-ISPR-amide

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A leading cause of death in Western society is due to the inappropriate formation of blood clots. Clots form due to the coagulation cascade, leading to the formation by thrombin of fibrin from fibrinogen, forming an insoluble polymer. Direct inhibition of thrombin would result in a reduction of clot formation. In the work presented here, blood clots were formed in a fibrinogen and thrombin-containing clotting assay. Triplicate assays each of uninhibited, inhibited using acet-ISPR-amide and acet-LSPR-amide, and inhibited using the commercial irreversible serine protease inhibitor Pefabloc®, were analyzed by visible spectroscopy to determine if clot inhibition occurred. Acet-ISPR-amide and acet-LSPR-amide provided slight but significant inhibition at 14 mM, compared to the uninhibited case; however the 30 μM concentration, for both the acet-ISPR-amide and acet-LSPR-amide, demonstrated more inhibition than the 14 μM and uninhibited case. The spectra were then fit to a sigmoidal curve using the three-coefficient Hill equation. Coefficient “a” provided the maximum clot density (clotmax), coefficient “b” showed the level of cooperativity in clot formation as a function of the sigmoidality of the curve, while “c” provided the time of half clot formation (time1/2clot). The clot density was similar throughout the first three cases; however Pefabloc® was slightly smaller. The time1/2clot increased as the concentration of each peptide inhibitor increased.

Probing the substrate specificity of lysine deacetylases using mutagenesis

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Lysine deacetylases (KDACs) catalyze the hydrolysis of ε-N-acetyl lysine residues in proteins to generate an unmodified lysine residue and acetate. KDACs play a critical role in transcriptional regulation, cell cycle progression, and developmental events. Perturbations in this process have been linked to diseases, including cancer and inflammation. While thousands of acetylated proteins have been identified, little information is known concerning the specificity profiles of KDACs and the role of several conserved active site residues in determining that specificity. In this study, selected residues were mutated in different deacetylates with the goal of expressing and purifying the resulting proteins to evaluate the effect of the mutations on the enzyme’s
activity, which was measured using a panel of model peptide substrates. The results provide insight into the selectivity and mechanism of KDACs.

CHED 526

Two systems for modulating back electron transfer between guanine radicals and 2-aminopurine in duplex DNA

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Electron holes produced upon DNA oxidation are mobile and can move throughout the base stack; guanine is the DNA base that is most susceptible to 1-electron oxidation. Once formed by photooxidation, the guanine radical can either undergo back electron transfer with the photooxidant or react further to give permanent products. Here, the fluorescent analogue, 2-aminopurine, was used as the photooxidant and two different systems were examined for modulating the amount of permanent products from guanine oxidation. In the first system, the formation of DNA-protein crosslinks was monitored as the trapping reaction for the guanine radical. 2-aminopurine was incorporated into a 29-mer DNA duplex containing a 5′-G(T)ₙX-3′ sequence (n=0,4 and X=2-aminopurine) to determine the relative rates of back electron transfer and crosslinking to protein. Crosslinking was detected by gel shift assay. Upon 325 nm irradiation, only a small change was seen in the mobility of the n=0 duplex, whereas the n=4 duplex showed a decrease in free DNA bands and the clear appearance of lower mobility bands. This result suggests that in the n=4 duplex, back electron transfer does not compete as well with the protein trapping reaction. In the second system, the distance between the photooxidant and the closest guanine was held constant, but the sequence was designed to either increase or decrease guanine oxidation potential with the distance from the photooxidant, to either localize or pull away the electron hole, respectively. In this case, the assay involved oxidation of cytochrome c by the guanine radical. Indeed, a less efficient oxidation of the cytochrome, as evidenced by the loss of the 550 nm absorbance band, was observed for the sequence designed to keep the electron hole in proximity to the photooxidant.

CHED 527

Conformational analysis of cyclic disulfides and selenenyl sulfides in peptide redox motifs

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The antioxidant activity of the biochalcogens sulfur and selenium is important to reducing the risk for cancer, cardiovascular disease, and other chronic illnesses. The
active sites of thio- and selenoproteins often contain a C(X)_nC(U) (n = 0-2) motif, where C = Cys, U = SeCys, and the spacer residue X varies with protein function. It has recently been shown that different conformations of the selenenylsulfide ring formed through the oxidation of these motifs can be detected through $^{77}$Se NMR and identified through DFT calculations of the $^{77}$Se chemical shift of model compounds. In this study, molecular dynamics (MD) simulations in AMBER are used to propagate the conformations of the disulfides CGGC and CGAC to understand the affect that spacer residues have on the oxidized form of thio- and selenoproteins. Unique conformations of the disulfide and the selenenylsulfide analogues were optimized using density functional theory (DFT). GIAO-DFT calculations were used to calculate the $^{77}$Se chemical shifts for comparison to experimental data. The theoretical chemical shifts for different conformations were in excellent agreement with resonances observed in the experimental $^{77}$Se spectrum of CGAU-containing selenopeptides.

CHED 528

DNA binding and selectivity of dapsone derivatives

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Small molecules that bind to DNA can inhibit DNA binding proteins and therefore disrupt biological functions associated with genetic disorders. Specificity in the binding patterns of novel small molecules would allow for the targeting of sequences linked to disease and subsequent development of therapeutics. The focus of this study is to assess the binding affinity, and therefore the selectivity, of dapsone derivatives. One particular derivative, KCA-I-24, was studied in conjunction with three hairpin DNA sequences. Filter binding and differential scanning calorimetry were used to quantify equilibrium constants, analyze stoichiometry in binding, and assess the possibility of specificity for KCA-I-24.

CHED 529

Using acute promyelocytic leukemic cells to test for receptor binding of ajulemic acid

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Ajulemic acid (AJA) and other cannabinoids are a current topic of interest for the treatment of Ewing’s sarcoma, a pediatric bone cancer with poor prognoses. AJA is structurally similar to tetrahydrocannabinol (THC), the active compound in the marijuana plant, but AJA has no psychotropic effects, making it a viable option for the pediatric
population. This compound has been shown to induce apoptosis in Ewing’s sarcoma cells, but the mechanism of action is not yet understood. Previous work in the lab has identified the retinoic acid receptor (RAR-alpha) as a strong candidate receptor mediating the induction of apoptosis. Acute promyelocytic leukemia (APL), a subtype of acute myelocytic leukemia, is treated with all-trans retinoic acid (ATRA). ATRA binds to the retinoic acid receptor, inducing differentiation of the promyelocytes. The goal of this study is to investigate the effect of AJA on APL cells. It was hypothesized that AJA, like ATRA, will force differentiation of this cell population. If true, this will confirm the ability of AJA to bind to the retinoic acid receptor and may elucidate the mechanism this compound uses to induce apoptosis in Ewing’s sarcoma cells.

CHED 530

Observing the folding behavior of bi1 group II intron

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RNA folding is involved in many biochemical processes, such as protein synthesis and gene regulation. When RNA is folded correctly, it can perform its function in the cell. By studying RNA folding using catalytic RNA, the process of RNA folding can be better understood. By using catalytic RNA, folding can be monitored by the fraction of intron spliced, which will give estimation of how much RNA was folded correctly. The primary goal of this research is to observe the splicing and folding behavior of bi1 group II intron under different reaction conditions in order to understand the specific folding pathway of the intron. By plasmid DNA linearization and through in-vitro transcription by T7 polymerase, the RNA can be quantified, and splicing reactions will be conducted. The different reaction conditions that will be used will represent near-physiological and non-physiological conditions under high salt concentrations to induce splicing. By analyzing the data through a capillary electrophoresis instrument, the identity of the peaks can be analyzed and correlated to different sections of the spliced RNA and the amount of precursor present. Efforts are underway to find the optimal conditions to visualize the RNA splicing products on the capillary electrophoresis instrument before the splicing reactions occur, in order to analyze the data properly.

CHED 531

Development of small molecules as potential RNA-binding molecules

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The diverse functionality and complex three-dimensional structure of RNA illustrates its promising potential as a therapeutic target. Inspired by established RNA-small molecule
interactions, a series of TAN-1057 analogs have been designed as potential RNA-binding molecules. TAN-1057 is a naturally produced antibiotic that is known to interact on the bacterial ribosome. The primary disadvantage of TAN-1057 is its indiscriminate binding to both pathogen and host RNA. Alterations at carbon four of the heterocyclic core of TAN-1057 will be made with the intent to generate a library of analogs all containing a common 2-amino-5-(methylamino) pyrimidine-4,6-dione core. These analogs will be evaluated for their potential to eliminate promiscuity while maintaining strong interactions with specific RNA targets. Current synthetic method consists of a two-step process designed for the rapid development of a diverse library of small molecules. The initial stage of synthesis has been successfully developed and utilizes a substitution reaction. Additional efforts are in progress involving the introduction of various functional groups as side chain decorations around the common core. Efforts are also underway towards the synthesis of the second step of the reaction scheme. Upon the development of a diverse set of analogs, testing for binding affinity to RNA targets of interest will be conducted.

CHED 532

Characterization of the disulfide crosslinking in lysyl oxidase

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Lysyl oxidase is a copper-dependent amine oxidase that catalyzes the oxidation of amino groups in collagen and elastin. The resulting aldehyde molecules are essential in the production of the crosslinkages in these proteins. Lysyl oxidase has been shown to be stabilized by five disulfide linkages; however the levels of stability provided by each linkage has not been fully studied. The main focus of this study is to investigate the role each disulfide bond has on lysyl oxidase. A LOX mutant, C238S, was generated via PCR mutagenesis program. Overexpression of this mutant yielded 16.01 mg of enzyme per liter of media. There was no catalytic activity for this mutant when compared to the wildtype. In order to facilitate overexpression and analysis of the effect of the mutants in lysyl oxidase, the mutant LOX gene will be moved to a vector carrying a solubility tag.

CHED 533

Use of solubility tags to characterize lysyl oxidase

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Lysyl oxidase (LOX) is a copper-dependent enzyme that activates the formation of crosslinkages in collagen and elastin in connective tissues by oxidative deamination of lysine and hydroxylysine residues. LOX requires one covalently bound cofactor, lysyl
tyrosyl quinone, and a copper ion in order to carry out catalysis. Currently, there is no crystal structure available for mammalian LOX, primarily due to the low solubility of the enzyme in aqueous buffers. The only crystal structure available for lysyl oxidase is from *Pichia pastoris* which uses a different catalytic cofactor. In order to overcome the low solubility of lysyl oxidase, a thioredoxin solubility tag has been engineered on the N-terminus of mature mammalian LOX in order to facilitate the elucidation of the crystal structure of lysyl oxidase. Overexpression of this enzyme yielded 4.4 mg of enzyme per liter of media. This is nearly double the yield obtained using the much larger Nus-A solubility tag, suggesting that this tag has less of an effect on overexpression. The enzymatic activity for this tagged enzyme appears to be unaffected by the tag. LTQ content will be quantified by detection of a phenylhydrazone adduct via visible spectroscopy, and the percent copper incorporation will be also determined. Once these parameters are established, crystallographic screens will be carried out in order to determine crystallography conditions leading to the elucidation of a crystal structure.

CHED 534

Cooperativity of TU100 and ascorbic acid in the production of reactive oxygen species

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12,13-dihydro-N-methyl-6,11,13-trioxo-5H-benzo[4,5]cyclohepta[1,2-b]naphthalene-5,12-imine, a novel naphthoquinone known as TU100, has shown potential as a chemotherapeutic agent, in part due to its cytotoxic properties in cancerous cells. Past research indicates that this cytotoxic mechanism involves the increased generation of reactive oxygen species (ROS), leading to apoptosis. Ascorbic acid is a common dietary supplement that participates in redox reactions and may interact with TU100 via a redox cycling mechanism, thus enhancing its effect. Stains that fluoresce in the presence of ROS indicate that TU100 and ascorbic acid demonstrate strong cooperativity in the production of these moieties. Implications for usage in targeted cancer therapy are discussed.

CHED 535

Supramolecular guanine-rich quadruplexes and their transfection into mammalian cells

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Guanine-rich nucleic acids have the ability to adopt quadruplex helical structures consisting of a core of four guanines arranged in stacked tetrads. These four-stranded
structures are commonly known as G-DNA and they exist as stable conformers readily observed in the chromosomes of eukaryotes or as isolated synthetic assemblies. Genome stability and the controlled expression of specific proto-oncogenes rely on G-DNA structures, where their presence in these locations interferes with events associated with neoplastic transformation. The potential for G-DNA stabilization to serve as an anti-proliferative mechanism is of great interest for drug development, as well as the design of theranostic devices. The work described here utilizes a supramolecular G-DNA (G-wire) that is self-assembled from a guanine rich oligonucleotide (GRO) as a potential decoy molecule that would disrupt normal cell function. G-wires possess nanoscaffolding properties that allow for external modification and the creation of potential novel carrier molecules. Recently, the conditions for introducing G-wires into a mammalian cancer cell line using a generation 5 dendrimer have been identified. Current work is underway to quantify the cellular uptake, dispersion, and proliferative response of affected cells.

CHED 536

Detecting DNA-protein crosslinking in DNA with 2-aminopurine via fluorescence polarization

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DNA-protein crosslinking can be detected by variety of methods, but most consume a considerable amount of DNA. Here, an artificial fluorescent DNA base, 2-aminopurine, was incorporated into a 29-mer DNA duplex, and the fluorescence polarization was measured using a custom-built filter system on an AB2 spectrofluorometer. Oxidative DNA-protein crosslinks were induced photochemically by the flash quench technique; then the samples were analyzed by gel electrophoresis and fluorescence polarization. Untreated samples showed very little polarization, whereas irradiated samples showed an increase in polarization. Analogous samples subjected to gel electrophoresis show decreased mobility, consistent with crosslinking. Treatment of the irradiated samples with proteinase K mostly reverses both the polarization increase and the gel shift. These results show that 2-aminopurine is a promising probe for detecting DNA-protein crosslinking.

CHED 537

Function of laforin in glycogen metabolism and lafora disease

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Lafora disease is a fatal, recessive neurodegenerative epilepsy caused by mutations in the EPM2A gene that encodes for the glycogen phosphatase Laforin. In the absence of laforin activity, glycogen transforms into hyper-phosphorylated, water-insoluble starch-like particles called Lafora bodies (LBs). LBs are the suspected cause of neuronal apoptosis, neurodegeneration, and eventual death of LD patients. Laforin is the founding member of the glucan phosphatase family and also the only known human phosphatase with a carbohydrate-binding module (CBM), followed by a dual specificity phosphatase domain (DSP). The CBM is responsible for glycogen binding while the DSP possesses phosphatase activity. At present, there are over 30 single-point mutations identified in LD patients. However, the molecular mechanism of glycogen dephosphorylation by laforin and the formation of LBs are not understood. The X-ray crystal structure reveals that the patient point mutations are scattered between specific regions of the CBM and DSP domains of laforin suggesting multiple mechanisms that causes LD. To understand the mechanism of phosphatase activity, stability, and glycogen binding of the mutants, we employed several biophysical methods (DSF, SAXS, AUC) and biochemical assays (glycogen phosphatase, ConA, etc.). Our data shows that patient mutations are described to have loss of functional interactions either in the CBM binding site, DSP active site, CBM/DSP interface, or at the dimerization interface. Moreover, the analyses of LD patient mutations define the mechanism by which subsets of mutations disrupt laforin function. Our data provides fundamental insights connecting glycogen metabolism to this neurodegenerative disease.

CHED 538

Analysis of antibacterial components of honey

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Honey is a complex natural product that has been used by the Egyptians, and mentioned by Aristotle, as a natural remedy. Today, honey continues to be studied for its medicinal applications, particularly in terms of wound care. Honey is particularly useful as an antibacterial due to its effectiveness against antibacterial-resistant strains of bacteria. While it is known that methylglyoxal (MGO) and hydrogen peroxide (H$_2$O$_2$) are among the components that give honey this quality, other components of honey are currently under study to determine their respective synergistic effects. The effect of osmolarity, pH, and concentration of MGO and H$_2$O$_2$ on the antibacterial property of honey was analyzed via agar well diffusion assay to determine the minimum inhibitory concentration. The zone of inhibition was recorded for increasing concentrations of each component studied in independent tests using S. aureus, S. epidermidis, and methicillin resistant S. aureus. The antibacterial activity equivalent to % w/v phenol for each component was determined from a calibration curve prepared of
varying % w/v phenol concentrations and the resulting zone of inhibition. Similar concentrations of MGO can have varying effects as an antibacterial agent due to the synergistic effects of other components within the honey. The antibacterial activity of identical concentrations of MGO in pasture, manuka, and control honey solutions was analyzed via agar well diffusion assay, and the zones of inhibition compared.

CHED 539

Encapsulation of superparamagnetic nanoparticles in mPEG-PLGA micelles for targeted drug delivery

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One of the problems encountered for the application of anticancer drugs such as chlorambucil-tempol (CT) is its solubility. CT has a cytotoxicity that proves powerful in in vitro testing against cancer cell lines. Poor solubility means that it cannot be tested or applied in vivo due to lack of ability to target the cancer-specific sites within the body. However, encapsulating CT in a methoxypoly(ethylene glycol)-polylactic-co-glycolic acid (mPEG-PLGA) nanoparticle micelle allows for increased solubility in water. This leads to a controlled drug delivery system wherein the contents of the micelle could be accepted in to the blood stream, and would be able to diffuse for evenly and more measured drug distribution; this would fix the problem of drug delivery and tumor targeting compared to applying CT to the body alone.

Studies done on anticancer drugs have focused on drug delivery systems that would have an effect throughout the entire body. The addition of superparamagnetic nanoparticle encapsulation within the mPEG-PLGA micelle along with the cytotoxic CT drug may allow for an alternative delivery system, as well as better tracking through the body. Magnetite (Fe₃O₄) is a biodegradable magnetic NP that can serve this purpose. The presence of magnetite allows for avoiding the exposure of the hydrophobic interior of the micelle that contains it. If the interior were exposed, there would be adsorption of proteins in the blood; avoiding this allows for extended blood circulation. Theoretically, the magnetite would also allow for specifically targeting cancer sites using electromagnetic fields to specify the location of the whole micelle after being administered, due to its superparamagnetic properties. This would create a novel system for administering anticancer drugs to tumors. The superparamagnetic properties additionally allows for boosted visibility when using an external magnetic field (EMF) such as magnetic resonance imaging machine (MRI).
CHED 540

Exploring simple pattern transfer using microcontact printing

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In microelectronics, patterned surfaces can be used to lay down wires, transistors, and other electrical components. Our aim was to prepare a microcontact (µCP) printed surface on silicon, and to use the pattern as a guidepost to attach soft nanostructures. Elastometric stamps fabricated via an established method using poly(dimethylsiloxane), (PDMS), in a two part pre-polymer mixture with a 20:1 mass ratio was cured at 70°C for 20 minutes. A commercial diffraction grating was used as the master to prepare a stamp. The fabricated stamp was dipped into silane inking solutions, and the pattern was made by pressing the inked stamp onto silicon. Imaging was performed using an Atomic Force Microscope (AFM). We obtained good pattern transfer on mica and polished silicon with a method that we developed to apply constant and reproducible pressure during transfer.

CHED 541

Identification of previously unsequenced viruses from wild-caught mosquitoes by metagenomic sequencing
Metagenomic sequencing (unbiased, high throughput sequencing directly from complex matrices) can be used to analyze the genetic material contained in a taxonomically diverse sample. This method has the potential to be used for several applications, including diagnostics and biosurveillance. Mosquitoes, which feed on a variety of organisms within their environment, are ideal subjects for this type of analysis.

Viral genomes from wild caught mosquitoes in the contiguous United States (CONUS) have not been fully characterized in public databases. Research in this area has primarily focused on only viruses with DNA genomes. This suggests that we have very little knowledge of the microbiota of an important disease vector on our own soil, and likely even less knowledge of the microbiota of disease vectors where our troops are deployed overseas. Small distances between collection locations can result in completely distinct mosquito viromes, thus illustrating the extent of diversity that exists within these tiny vectors.

The aim of the current study is to determine if samples of mosquitoes collected from different sites (CONUS, east coast) could be differentiated using metagenomic analysis of the RNA fraction. Mosquito samples were collected from several locations, sequenced, and analyzed. Both total and viral enriched RNA samples were created from each site. Preliminary data suggest the presence of multiple previously unsequenced viruses within these samples. Genome characterization of these apparently novel viruses is currently in progress.

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CHED 542

Modified coarse-grained DNA model and its application to surface density effects on decamer hybridization

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DNA microarrays are used to detect specific sequences within DNA samples, and consist of known single stranded DNA fragments, referred to as probes, which are attached to a solid surface. Labeled sample DNA, if complementary, will then hybridize
with the probes. As microarrays have multiple probe strands on a given surface, their proximity can effect hybridization. The effect of surface density and of temperature on DNA decamer duplexes in a model microarray is studied in this work with Monte Carlo molecular simulation and a coarse-grained model.

CHED 543

Proof-of-concept for rapid point-of-care LFCC detection of serum cancer biomarkers

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Current cancer detection methods are costly and require off-site analysis of the patient’s serum. In an effort to develop a new method of detection, methods previously developed by this lab are being applied to this area. Previously, lateral flow capillary concentration (LFCC) was developed as a technique to quantify the amount of specific bacterial strains present in various applications. The current prototype has a 100µL polycarbonate capillary encased in acrylonitrile butadiene styrene (ABS). Sample wells feed into the capillary tube and an underlying, removable magnet allows for the concentration of paramagnetic analytes along the magnet. This technique is highly analyte-specific, which broadens the potential applications for it. Now, it is being applied to cancer biomarkers, in an attempt to replace or supplement current analysis of these biomarkers. Prostate and breast cancer have well known and specific biomarkers, prostate specific antigen (PSA) and CA 15-3, respectively. Monoclonal antibodies were created for these proteins; these antibodies were then conjugated to Raman-active, thiol-modified SERS particles and paramagnetic particles. These solutions were then bound using the cancer proteins and run through the LFCC device. They congregated where the magnet is located in the device and this area was analyzed using Raman spectroscopy to quantifiably measure the amount of cancer protein present in a given sample. The goal is to show this technique is comparable to current techniques, as it is much cheaper and could provide in-office testing to many locations.

CHED 544

Sensor circuit for streamlining E. coli cell phase determination

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In biological applications involving prokaryotic cells it is necessary to know the cell stage to produce consistent results in biotechnical procedures such as DNA amplification or protein overexpression. Cell phase is relevant because during logarithmic growth cells maintain a reproducible environment favorable to manipulation. Standard practice
involves determining cell phase by measuring optical density via a spectrophotometer, but such determination is only indirect. Additionally, it can be time consuming to carry out repeated optical density measurements. To address this issue, we have designed a genetic circuit consisting of an RpoS-responsive promoter, a library of ribosomal binding sites and a chromophoric protein. This system will indicate with a visible color change when cells leave logarithmic phase. Incorporating this system in commonly used laboratory bacteria like *E. coli* would streamline procedures for cloning and protein expression by allowing a quick visual observation to check if cells have exited logarithmic phase.

CHED 545

**Development of a cellular probe based on a synthetic receptor**

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The focus of this project was to develop a molecular probe for interfacing with biological systems. The probe was constructed from a synthetic receptor, cucurbit[7]uril (Q7), and a fluorescent dye, tetramethylrhodamine (TMR). The Q7-TMR conjugate was added to cultures of N27 and HT22 neuronal cells, and imaging was performed using confocal microscopy. Fixed cell experiments show the Q7-specific internalization of the Q7-TMR conjugate, but it remains to be determined specifically where the conjugate localizes or whether that localization is driven by the binding of Q7 or another process. Live cell experiments corroborate the fixed cell data, and experiments with organelle markers show preliminary evidence of localization to specific organelles.
Characterization of a cucurbit[7]uril-rhodamine conjugate as a chemical sensor

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Cucurbit[7]uril (Q7) is known for its binding to molecules such as insulin in aqueous solution. Previously, fluorescence assays using Q7 and fluorescent dyes were use to determine the binding affinities of Q7 with various analytes, but the working concentrations of the assays depended heavily on the binding affinity between Q7 and the dye. The covalent attachment of Q7 to a fluorescent dye should remove this concentration dependence. The two-step synthesis of a Q7rhodamine conjugate produced four isomers which were separated by HPLC and isolated in pure form. Preliminary studies with one of these isomers (P1) demonstrated similar binding affinity as unmodified Q7 to peptides. Binding affinities were determined using the change in fluorescence of the rhodamine moiety upon binding. While replicating these data, several variables have been encountered which impact the fluorescence of the conjugates as a function of time, concentration, and container material. These variables suggest the influence of nonspecific adsorption of the conjugate to the walls of the container and potentially photobleaching of the dye. Ongoing studies are in progress to overcome this obstacle and validate the conjugates as chemical sensors.

CHED 547

D-Lactic acid biosynthesis from corn stover using engineered Lactobacillus plantarum

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A sustainable replacement option for petroleum derived plastics are poly-lactic acid (PLA) plastics which are able to be derived from renewable resources. Mixtures of L- and D-poly-lactic acid have higher melting points than poly-L-lactic acid alone. This higher melting point characteristic of stereocomplex PLA will allow for broader applications of PLA.

There have been many studies on the production of L-lactic acid but few on the biosynthesis of D-lactic acid. In our study, corn stover was hydrolyzed using CTec2 and HTec2 to provide sugars for the biosynthesis of D-lactic acid. L. plantarum NCIMB 8826 ΔldhL mutant with the ldhL gene knocked out and a recombinant L. plantarum NCIMB 8826 ΔldhL carrying pCU-xyAB plasmid were used in our study to produce lactic acid from different carbon sources. L. plantarum NCIMB 8826 ΔldhL produced D-lactic acid with an optical purity of 99.1% and a yield of 0.94 g. The recombinant strain with pCU-xyAB was able to use xylose and produced D-lactic acid with a yield of 0.51 g.
The high optical purity, yield and productivity of the mutant strain shows an efficient production of D-lactic acid from corn stover which may be used to create innovative PLAs in the polymer industry and the results with the recombinant strain showed evidence that the recombinant strain of *L. plantarum* may be able to produce higher concentrations of lactic acid by utilizing all of the sugars present in biomasses.

CHED 548

**Engineering light-gated, transmembrane proteins for use in hybrid systems**

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Nature provides a wide array of molecular machines that not only perform important biological functions, but also serve as potential building blocks for hybrid materials, devices, and systems. For example, bacteriorhodopsin (bR) is a transmembrane protein that functions as a light-gated proton pump as part of ATP synthesis and has been used in engineered systems for optical memory storage. Similarly, channelrhodopsin (cR) is a light-gated cation channel that has recently been used in optogenetic applications, such as remote control of neurons. Because both of these proteins use well-controlled photocurrent generation, they could potentially serve as functional components of hybrid materials with enhanced optical and electrical properties. Central to this objective is the ability to engineer these proteins with specific characteristics to enable better understanding of the fundamental nature of these proteins as well as provide seamless integration into artificial environments. To this end, site-directed mutagenesis (SDM) was used to create mutations involving single amino acids that are to achieve novel function of these proteins in hybrid nanomaterials. This presentation will discuss the selection, modification, and function of specific mutations in both bR and cR. More specifically, mutational changes to bR will be discussed in terms of creating unique “chemical handles” for directed orientation bR on functionalized polycarbonate surfaces, as well as a mutation (Asp-85 residue with Thr) that enables bR to pump chlorine ions inward and protons outward under green light and reversibly, proton pumping inward under white light. The use of SDM in cR to mutate residues Cys-128 and Asp-156, which have a large effect on the conducting state and photocycle kinetics of cR, will also be presented.

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CHED 549
Measuring amyloidogenic protein interaction with lipid membranes via colorimetric assay

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Neurodegenerative diseases such as Alzheimer’s disease (AD) and prion-related encephalopathies (PRE) are commonly identified by proteaceous fibrillar aggregate deposits known as amyloids. Here we utilize a colorimetric, vesicle-binding assay to study protein-surface interactions of amyloid-forming proteins with lipid membranes. The assay consists of vesicles incorporated with polymerized polydiacetylene (PDA) molecules which provide a model system to mimic cell membranes. Lipid/PDA vesicles undergo a visible blue to red conversion in response to environmental conditions. From our spectroscopic data, we obtained time-resolved absorbance measurements of the “blue” (630 nm) and “red” (490 nm) components from lipid/PDA vesicles exposed to various amyloid-forming proteins such as β-amyloid (Aβ) and prion peptide fragments (PrP). Upon exposure to each amyloid-forming protein, we demonstrate the colorimetric responses of the lipid/PDA vesicles vary depending on the magnitude of protein association with the membrane. These studies illustrate the potential for this colorimetric assay to become a useful technique in studying biological systems.

CHED 550

Gold(I) complexes of benzene-1,3,5-tricarboxamide ligands for Conia-Ene Catalysis

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Metal complexes of benzene-1,3,5-tricarboxamide (BTA) based ligands are known to self-assemble into supramolecular stacks in non-polar media generating a tunable platform for asymmetric catalysis.¹⁴BTA¹⁴ ligands (R=m-PPh₂, p-PPh₂) were synthesized at high yields using a modular multi-step approach. Their respective gold complexes were prepared to examine catalytic Conia-Ene reactivity. Conditions were screened to optimize conversion for the Conia-Ene reaction. Initial results aim to display some of the challenges and potential for successful gold (I) supramolecular catalysis performed with BTA ligands.

Inimines are a family of compounds known to have a variety of uses. For example, inimines have been shown to have antibacterial, antifungal, and antiviral activity. In addition, some inimines are used to synthesize common prescription drugs (e.g., Zetia and Taxol). Outside of their medical applications, inimines have found use as corrosion inhibitors and in organic light emitting diodes (O-LEDs). This project was undertaken to identify simple inimines that display electroluminescent properties, improve the synthesis of inimines known to be electroluminescent from the literature, and to synthesize new electroluminescent inimines. Ultimately, we hope to develop a project for organic chemistry laboratory where students synthesize electroluminescent inimines, analyze it using standard organic laboratory techniques (e.g., melting point and NMR), and create a simple O-LED.
Development of a simple, qualitative tyrosinase inhibition assay for organic chemistry laboratory

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When plant tissue is damaged, oxygen in air reacts with the enzyme tyrosinase in cells to carry out a process that ultimately changes the injured tissue brown. Our research group has recently developed a greener synthesis for a group of compounds known as thiosemicarbazones (TSCs), some which are known inhibitors of tyrosinase. This synthesis project was designed to be performed in a one- or two-semester organic chemistry course and we wanted an assay that could be performed using the equipment and skills found in this course. While many inhibition studies have been performed to test tyrosinase after first isolating and purifying it, we needed a more organic chemistry friendly approach. Since our students do not yet have the skills to isolate an enzyme nor the equipment to do so, we developed an assay where solutions of inhibitors and control compounds were applied directly to fresh plant slices of interest, apples and potatoes, for quick and easy analysis of inhibitory activity in an organic laboratory setting. Different solvents, starting materials, and TSCs were analyzed in this way to identify promising TSCs with inhibitory activity against tyrosinase. An upcoming collaboration with biochemistry students will allow our organic students to pass on promising inhibitors they synthesized for quantitative analysis in the biochemistry laboratory.

CHED 553

Greener synthesis of thiosemicarbazones

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Thiosemicarbazones (TSCs) are a class of compounds with antibacterial, antifungal, and antiviral properties. Recently, they have been found to be useful in the development of antitumor drugs, making them a topic of extreme interest. Some TSCs are also known to inhibit the enzyme tyrosinase, which is responsible for the browning that occurs in damaged plants. The purpose of this project was to synthesize thiosemicarbazones using green chemistry methods, as opposed to traditional, less benign methods. Green chemistry focuses on the development of products and processes that minimize the use and production of hazardous materials. The traditional methods for synthesizing these compounds required reflux in organic solvent, usually methanol or ethanol, with acid catalyst for several hours. These traditional solvents are flammable and have other adverse health effects. Our greener method uses mostly water containing some lactic acid as the solvent. Lactic acid is an additive and preservative for food products, and is found naturally in many foods, especially dairy products. Our aqueous system is a safer alternative than the traditional solvents. The
reactions in our greener method require no reflux, are complete in less than 15 minutes, and result in good to excellent purities and yields without recrystallization. A total of 18 thiosemicarbazones have been made thus far using this method. This synthesis has been class tested in two courses: second-semester organic chemistry with analysis by NMR and a one-semester introductory organic chemistry course with analysis by a simple fruit and vegetable browning assay our group developed.

CHED 554

Synthesis of C-glycosides as potential antihyperglycemic agents

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Type II diabetes mellitus is a disease characterized by hyperglycemia which is becoming of increased prevalence in the world. The goal of this project is to synthesize potential anti-hyperglycemic agents, specifically, C-glycosides with variations on the aromatic moiety. One proposed compound is shown in Figure 1. These variations will provide understanding in regards to their effectiveness and potential for further research as an anti-hyperglycemic treatment. Synthesized compounds will be evaluated using an alpha-glucosidase assay to test for efficacy of inhibition of this enzyme. This particular enzyme is responsible for breaking down polysaccharides, such as starch, into its monomers. This allows the small intestine to absorb monosaccharides that can lead to an increase in blood glucose levels which is characteristic of diabetes. The synthesis and characterization of these C-glycosides will be discussed in this presentation.

CHED 555

Characterization of self-assembled monolayers on zinc selenide
Self-assembled monolayers (SAMs) are organized, single layers of organic molecules which spontaneously form on certain surfaces. SAMs are widely used in the design of surfaces for a wide range of applications, such as biosensors, and directing different orientations of liquid crystals. SAMs are usually studied on gold substrates, but SAMs can be formed on a variety of surfaces, such as silver, copper, and zinc selenide (ZnSe). ZnSe is advantageous to use because it is transparent in the infrared region of the electromagnetic spectrum and is a common element in FTIR spectroscopy. The formation of SAMs on ZnSe has not been fully characterized. In our work, surface energies for several different thiolate SAMs were determined using contact angles and the Owens-Wendt-Rabel-Kaelble (OWRK) method, where Young’s equations is rewritten with two components of surface energy, polar and dispersive. Current work is focused on determination of monolayer density and defects using a variety of characterization methods including static contact angles, XPS, and ellipsometry. We anticipate extending the work toward the formation and characterization of carboxylate SAMs on ZnSe as well.

CHED 556

Reduction of infectious biofilms on the native oxide surface of titanium

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Titanium is a key biomedical material used for surgical implants, due to its biocompatibility, high strength, low density, corrosion resistance, and non-toxicity to the host. However, titanium implants can be infected by Staphylococcus aureus and Pseudomonas aeruginosa biofilms. Biofilms formed by microbial colonies can be resistant to antimicrobial treatments. Nitric oxide can be a biofilm dispersant by inducing nitrosative and oxidative stress on the bacteria, transitioning sessile biofilm cells to free swimming planktonic cells, which are more susceptible to antimicrobial treatments. It is hypothesized that the oxidized surface of titanium can be modified with a self-assembled monolayer containing a functional group that releases nitric oxide under physiological conditions. Diffuse Reflectance Infrared Fourier Transform spectroscopy and contact angle measurements were used to analyze the change in the organization of the monolayer on the surface. These substrates were then be modified for nitric oxide release using nitrosoamines.

CHED 557

Development in undergraduate organic chemistry laboratory curriculum
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Because of a noted shift towards inquiry-based learning in the chemical education literature, new laboratory experiments for the Luther College undergraduate organic chemistry curriculum were selected and optimized. The new experiments were selected on the basis of incorporating inquiry-based and/or green chemistry techniques in order to facilitate a more comprehensive learning experience for undergraduates. The three main experiments that were adjusted for successful implementation at Luther College were an Olefin Cross Metathesis reaction, a redox reaction using Oxone®, and a reaction employing the Wittig mechanism. The first two experiments are focused on teaching green chemistry, using a green solvent and a green oxidizing agent, respectively. The third is focused on letting students make and test predictions based on the accepted Wittig mechanism and a group of possible reagents. The labs developed here are important to the undergraduate curriculum because they encourage critical thinking and let students experience the research process.

CHED 558

Extraction and functional assay of cloned thymopentin 5

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Thymopentin 5 is a synthetic immunomodulatory peptide derived from the thymic hormone known as thymopoietin. It has been demonstrated that thymopentin 5 can be used to enhance immune response to vaccinations and cancers, rectify immune system imbalances, and increase the production of an important cytokine called interleukin-2. Organic peptide synthesis is the current method used to produce thymopentin 5, which is a time-consuming and expensive process that does not always result in a functional protein product. If thymopentin 5 can instead be produced using genetic engineering the peptide can be synthesized in a faster and less costly manner with a higher degree of folding accuracy. Previous work has already been performed to insert the DNA for thymopentin 5 in to the pETFVA vector. This research will attempt to transfet this vector in to COS monkey kidney cells and determine whether a functional thymopentin 5 protein product is produced. This will be done by performing an ELISA to determine whether there is an increase in interleukin-2 production in the transfected cells compared to the non-transfected COS cells. Thymopentin 5 has the potential to be used in clinical settings as an immune enhancing therapy; however, it is not naturally produced in the human body. In this project thymopentin 5 will be transfected in to COS cells and a functional protein product will be produced, which therefore could possibly be a new therapy for combating immune deficiencies.

CHED 559
Modification of FTY720 for use as a prodrug for cancer therapy

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2-Amino-2-[2-(4-octylphenyl)]-1,3-propanediol (FTY720), also known as Fingolimod, is approved by the Food and Drug Administration (FDA) to treat relapsing episodes of Multiple Sclerosis (MS). FTY720 is a structural analogue of endogenous sphingosine. Once ingested, it undergoes phosphorylation to produce FTY720 phosphate, the biologically active compound. At MS doses (0.5 mg/day), FTY720 phosphate causes a drop in resting heartbeat (bradycardia), which can be lethal. Studies have indicated that higher doses (10 mg/day) are therapeutic for cancer treatment. At these higher doses, there is concern that the chance of a patient experiencing bradycardia may be higher. In an attempt to prevent this potentially lethal side effect, we are interested in modifying FTY720 and using it as a prodrug for cancer treatment. Herein, we have optimized the reaction conditions using 2-Amino-2-methyl-1,3-propanediol (AMPD), a model for FTY720, and are now testing their efficacy for the modification of FTY720.

CHED 560

Auto-oscillatory/excitable boundary and complex dynamics in the Belousov-Zhabotinsky reaction

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The ferroin catalyzed Belousov-Zhabotinsky (BZ) reaction is a prototypical oscillating chemical reaction with a visible cue of oxidation state given by the complex autocatalytic reaction of bromide, malonic acid, bromate, and ferroin. As discovered by Showalter et al., initial conditions determine whether the system will be in an auto-oscillatory state ([H+][BrO3-] >0.045 M2) or an excitable state ([H+][BrO3-] <0.045 M2) where oscillations may be induced. Therefore, the BZ reaction exhibits an auto-oscillatory/excitable boundary. The focus of this research is to demonstrate that through manipulation of reagent concentrations, the BZ reaction can be used as a qualitative model for other natural systems that exhibit this behavior, such as the electromagnetic heartbeat or nerve impulses. Theoretical models were created to approach the system’s behavior with changing initial conditions and introducing perturbations to it in the form of pH changes in a sinusoidal pattern (heterodyne model). The model showed very little change in period. Experimental work used base pulses as its perturbations in a ‘square wave’ pattern in an attempt to mimic the sinusoidal behavior of the theoretical model. Introducing pulses 15s after each oscillation had no effect on period, whereas the introduction of a base pulse every 60s after the first oscillation increased period time.
Ascorbic acid enhances cytotoxicity of a novel naphthoquinone containing a modified anthracycline Ring System

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A naphthoquinone compound (12,13-dihydro-N-methyl-6,11,13-troxo-5H-benzo[4,5]cyclohepta[1,2-b]naphthalene-5,12-imine) known as TU100 was previously synthesized as a potential chemotherapeutic agent. Evaluation of its biological activity using cancer cell lines revealed that TU100 is cytotoxic in part because it generates reactive oxygen species that likely cause DNA damage, cell cycle arrest, and ultimately apoptosis. Based on these results we hypothesized that ascorbic acid might promote TU100 production of reactive oxygen species via a redox cycling mechanism. To test this idea cancer cell lines were treated with varying concentrations of TU100 in the presence and absence of ascorbic acid, followed by evaluation of cell viability using a resazurin-based fluorescent assay. Our results show that ascorbic acid greatly enhanced the cytotoxicity of TU100, such that the cancer cells died at much lower concentrations of the drug. To determine if this enhanced cell death was due to increased production of reactive oxygen species, we utilized dihydroethidium bromide to measure their production in cells treated with TU100 with and without ascorbic acid. Both fluorescence microscopy and quantitative measurement of fluorescence using a plate reader revealed that ascorbic acid greatly increases the production of reactive oxygen species produced in the presence of TU100. These results provide further evidence that TU100 cytotoxicity is mediated by production of reactive oxygen species, and raise the possibility of using ascorbic acid to enhance this effect in order to promote cancer cell death.

Site selective Pd-catalyzed intramolecular cyclization of oxygen nucleophiles

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Natural product synthesis has been a chief goal for organic chemists and continues to present a formidable challenge due to their complex molecular architecture. Due to the complex nature of these naturally occurring molecules and their relevance in drug targets, there is high demand for reliable synthetic methods to efficiently synthesize natural product scaffolds. A structural motif ubiquitous in natural products is the heterocycle; traditionally synthesized through substitution pathways that are often unpredictable and difficult to control as the molecule becomes increasingly complex. Here we report a removable directing group approach to the intramolecular cyclization
of alcohols via directed Pd catalyzed activation of sp3 C-H bonds to provide heterocyclic compounds. Under our conditions, various ring sizes have been achieved in moderate to high yields, where primary secondary and tertiary alcohols are all tolerated. In addition, the intramolecular cyclization to form spirocyclic compounds have also been observed in moderate yields. This discovery provides a novel method for intramolecular cyclization that is both catalytic and site selective, a promising tool for natural product synthesis.

CHED 563

Comparison of nutrient deprived cellular behavior in transformed and untransformed cells

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During early tumor formation, before angiogenesis, cancer cells must proliferate in a nutrient poor environment. One way to acquire carbon sources would be to cannibalize surrounding cells. This hypothesis is being investigated in a tissue culture model system in which a cancer cell line is allowed to reach confluence, at which point they begin to form tumor-like structures called foci. In contrast, normal cells undergo contact inhibition and so exit the proliferative cycle. Cell death in foci and untransformed cells under various growth conditions has been investigated using immunofluorescent microscopy. Critical carbon sources like glucose and glutamine were removed from the media and effects on cell organization and viability were evaluated. Results suggest cells in the center of the foci preferentially died, which may reflect their ability to obtain nutrients. Alternatively, they might be cannibalized by exterior cells due to their weakened state. Untransformed normal human fibroblasts also died under nutrient depleted conditions, but in marked contrast to transformed cells showed no apparent pattern in the cell population.

CHED 564

Photographic evidence of reactions in organic chemistry: The formation of trans-diols from cyclohexene and meta-chloroperbenzoic acid

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Organic chemistry plays an important role in many areas of science; however, students are faced with severe challenges in studying the subject. One crucial problem is that the subject has been taught in a rather abstract fashion using text and line art accompanied by some figures, most notably electrostatic potential maps, and various spectra. This pedagogy is especially challenging for students who need visual reinforcement of
course material. In this photographic study we focus on the transformation of cyclohexene into trans-1,2-cyclohexanediol via cyclohexene oxide. In addition to providing visual evidence for the reaction outcome, the experiments provide evidence for the reaction stereochemistry, which is a central feature of the reaction mechanism. Cyclohexene reacted with pure meta-chloroperbenzoic acid (MCPBA) to form cyclohexene oxide and a precipitate of meta-chlorobenzoic acid (MCBA) byproduct. Visual evidence of cyclohexene oxide formation was supplied by boiling point and formation of a green color with Reichardt’s dye. The MCBA was confirmed by comparison of its \( pK_a \) 3.82, with that of MCPBA, \( pK_a \) 7.52. Hydrolysis of cyclohexene oxide yielded trans-1,2-cyclohexanediol. Proof of the trans-diol formation was generated by melting point and from a study of the rates of decolorization of the red complex formed by reaction of the diol and ceric ammonium nitrate (CAN). 1,2-trans-cyclohexanediol is decolorized (as a result of oxidation) much more rapidly than the complexes of simple alkyl alcohols. In contrast, the cis-1,2-cyclohexanediol complex decomposes significantly faster than the trans-product.

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CHED 565

Carbonic anhydrase as a model for matrix metalloproteinase inhibition

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Carbonic anhydrase (CA) is being used as a model for matrix metalloproteinases (MMPs). CA is a more ubiquitous protein that binds zinc in the same manner as MMPs, in a tri-histidine manner. Potential pharmaceutical building blocks are being evaluated using CA as a model due to this structural similarity in order to probe binding information.

CHED 566

Completing a green chemistry laboratory manual for general chemistry

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Green chemistry is the philosophy of designing safer chemical products and processes from the beginning. Greener laboratory procedures reduce or eliminate hazardous materials and hazardous waste. These procedures are typically safer for the
environment as well as students. There is a need for educational laboratory materials that not only make experiments greener, but also teaches students how to implement green chemistry. This research involved completing the writing of a green chemistry laboratory manual for the general chemistry level that provides greener experiments and teaches the principles of green chemistry.

CHED 567

Utilization of polymeric quaternary ammonium salts-clay composite in triphase catalysis

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A series of novel heterogeneous catalysts have been synthesized through intercalation reaction of sodium montmorillonite clay (Na-MMT) with polymeric quaternary ammonium salts. The resulting solid catalysts have been utilized in triphase catalysis which is a unique branch of phase transfer catalysis (PTC). In triphase catalysis, reactants and the catalyst are located in various phases such as water, organic and solid phase. In this study, low molecular weight polyimide as well as various molecular weight poly (propylene glycol)bis(2-aminopropyl ether) with an average molecular weight of 2000 and 4000 has been used to synthesize the polymer-MMT composites as a catalyst. Catalytic activity of these organo-clays structures have been tested in several nucleophilic displacement reactions such as conversion of n-butyl bromide to n-butyl acetate and iodide under a triphase reaction condition. Pseudo-first order kinetics has been observed with various catalytic activities. These kinds of polymer-MMT composite may provide a potential for synthesizing more robust and heat resistant heterogeneous catalysts than traditional organo-clay using quaternary ammonium catalyst.

CHED 568

Efficiency of synthetic pyrazoline derivatives on inhibiting Entamoeba histolytica growth as novel treatment against amebiasis

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Amebiasis causes 100,000 deaths per year worldwide. The current treatment, metronidazole has toxic side effects. Alternative treatments are of interest. We examined the efficiency of four series of synthetic pyrazoline compounds on inhibiting growth of E. histolytica, the causative agent of amebiasis. The efficacy of these compounds depends on the functional halogen group; for example, chlorine affects activity more than bromine. Four series (sets of 3-8 compounds per series) of pyrazoline
analogues were synthesized and evaluated in their abilities to inhibit amoebic growth. Series 1a (1,3-diphenyl-1-carbamoyl-2-pyrazoline), series 1b (3-diphenyl-1-propylcarbamoyl-2-pyrazoline), series 2 (1,3,4-triphenyl-1-carbamoyl-2-pyrazoline), pyrazoline derivatives showed capabilities to inhibit amoebic growth. The following compounds show promising results: from series 1a [3-(4-chlorophenyl)-1-(bromophenylcarboxamide)-2-pyrazoline]; series 1b [3-(4-chlorophenyl)-1-N-propylcarboxamide-2-pyrazoline]; and series 2 [3-(4-chlorophenyl)-4-phenyl-1-(4-chlorophenyl thiocarboxamide)-2-pyrazoline]. The inhibitors were tested on their abilities to block growth of *E. histolytica* at varying concentrations compared to metronidazole. At a concentration of 120 µM, series 1a [3-(4-chlorophenyl)-1-(bromophenylcarboxamide)-2-pyrazoline], and series 1b [3-(4-chlorophenyl)-1-N-propylcarboxamide-2-pyrazoline] pyrazolines significantly inhibited trophozoite growth at a rate similar to metronidazole. Series 1a and 1b pyrazolines are less bulky with one less substituent on the pyrazoline ring than series 2 pyrazolines, which may allow them to more easily bind and inhibit EhADH2, which has been shown to be the site of inhibition. Future studies will elucidate the mechanism of action of these compounds.

**Growth inhibition of *E. histolytica***

Pyrazoline Inhibitor # 15

![Growth inhibition graph](image)

Dr. Siegler, John Hopkins University, Small Molecules X-ray Crystallography

CHED 569

**Role of GRK4 in bladder exstrophy-epispadias complex**
Bladder Exstrophy-Epispiadias Complex (BEEC) is a congenital anomaly of the urinary tract that occurs in 1 in 20,000 to 80,000 births. However, in families with a previous occurrence of BEEC, the incidence is 1 in 100 births, a significant increase over the population incidence, indicating a possible genetic factor. Analysis of array Comparative Genomic Hybridization (aCGH) results from a BEEC patient population revealed a patient with a microduplication encompassing the G Protein-Coupled Receptor kinase 4 (GRK4) gene. Copy number variations of GRK4 are rare in the general population, with a frequency of 0.162% (https://decipher.sanger.ac.uk). Also, we identified 10 patients with urological defects, mainly of the kidney and bladder, with CNVs containing GRK4. The low frequency CNVs containing GRK4 and their association with urological defects makes GRK4 a promising candidate for study.

GRK4 is one of six members of a G protein-coupled receptor kinase family that desensitize activated, agonist bound G protein-coupled receptors (GPCR) through phosphorylation. GRK4 is known to phosphorylate the dopamine D1 receptor, which leads to a decrease in cellular levels of cyclic AMP (cAMP).

Sequencing and analysis of patient DNA revealed four patients with potentially dangerous mutations in the GRK4 gene. The object of my research was to identify the effects of GRK4 mutations found in BEEC patients on protein function, by measuring cAMP levels of cells containing mutated GRK4 transcripts.

CHED 570

Impact of nanoparticles on bacterial community

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Despite the successful and useful application of nanoparticles (NPs) for creating new types of analytical tools for biotechnology and life sciences as well as for new engineering and energy materials, studies have identified an importance of understanding the fate and transport behavior of NPs in natural environments and the subsequent effects of them on ecosystems. For example, toxicological investigations of NPs on bacteria and living organisms have shown that they pose a significant adverse impact over a wide range of microbial communities. However, such studies require more systematic and fundamental approaches because NPs vary widely in their physicochemical properties depending on the environmental factors. This study presents the interactions between zinc oxide (ZnO) and iron oxide (FeO) NPs with Shewanella oneidensis MR-1 strain. We examined the cytotoxic effects of these specific NPs on S. oneidensis by varying the concentrations of NPs, particles sizes of them, and the types of NPs. Microbial growth was continuously monitored after incubation of NPs with cell suspensions, and the samples were tested for cell viability by absorbance.
spectroscopy. Tests including attenuated total reflectance- Fourier transformed infrared (ATR-FTIR) spectroscopy, x-ray diffraction (XRD), and bioassays were conducted to identify the extents of the effects of the investigated variables. We believe that results of this study will provide a fundamental milestone for enhancing our knowledge on NPs and their impact of ecological environment.

CHED 571

Hands-on activity incorporating the threefold representation on the limiting reactant concept

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According to Johnstone’s model, chemistry can be taught at three levels of representation: macroscopic, submicroscopic, and symbolic. The model suggests that to gain a full understanding about chemistry concepts, a learner has to be able to connect the three levels of representation. Following Johnstone’s model, a hands-on activity that incorporates the three levels of representation for the limiting reactant topic has being developed. The activity was designed to help students hone their understanding of the limiting reactant concept in an active environment, after the topic has being introduced in class. The main objective of the project is to measure the impact that the hands-on activity incorporating the three-fold representation has in students’ understanding about the limiting reactant concept. The activity was implemented with undergraduate students enrolled in the first sequence of a general chemistry course at a four-year undergraduate institution in Puerto Rico. To assess the learner’s conceptual understanding, an assessment instrument was developed and implemented before and after students worked on the activity. In addition, qualitative data from observations and students’ comments during their work on the activity was collected. The results gathered during the implementation will be presented.

CHED 572

Probing the question-order effect on chemistry concept inventories

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Previous research shows conflicting results as to whether or not question order on exams would have an effect on student performance. Since many teachers randomize test questions in order to prevent cheating, there is some concern as to whether this would give certain students an conceptual advantage. The purpose of this research
The project is to address this concern by analyzing the question order effect, or lack thereof, on chemistry concept inventories. The primary research question being investigated is: How does question order influence student performance on conceptually isomorphic questions when presented with pictorial and verbal versions of the questions? In particular, we probe the effect of priming of verbal versus pictorial questions, relative question location, and students’ level of chemical expertise on student performance.

This project follows a Mixed Methods Explanatory research design, incorporating quantitative and qualitative data analysis. First, students complete an online twenty-question concept inventory over acid-base concepts. Our conceptually isomorphic pictorial and verbal questions are inserted into the concept inventory at specific places among a static set of questions, resulting in four different test versions. Student scores are analyzed using SPSS. Quantitative analysis compares students’ scores across the four test versions for accuracy, as well as to determine which misconceptions in the answer choices were the biggest distractors. A sub-sample of the students are then asked to come in for think-aloud interviews, during which they work problems from their original test version. Interviews are then transcribed and coded based on grounded theory. We will present in this poster the preliminary analysis of the survey and interview data.

CHED 573

Impact of an intensive workshop on STEM faculty’s fidelity of implementation of peer instruction

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Peer instruction is an example of an evidence-based instructional practice, i.e., practice that has been empirically proven to enhance students’ learning and attitude toward science. It consists of presenting a question to students, having the students think individually and vote using a personal response system which is followed by peer discussion and revote if the majority of the class chose wrong choices on the individual vote. Research investigating faculty’s implementation of evidence-based instructional practices has demonstrated that faculty often adapt the practices rather than following the prescribed method. This potentially low level of fidelity of implementation can result in lack of effectiveness of the practice. Physics education researchers have demonstrated that knowledgeable Peer Instruction users substantially adapt the strategy, most notably by skipping the individual vote. In this study, we investigate the fidelity of implementation of Peer Instruction by STEM faculty who participated in a semester-long professional development solely focused on the implementation and the research supporting Peer Instruction. We collected video recordings of STEM faculty participating in this training program before and after their participation. Each clicker question asked during these recordings were analyzed using an adapted version of the observation protocol developed in physics by Turpen and Finkelstein. Changes in instructional behaviors and adherence to the empirically developed Peer Instruction
method by the STEM faculty who participated in the professional development program will be presented.

CHED 574

Elimination reaction of tropic acid as a simple example of an E1cb reaction

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We have developed an economical and simple laboratory exercise that demonstrates an E1cb mechanism using inexpensive tropic acid and potassium hydroxide. The reaction involves a 40 minute reflux followed by neutralization and recrystallization. Student results generally yield 50 – 70% of pure atropic acid (2-phenylpropenoic acid) product. This exercise involves reflux, neutralization, recrystallization, and melting point analysis. If one chooses to run the NMR on the final product, there is an opportunity to teach about diastereotopic protons on terminal alkenes as well. Both the starting material and final product have no known health hazards and the only solvent used is water. The hazards are confined to the small amount solid potassium hydroxide and dilute hydrochloric acid that are used.

Mechanism of the E1cb reaction showing intermediates.
Resonance stabilized carbanion intermediate.

CHED 575

Chemistry teaching laboratories: What is the point?

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The periodic review of goals for a course is important for proper student learning. Reviewing course goals may also lead to curriculum changes to better align them with the needs of the current student population within a course. In this study, faculty and student opinions of the introductory chemistry laboratory at the University of Northern Colorado are compared and contrasted. Data was collected via the use of Likert-style surveys, which were informed by open-ended faculty interviews on their opinions of what students should get out of the laboratory. From these surveys, faculty and student choices were grouped into agree and disagree categories for faculty and agree, disagree, and neutral categories for students. These categories were used to ascertain overall agreement or disagreement with each statement for faculty and student data. In addition to the overall results, student data was broken down by major to analyze for potential differences. It was discovered that there are currently several areas in which faculty expectation of what should be taught in the course largely outweigh what students report learning. Based on the faculty and student results, suggestions are
made for potential curriculum improvements to enhance future faculty/student coherence.

CHED 576

Effect of *Azadirachta indica* tree in the CYP450 system of chinese hamster ovarian cells

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The *Azadirachta indica* tree, better known as Neem, has been used since ancient times as a medicinal plant. It is originally from India, besides being known for its medicinal properties is used in agriculture as a fertilizer and insect repellent. It is associate with the prevention of various diseases including diabetes, cancer, Alzheimer, psoriasis, AIDS, dental disorders, allergies, ulcers, dermatology, herpes, and other conditions. Effect of extracts from Neem leaves and stems, dried and not dried, were tested. Chinese Hamster Ovarian cells were cultivated to study the effect of the extracts on the CYP450 system. Cell microsomes were prepared to perform biochemical assays. Assays included: Bradford, hydroxylation of p-Nitrophenol, activity of 7-Ethoxyresorufin (EROD), Erythromycin N-demethylase-(ERND) and cytochrome P450. Toxicological tests were carried out using brine shrimp. Assays were repeated three times to apply statistical analysis. Cells will be treated with cadmium to measure the effect on cell proliferation. Neem extracts will be used in treated cells and biochemical assays will be performed to measure the effect on CYP450 system.

CHED 577

Dioxygen activation by mononuclear non-heme iron oxygenases and the corresponding model complexes

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The activation of O₂ is a process that occurs naturally when enzymes containing iron centers, known as mononuclear non-heme iron oxygenase (MNO) enzymes, oxidize challenging substrates. The objective of this project is to develop synthetic model complexes that can mimic the reactivity properties of these MNO enzymes. The use of iron in these catalytic systems is particularly attractive as this metal is earth-abundant and non-toxic and thus this effort opens new avenues in inexpensive and sustainable catalytic transformations. An N₂O₅ ligand set and its reaction with α-ketoglutarate to generate the Fe³⁺/α-ketoglutarate complex was investigated as an MNO enzyme mimic.
We have experimentally observed that the structurally characterized fac-[Fe$^{II}$$(N_2O_1)(sol)_3]^{+}$ complex: (i) rapidly reacts with a variety of $\alpha$-ketoacids to form 1:1 complexes, (ii) shows significantly enhanced oxygen sensitivity when coordinated by $\alpha$-ketoacids, (iii) rapidly decomposes the $\alpha$-ketoacid ligand to CO$_2$ and the corresponding carboxylate ligand, and (iv) generates an Fe-based reactive intermediate that is kinetically competent. A cyclic reaction was observed, where each mole of $\alpha$-ketoglutarate added, gave rise to 1 mole each of water, formaldehyde, and succinic acid (completely coupled reaction). A Nash Assay was performed to determine the amount of formaldehyde within each sample. A Karl Fischer titration was used to determine the amount of water within each sample.

Supported by NSF-REU, Boston University

CHED 578

Developing and evaluating a collaborative learning environment in analytical chemistry

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Collaborative learning, argumentation and development of critical thinking are skills students need to succeed in the STEM fields. Building upon the ideas of inquiry, communication and application, we converted a traditional analytical chemistry lecture to a collaborative learning course using an Active Learning and Technology (ALT) classroom. The flipped classroom approach included online tutorial-based homework, in class problems sets and a combination of individual and collaborative assignments and assessments. Information about student motivation, study techniques and exam scores were collected and analyzed based on the ALT room experience. Daily quizzes reflected students attendance, which influenced exam scores. The America Chemical Society (ACS) Analytical Exam, standardized exam, has been given as the final exam for this course over the progression from a tradition lecture style class to a full collaborative learning environment. We observed that students who objected to the collaborative approach and refused to participate were less successful than those who engaged. Results from this semester’s class show both active and reflective students have the potential to succeed in an ALT classroom. Currently, it can be concluded that both active and reflective students can succeed in a collaborative classroom environment. In this presentation we will present the statistical results and detailed conclusions of this study. Further work will establish the most efficient ways to motivate students, the most effective way to connect with every student, and solid structure so that all students feel that they can succeed by collaborative learning.

CHED 579

Holistic trace analysis: Development of an upper-level chemistry experience
Chemical analyses using analytical chemistry are engrained within all sub-disciplines of chemistry and thus encompass a far-reaching skill set all undergraduate students should acquire. Rarely do undergraduate students experience a complete analysis from conception to completion. Herein we present an upper-level educational laboratory experience designed for Hendrix College’s Advanced Techniques in Experimental Chemistry, an interdisciplinary laboratory combining physical, inorganic and analytical chemistry techniques. This four week experiment requires students to design an experiment to analyze PM10 and PM2.5 aerosol samples collected using a Tisch volumetric flow controlled Hi-Vol sampler. Opportunities for analysis include trace metals, organics or ions using graphite furnace atomic absorption spectroscopy (GFAAS), gas chromatography/mass spectrometry or ion chromatography, respectively. The focus of assessment is on analysis development and execution. This experiment takes a holistic approach to trace analysis by encompassing all the elements of experimental design while providing students with an opportunity to think about the chemical composition of atmospheric particles, emission sources and human health effects.

CHED 580

Paper microfluidic method to quantify taurine in urine samples: A college-level introductory chemistry experiment

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This laboratory experiment is designed to introduce college students to paper microfluidics and the role of biomarkers in detecting various diseases. The procedure allows students to design paper microfluidic systems using inexpensive materials that are available in most college laboratories. In this experiment, taurine an organic acid which can also act as a cancer biomarker is prepared in a synthetic urine-phosphate buffer solution (pH = 10.3), and is allowed to react with sodium hypochlorite and phenol on rectangular filter paper. The reaction can be observed through the purple-colored indo-phenol dye formation on the filter paper. The intensity of this color change is measured with graphics software, such as Adobe Photoshop™. Over a three-hour laboratory period, students work in teams to prepare the necessary solutions and design paper microfluidic devices to quantify the intensity of the end product after the reaction. Calibration standards are prepared in a synthetic urine matrix in order to account for the matrix effect. Students can use the mean intensity versus taurine concentration calibration curve to quantify taurine in an unknown urine sample. The experiment can be done within two hours, which provides the students with the opportunity to use their additional time to redesign the systems and improve the precision of their work. This experiment is designed to help students explore the
relationship between the concentration of taurine and the intensity of the indo-phenol dye through the construction of a calibration curve. They also learn the importance of the matrix effect in the quantitative analysis. Additionally, students are introduced to non-traditional methods of quantitative analysis. This shows them that although some things may seem unrelated to any field of scientific research, such as graphics editing software, they can still be combined with chemistry to make an ideal analytical tool. Finally, with simple modifications, this method can be used to quantify taurine in other types of samples, in addition to urine.

CHED 581

Epoxyeicsatrienoic acid analog mitigates kidney injury in experimental radiation nephropathy

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In this study, we investigated the kidney protective effects of eipoxyeicosatrienoic acid analog (EET-A) in experimental radiation nephropathy caused by total body irradiation (TBI) of 11 Gray (Gy). Male WAG/RijCmcr rats were divided into four groups: normal rats (control), TBI rats treated with vehicle (TBI-V), TBI rats treated with EET-A (10 mg/kg/d, TBI-EET-A) or captopril (30 mg/kg/d, TBI-Cap) in drinking water. Urine and plasma samples were collected after 12-week treatment to assess kidney protective effects of EET-A and captopril by determining blood urea nitrogen (BUN), proteinuria, albuminuria, nephrinuria, and histopathological examination. 12-week post TBI blood samples demonstrate elevated BUN level in TBI-V compared to control group (44±5 vs. 18±1 mg/dL, P<0.001). EET-A and captopril treatments reduced BUN levels compared to TBI-V group (EET-A: 27±3 mg/dL and TBI-Cap: 18±1 mg/dL, P<0.01). The TBI-V group had elevated urinary albumin (310±50 mg/d) compared to control (0.9±0.1 mg/d), and both EET-A and captopril treatments reduced it (P<0.001). Moreover, TBI-V group demonstrate elevated urinary nephrin level (5.7±0.9 mg/d) compared to control (0.07±0.01 mg/d), and EET-A as well as captopril treatments attenuated this (P<0.001). In brief, we demonstrate that the captopril and EET-A treatments mitigate kidney injury in radiation nephropathy, and EET analog could be a new therapeutic target to treat radiation nephropathy.

CHED 582

Toward a comprehensive integration of calorimetry across the curriculum

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Student comments indicate that calorimetry is one of the most difficult labs currently in our General Chemistry sequence. Research was focused on developing a multi-week laboratory experiment for General Chemistry students to study and explore various aspects of calorimetry. The goal was to replace the current one-week calorimetry lab with a two-week lab allowing students to better process and understand the techniques of calorimetry.

In addition to the General Chemistry lab we have been able to add the concept of constant volume calorimetry to the allied health General, Organic, and Biological Chemistry course. Students have traditionally only used constant pressure calorimetry to measure the heat liberated from a burning nut. To include constant volume calorimetry, a video was produced showing the use of the bomb calorimeter and the data for burning the nut. By burning food in both calorimeters and determining the total calories obtained from each, students will be able to learn the differences in accuracy for each type. To further cement the concept of heat transfer, an inquiry lab related to heat transfer was developed for students to understand how different container materials insulate a system from its surroundings.

Analysis of student synthesized biodiesel and other organic samples allows the concept of calorimetry to be continued in the Organic Chemistry sequences, which helps validate its usefulness as an analytical tool. By bringing constant volume calorimetry into a variety of classes we can improve students' understanding of heat transfer and analytical tools for measuring this transfer.

**CHED 583**

**Documenting collective activity in a large scale introductory chemistry class**

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My project focuses on Process Oriented Guided Inquiry Learning (POGIL), a teaching method intended to help students learn chemistry by using process skills such as critical thinking, assessment and communication. Typically, POGIL is implemented in smaller classes, but this project observes POGIL on a large scale in a freshman General Chemistry lecture of over 100 students. The data was collected by recording teacher-student interactions during the whole class discussions and one group of students during small group work. This data was then transcribed verbatim for analysis. The class went over the following topics during our research: stoichiometry, Lewis structures, bonding, and thermodynamics. The purpose of this project was to analyze how an instructor’s implementation of the POGIL materials influenced student argumentation and conceptual understanding of chemistry. This data was studied with an analytical approach utilizing Toulmin’s Model of Argumentation and the Inquiry Oriented Discursive Moves framework to examine how the class translated between
macro, sub-micro, and symbolic levels of representation. Analysis of the materials indicated which questions prompt which levels of conceptual thinking. Analysis of the instructor’s pedagogy and student interactions provided insight into the dynamics of small group and whole class discussions, the instructor and course material influences on the quality of scientific arguments developed by students, and students’ conceptual understanding of freshman-level chemistry.

CHED 584

Synthesis of highly functionalized nitrogen containing monoadducts via copper catalyzed atom transfer radical addition (ATRA)

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Atom transfer radical addition (ATRA) is a technique used for the formation of C-C and C-X (X = halide, pseudohalide) bonds by the addition of alkyl halide across the double bond of an alkene. The final product, monoadduct, is a highly functionalized molecule and can be used as a precursor for drug discovery and natural product syntheses. Nitrogen containing monomers such as 4-vinylpyridine, 2-vinylpyridine, 4-acryloymorpholine, N-methyl-N-vinylacetamide and 1-vinylimidazole were utilized for the first time in ATRA, catalyzed by [CuII(TPMA)X][X] (TPMA = tris(2-pyridylmethyl)amine; X= Cl, Br) with carbon tetrahalide (CX₄; X = Cl, Br). According to the preliminary kinetic studies, almost complete conversion was observed in less than 6 hours, which is not typically observed in ATRA with α-olefins and acrylates, indicating the high activity of N-based monomers. The monoadducts were successfully isolated and characterized using different spectroscopic techniques such as ¹H, and ¹³C NMR, HETCOR, IR and UV-Vis spectroscopy.
CHED 585

Targeting Glutaminolysis to selectively kill cancer cells with deregulated p27

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P27kip1 is a tumor suppressor protein commonly deregulated in aggressive cancers. It is thought to function as a cyclin-CDK inhibitor that blocks cell cycle progression. However, we recently discovered p27kip1 also controls a metabolic switch regulating nutrient usage. Like cancer cells, immortalized fibroblasts typically rely on aerobic glycolysis rather mitochondria for energy production because they need glucose carbons for cell proliferation. Surprisingly, however, cells lacking p27 (p27−/−) switched to metabolizing glutamine when glucose levels modestly declined, which would require TCA cycle and mitochondria to produce energy. This metabolic switch could provide a growth advantage during early tumor development before blood vessel formation. We hypothesized aggressive cancers with deregulated p27 could be targeted by artificially decreasing glucose levels and then inhibiting glutamine metabolism. To test this idea, p27 +/+ and p27−/- cells were treated with 2-deoxy-glucose followed by exposure to the mitochondrial inhibitor rotenone. Cells lacking p27 were preferentially killed by this drug protocol, indicating they switched to glutamine and thus required functioning mitochondria. In marked contrast, cells containing p27 were relatively unaffected because they continued to rely on available glucose and aerobic glycolysis rather than...
mitochondria for energy production. These observations provide a novel method for targeting aggressive cancers with deregulated p27.

CHED 586

Impact of cost on chemistry laboratory teaching practices

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Laboratory-based activities have been shown to be important and valuable learning opportunities in high school chemistry. However, there are different costs associated with laboratory-based learning, such as money, time and space. By gaining a better understanding of cost in the laboratory setting, the impact of cost on chemistry teachers' laboratory practices can be evaluated. This project studied Iowa secondary chemistry teachers' classroom laboratory teaching practices and how the teachers perceive laboratory-related costs in their classrooms. It aims to understand how the various costs may impact laboratory teaching practices. An online survey and semi-structured phone interviews were used in an effort to better understand the role of cost in the chemistry classroom laboratory setting. A majority of teachers reported that they incorporate laboratory-based activities three to five times per month, though many teachers also stated that they sometimes use computer simulations or teacher demonstration in place of a laboratory-based activity. Teachers indicated that their laboratory teaching practices are sometimes influenced by the materials readily available to them. Nearly all respondents claim to have spent personal funds on laboratory materials. Additional findings will be presented on the poster. Based on the findings, recommendations are made to encourage the use of laboratory-based activities in high school chemistry.

CHED 587

Developing a redox themed assessment instrument using the three levels of representation

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A deep conceptual understanding of redox reactions requires the interpretation and interconnection of the three levels of representation: macroscopic, submicroscopic, and symbolic. According to Johnstone’s model, meaningful learning is achieved when a subject is capable to make interconnections between the three levels of representation for a concept. In this project an assessment instrument was developed to measure students' understanding about the concepts involved in redox reactions, based on the
subjects' ability to interconnect and analyze the three levels of representation. The instrument consists of multiple-choice and open-ended items. For each multiple-choice item, a gradient was developed that allows classifying students' answers by levels of understanding. The instrument was administered to 31 first-year chemistry major students enrolled in the second semester of general chemistry course at an undergraduate institution. The results of the implementation and the alternative conceptions identified with the instrument will be presented.

CHED 588

Use of organic base to restore catalytic activity of [Cu(Me₆TREN)Cl][Cl] in Atom Transfer Radical Addition (ATRA) in the presence of ascorbic acid as a reducing agent

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Copper-catalyzed atom transfer radical addition (ATRA) is used for C-C bond formation through the addition of alkyl halides across various alkenes. According to electrochemical and mechanistic studies, copper complexes with Me₆TREN (tris(2-dimethylaminoethyl)amine ligand should be theoretically ~10 times more active than with TPMA (tris(2-pyridylmethyl)amine). However, catalytic studies in ATRA with different alkenes and alkyl halides showed the opposite trend. Catalyst regeneration is necessary for ATRA due to unavoidable diffusion controlled radical-radical terminations. The side product of the oxidation of ascorbic acid is the generation of H-X which protonates the Me₆TREN ligand, rendering it unable to coordinate to the copper. In this ATRA study, several weak bases were employed to inhibit the degradation of the ligand and restore the catalytic activity. These bases were used in different stoichiometric ratios relative to ascorbic acid with the addition of CCl₄ across various alkenes catalyzed by [Cu(Me₆TREN)Cl][Cl]. In this study, it was found that the 5:1 ratio of base to ascorbic acid was the most effective and increased the catalytic activity of [Cu(Me₆TREN)Cl][Cl] to nearly quantitative yields. In addition, kinetic studies demonstrated faster reaction completion with the ligand reducing the reaction time from 24 hours to 4 hours and decreased the reaction temperature from 60 °C to room temperature.

CHED 589

Investigation of HOBS methodology in nucleic acid NMR studies

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Homodecoupled band-selective (HOBS) NMR methodology was tested to see how it could enhance the resolution of sugar (cellobiose octaacetate) and nucleic acid (6-, 10-, and 16-mer oligonucleotides) spectra. Using the basic HOBS acquisition sequence for
one-dimensional proton experiments, pulse programs were generated and tested for advanced NOESY, ROESY, and TOCSY experiments. The efficacy of HOBS acquisitions was compared to those of both normal and purely band-selective pulse programs in both one- and two-dimensional methods. With the 6-mer, direct comparisons were made between measurements of $T_1$ relaxation delays in both HOBS-style and normal acquisitions. Using HOBS methods, values obtained for $T_1$ were more precise than those measured under a standard method due to the enhanced resolution brought forth by decoupling – in the H5 region of the spectra, the standard deviations of $T_1$-values determined by peak-picking decreased by as much as 0.033 s when implementing HOBS techniques. Finally, HOBS methods were compared to two other pure-shift related methods – instantaneous pure shift (IPS) and pure shift yielded by chirp excitation (PSYCHE).

**CHED 590**

**Enantiomeric interactions of amino acids adsorbed in zeolites: An investigation, using solid-state NMR, thermogravimetry (TGA) and differential scanning calorimetry (DSC)**

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Chemistry of life depends on chirality, whose origination is a fundamental question. We study zeolites as a possible medium for enriching the enantiomeric excess of solutions. Achiral Zeolite lattices do not prefer one enantiomer over the other, and adsorb the enantiomers equally well. However, if the D- and L- enantiomers adsorb together as a heterodimer, the enantiomeric excess of the solution they leave behind is augmented. We used NMR, TGA, DSC to explore the adsorption behaviors of D-, L-, and DL- N-acetyl Leucine, Alanine and Methionine into Zeolite NaY. The solid state NMR spectra of the pure D- and L- acetyl Leucine showed the same results as the racemic mixture of N-acetyl-DL-Leucine, indicating a preference to form microcrystals of pure D and L forms. In contrast differences in the solid state NMR spectra are observed for N-Acetyl -DL- Methionine and N-acetyl-DL -Alanine from their pure enantiomers. This implied that both form a mixed crystal. However when adsorbed onto the zeolite, N-Acetyl Methionine and N-acetyl-Alanine exhibit the same behavior as its Leucine counterpart indicating that they are adsorbed as homodimers. NMR line widths of all compounds show a 10 fold increase when adsorbed in NaY indicating restricted molecular motion. TGA data for all compounds exhibits roughly 12-15% adsorption of the amino acids under air. Pure NaY shows 34 % water adsorption; which decreases to 4% after drying at 425°C for 4.5 hours. Exothermic decomposition of the samples is observed with DSC, and TGA performed under Argon.
CHED 591

Synthesis of pyridone-based ligands for homogenous hydrogenation iron-based catalysts

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The amount of waste produced by the chemical industry as a whole is in the millions of tons per year. Many processes are very sustainable, but the sizeable scale of reactions inevitably mean the amount of waste is also large. To date, catalysis has helped tremendously to reduce waste in the industry and increase the efficiency of reactions. For example, catalytic homogenous hydrogenations are prevalent in pharmaceutical syntheses. The catalysts currently available for homogenous hydrogenations are efficient but are not perfect: they are expensive, toxic, and environmentally unsustainable. The synthesis of new catalysts based on iron – an abundant, cheap, and environmentally friendly metal – would address several of these serious limitations. Research in our lab has been focused on the development of iron-based homogenous hydrogenation catalysts that work through a ligand-assisted heterolytic cleavage mechanism. Our system involves a pyridone-based ligand-assisted heterolytic cleavage of dihydrogen. The focus of this presentation will be on the synthesis of eight pyridone ligands. We will also briefly discuss strategies being used to form the corresponding iron complexes.

Pyridone-based ligand-assisted heterolytic cleavage of H₂

CHED 592

Adapting a set of organic chemistry experiments for delayed analysis time

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One of the experiments we carry out in our first semester organic chemistry laboratory course is a substitution reaction to synthesize an alkyl halide. Subsequently, the alkyl halide product is used as the starting material for an elimination reaction. Our lab schedule is such that we synthesize a compound one week and then analyze it the
following week. Initially, we used an experiment involving the synthesis of 2-chloro-2-methylbutane from 2-methyl-2-butanol. However, the products of the subsequent elimination reaction, 2-methyl-1-butene and 2-methyl-2-butene, were produced in such small amounts and were volatile enough that many of the students’ products evaporated before analysis, even when stored at 4°C. Therefore, we have undertaken modification of the experiment to use 3-methyl-3-pentanol in synthesizing 3-chloro-3-methylpentane, and subsequently performing the dehydrohalogenation reaction to produce 2-ethyl-1-butene and 3-methyl-2-pentene. We have tested the feasibility of this change and are working to optimize the modified procedures. We will present the results of our studies.

CHED 593

Preparation of NiFe supported catalysts for hydrotreatment

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Bimetallic Ni-Fe alloys are theorized to be more active than Ni or Fe for hydrotreatment of biofuels and allow for fine tuning of the properties of the catalyst. However, it has previously been a challenge to devise a consistent method of preparation which gives nanoparticles of homogeneous composition in a uniform size distribution. There is also little firm consensus on the exact catalyst composition which is most active. Here, two synthesis methods for bimetallic nanoparticles were attempted, deposition-precipitation (DP) on carbon or silica and colloidal synthesis. X-ray diffraction, X-ray fluorescence and temperature-programmed reduction were used to analyze the samples. The deposition-precipitation method produces bimetallic nickel-heavy nanoparticles (> 60 wt%) only when the DP reaction is carried out under inert atmosphere, otherwise predominantly iron deposits on the supporting material. When the reaction mixture contains too much iron (> 60 wt%), the particles adopt two separate compositions, that of pure iron and a nickel-heavy alloy. Colloidal synthesis forms bimetallic nanoparticles but further work needs to be done to investigate their stability.

CHED 594

Near infrared spectroscopy chemical Imaging for the determination of component segregation

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Most analytical methods report the content of an analyte within a sample. However, to understand the performance of many materials, the spatial distribution of its components must be known. This work serves the purpose of making most out of data handling, by facilitating its interpretation and accessibility for future generations of
Process Analytical Technologies (PAT) scientists. In this study, Near Infrared Chemical Imaging (NIR-CI) has been used to determine the spatial distribution of an active pharmaceutical ingredient (API) in a pharmaceutical formulation. NIR-CI is the combination of near infrared spectroscopy and image analysis. It is capable of providing information about the spatial distribution of the compounds in the samples. Each sample generates a hypercube containing thousands of spectra. NIR-CI is a powerful technique for providing high quality spectral information of the surface of samples. The advantages of this technique include no destructiveness of the sample, rapid analysis and real time monitoring.

The aim of the study was to obtain chemical images to determine the spatial distribution of the API, Acetaminophen (APAP). NIR chemical images provide characterization of heterogeneous solid dosage forms and were compared to different micrograph magnifications. Thus, spatial and chemical information of granules at different micron scale were obtained. The feasibility of this technique is assessed in order to describe granule properties. A concentration range of 50-100% w/w APAP was used for the analysis of tablets, with varying excipient concentrations. NIR-CI was used to evaluate the distribution of the chemical components throughout the tablets. The NIR-CI instrument used was a Malvern Spectral Dimensions SyNIRgi Chemical Imaging system with a wavelength range from 1200 – 2400 nm with an image matrix of 320 x 256 pixels. The NIR chemical imaging system showed the distribution of APAP at 1660 nm.

CHED 595

Preparing and screening brominated phenols: An organic laboratory experience

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This work will bring an experience to the organic teaching lab which is typically overlooked. That is the true experience or life of a synthetic chemist. In so many teaching labs, within the sciences, we focus on just doing experiments and force the experience into a “recipe.” This work evaluates the practical applications of preparing brominated phenol derivatives in a teaching lab setting. We will be laying the foundation for a semester long laboratory experience that involves preparing a multi-step small molecule and carrying it through biological screening.

CHED 596

Applying a greener approach to the Grignard reaction

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Environmental pollution that has accumulated from hundreds of years ago has reached alarming levels that are generating an environmental awareness. That’s an important reason to apply green chemistry to new methods of research in the field of chemistry. Moreover, we must educate the future generations to redesign existing methods to follow the green chemistry concepts. This research is focused in the design of a greener Grignard experiment for the organic chemistry laboratory course, in which the steps that students are intended to take are through the simulation of research that is performed nowadays. Also it allows them to correlate and integrate different concepts learned throughout the organic chemistry course. This experiment aims to involve students in the process of creativity and critical thinking, through a greener synthesis of a tertiary alcohol using three different routes. To meet the green chemistry principles, the solvent used was switched for one that is less harmful to the environment and less dangerous. Also the amount of solvent was reduced and a nitrogen atmosphere is not necessary. The results and limitations of this study will be presented.

CHED 597

Total synthesis of a calixarene cage

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Calix or chalice refers to a vase like structure. Calixarenes can be modified into specific types of host which could have many modern applications such as encapsulation, detection and delivery. Our calixarene-based host structure, contains a highly conjugated dithiepin-anthracene linker which should prove useful in exploring is applications to modern medicine or biochemical processes. The electron rich dithiepin framework will potentially provide a detectable change in UV absorption when interacting with a guest. This UV absorption change can be used as a detection method for a small organic molecule (drug) or metal ion. Previous research projects have established the dithiepins UV activity and the synthesis of some of the necessary fragments/precursors to synthesize the calixarene-based dithiepin host. The current project outlines the total synthesis, characterization and electronic properties of a calixarene-based dithiepin Host.

CHED 598

Human carbonyl reductase as target for alleviating anthracycline cardiotoxicity: Understanding small molecule binding by human carbonyl reductase

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Anthracyclines, commonly used chemotherapy drugs, are reduced by the enzyme Human Carbonyl Reductase (HCBR) into their alcohol metabolites, which lack cytotoxicity and possess cardiotoxic properties. Understanding how HCBR recognizes
and binds small molecules such as anthracyclines promises to provide insight into the
design of non-substrate anthracyclines, or inhibitors that could be coadministered with
the anthracyclines. A novel substrate, 2-acetyl-1-tetralone, was identified. Steady-state
kinetic measurements estimated values of 2.5±0.5s⁻¹, 220±20μM, and 0.011±0.002μM⁻¹s⁻¹
for kcat, Km, and kcat/Km values, respectively. Substrate inhibition was observed for
concentrations above 400μM, and its kinetic properties were similar to that of the
anthracycline Daunorubicin, suggesting its regioselective reduction by HCBR. Molecular
modeling experiments led to the identification of a novel inhibitor candidate and to the
hypothesis that the Met234 residue plays a role in anthracycline substrate specificity.
The rate observed for 2-acetyl-1-tetralone compared to known substrates was
anticipated by other molecular modeling experiment results.

CHED 599

Comparison of metacognitive abilities of introductory chemistry students

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A student’s ability to make judgments about their own knowledge and thought
processes is one aspect of metacognition. Students with high levels of metacognitive
skills are more academically successful. Being able to organize as well as reflect upon
one’s thoughts plays a crucial role in one’s educational experience, especially in STEM
fields. This study examines the relationship between students’ confidence in their ability
to answer a question correctly versus their performance on a subsequent assessment.
We administered a knowledge survey one week prior to a cumulative assessment.
Knowledge surveys encompass a range of topics from the entire course written at
various Bloom’s levels. Students are asked to respond about their confidence in their
ability to answer a question correctly. Their confidence has been compared to their
actual ability to answer a paired question on a cumulative assessment. This analysis
was done with sections of an introductory level chemistry class, using both a lecture
format and a student-centered learning approach.

CHED 600

Biochemical analysis of G-quadruplex secondary structures in CDK5R2 mRNA
and of their role in fragile X syndrome

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Fragile X syndrome (FXS) is a genetic disease that accounts for a majority of the cases
of inherited intellectual disability in humans. FXS results from the silencing of the fragile
X mental retardation 1 (FMR1) gene which is critical for proper brain development. In
the healthy brain, the FMR1 gene expresses high levels of fragile X mental retardation
protein (FMRP) which has been shown to be an important nuclear shuttling protein that also partakes in translational regulation of messenger RNAs (mRNAs). Although the root cause of this disorder is relatively well understood, the exact mechanism of its development is not. Because the FXS phenotype results from a lack of FMRP, a translational regulator, we have decided to study its possible mRNA targets to better understand the pathogenesis of the disorder. One way to select these mRNAs is to search for those with a high probability of forming G-quadruplex secondary structures, which are known to be targeted by the arginine-glycine-glycine (RGG) domain of FMRP. We have selected the cyclindependent kinase 5, regulatory subunit 2 (CDK5R2) mRNA for study because in silico energy modeling has predicted a high probability of G-quadruplex formation, and this mRNA has been shown to play a vital role in early brain development. Circular dichroism spectroscopy, $^1$H-nuclear magnetic resonance spectroscopy, UV spectroscopy, thermal denaturation experiments, and polyacrylamide gel electrophoresis were utilized to confirm the presence of and characterize G-quadruplex structures in the selected sequence. Electromobility shift assays and fluorescence spectroscopy experiments were performed to demonstrate the binding of FMRP to CDK5R2 mRNA, illustrating that FMRP may perform in vivo regulation of the mRNA in healthy (non-FXS) individuals, and therefore implicating it in the development of FXS.

CHED 601

Theoretical description of chemical shift anisotropy


Nuclear magnetic resonance (NMR) is a technique that takes advantage of a magnetic field to perturb a molecule in order to study the physical, chemical and biological properties of matter. The fundamental NMR parameter that allows for its successful application in a wide array of disciplines is the chemical shift. The theory behind the chemical shift phenomenon involves advance topics of electromagnetism and quantum mechanics. The objective here is to describe mathematical theory of magnetic resonance for the undergraduate student who wishes to pursue research in NMR spectroscopy. While numerous textbooks describe the chemical shift phenomenon, they are written for those with the proper background. By writing down the quantum mechanical expressions for magnetic shielding of nuclei at the undergraduate level, basic principles of quantum chemistry are reviewed and highlighted here. Due to the orientation dependence of shielding, the concept of anisotropy and tensorial math is also demonstrated.

CHED 602

Designing catalytic N-heterocyclic carbene complexes for enantioselective allylic oxidation
Due to the ubiquity of allylic alcohols, the efficient installation of a hydroxyl group adjacent to doubly bonded carbons has garnered considerable attention. Kharasch and Sosnovsky’s allylic oxidation has been shown to yield an effective conversion, with recent examples attaining moderate to excellent e.e.’s by employing chiral bis(oxazoline) ligands. Herein, we report the application of N-heterocyclic carbenes as ancillary ligands under these oxidative conditions. Achiral moieties have been synthesized and steps towards the synthesis of a chiral ligand are on going. Response surface methodology is currently being employed to model and optimize the NHC mediated oxidation by elucidating the effects of catalyst loading, time and temperature.

CHED 603

Development of a selection marker for automated genome construction

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Introduction:
Both selectable and counter-selectable markers are useful tools for genome engineering. Selectable markers are mainly used for plasmid maintenance, engineered conjugation and genome manipulation. On the other hand, counterselectable markers can aid in scar-less gene deletion, plasmid curing, and engineering double-crossovers. Since selectable and counter-selectable markers both have practical applications that can be of great utility, it is desirable to optimize dual-selectable markers, which can serve as both selectable and counter-selectable markers. Like counter-selectable markers, dual selectable markers also suffer from high counter-selection escape; this is one of the primary complications of finding suitable dual selectable markers.

Methods:
In this project we will aim towards the development of a selection marker for automated genome engineering. We will be working with the enzyme thymidine kinase (tdk) and demonstrate whether it can be used for coselection Multiplex Automated Genome Engineering (coS-MAGE). We will be alternating between selections that utilize either azidothymidine (AZT) or 5-Fluorodeoxyuridine (FDU) and thymidine through the cycles and determining where the break out point lies.

Results and Future Directions:
An effective dual-selectable marker is one that can survive for at least 10 cycles without breaking down. Our marker managed to survive and maintain stability
throughout 10 cycles at three different concentrations (0.2μM, 0.5μM, and 2.0μM). The next steps in our project are verification and segment integration. If successful, tdk will serve as a useful tool for genome engineering applications and prospective synthetic biology research.

CHED 604

Expression of major hominoid seminal proteins in a mammalian cell culture system

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There are great differences in mating behaviors between humans (Homo sapiens), chimpanzees (Pan troglodytes), and gorillas (Gorilla gorilla). The variability in mating behaviors directly correlates with differences in several aspects of anatomy and physiology among the three species. Much of the variation in semen physiology may be caused by remarkable molecular differences in the length, sequence, and structure of several high abundance proteins of interest. This connection between protein function and physiology could potentially be used to make inferences about the mating behaviors of extinct species, including the common ancestors of humans, chimpanzees, and gorillas. To do this, we will express recombinant proteins from these species in a human cell line (293T cells) and test for functional differences. For the first step of this project, I optimized choice of expression vector, transfection reagents, and transfection conditions using a green fluorescent protein (GFP) expression system. Next, we cloned the KLK3, TGM4, ACPP, SEMG1, and SEMG2 coding sequences of human, chimp, and gorilla into the pFLAG vector, which yielded the best expression during optimization. We detected and quantified expression of these recombinant secreted proteins from media with SDS-PAGE and Western blots. Future work will include purification and functional analysis of these proteins.

CHED 605

Adsorption of thioethers on Au(111) using scanning tunneling microscopy

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The goals of this research include finding evidence that thioethers can physisorb and self-assemble on the surface of Au(111) under ambient conditions, and gaining better control of the nano-patterning of the molecules on the surface of the substrate. The tools employed to achieve these goals include the scanning tunneling microscope (STM) and gas chromatograph/mass spectrometer (GCMS). The STM is used to show evidence of thioether monolayers on the gold surface, and the GCMS is used to verify
that thiol impurities have not contaminated the thioether self-assembled monolayers (SAMs).

CHED 606

Heavy metal isotope analysis of historic skeletal remains using ICP-MS

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Analytical techniques and instrumentation have been integral in the identification and quantification of trace amounts of heavy metal isotopes in human remains. The presence of heavy metals in skeletal remains can give insights into the socioeconomic status of historic and prehistoric populations. This is especially true for the examination of trace amounts of lead (Pb), arsenic (As) and mercury (Hg) in human bone from colonization through the 19\textsuperscript{th} century in America. In this research human bone and teeth, from archaeological excavations of historic sites in the Chesapeake area, were analyzed using time of flight inductively coupled plasma mass spectrometry (TOF ICP-MS) to determine and quantify trace amounts of heavy metal isotopes in the remains. TOF ICP-MS has low detection limits for heavy metals with high accuracy and precision, making it ideal for this study, despite the high time and cost associated with sample preparation, and destructive nature of the analysis. Given the concentrations of heavy metals in the bone samples, we are able to better understand the extent of historic populations’ exposure to heavy metals through household goods, medicinal use, and occupational tasks.

CHED 607

Detection of the $cp4$ epsps gene in maize line NK603 and comparison of related protein structures: An advanced undergraduate experiment

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In light of genetic engineering advancements and its surrounding controversy, we sought to develop a flexible, rigorous laboratory experiment for upper-level biochemistry undergraduates that focuses on the Roundup Ready maize line. The work is appropriate for undergraduate laboratory courses that integrate biochemistry, molecular biology, or bioinformatics. In this experiment, DNA is extracted and purified from maize kernel and leaf samples collected from a Roundup Ready maize grower’s field. A small
segment of DNA (108 base pairs) specific to the Roundup Ready transgene that codes for CP4 5-enolpyruvylshikimate-3-phosphate synthase (CP4 EPSPS) is then amplified with polymerase chain reaction (PCR) to detect the presence of the gene in the maize samples. Students additionally choose a protein closely related to CP4 EPSPS as determined by amino acid sequence alignments. The selected amino acid sequences are then submitted to an online protein modeling program, where students are able to compare their protein with the herbicide-resistant enzyme found in Roundup Ready crops.

CHED 608

Investigating the synthesis and role in molecule-based-magnets of bis(4-pyridyl)acetylene

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Traditional magnets, which are used in current technology, are created in conditions that require large amounts of energy to maintain, such as high temperatures and pressurized environments. Another option to the traditional magnets, which has yet to be fully researched, are molecule-based magnets (MBM), which require only the stable ambient pressures and room temperatures to synthesize. Currently, the MBM complexes that are known that have high ordering temperatures adapt an undesirable amorphous behavior in their solid structure. On the other hand, other MBM compounds that have crystalline structures have lower ordering temperatures. The goal of this research is to investigate various metal salts and inorganic syntheses as a way to form unidentified 3D MBM structures thus opening the door to further understanding of molecule-based magnets. Bis(4-pyridyl)acetylene (BPA) will be incorporated in MBMs as a ligand and its effects on the structure and magnetic properties of these compounds will be investigated.

CHED 609

Laboratory course as journal house: An advanced organic chemistry course incorporating writing/reviewing scientific manuscripts and green chemistry

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The second-semester organic chemistry laboratory course for Chemistry and Biochemistry majors at the University of Detroit Mercy is a multi-faceted educational experience aimed at training future scientists. Students prepare for writing and editing scientific manuscripts by studying The ACS Style Guide and similar texts, all while practicing firsthand usage of NMR, GC-MS and FT-IR instrumentation for structural data acquisition and interpretation. Weekly, one half of the course’s students perform advanced organic synthetic techniques and accrue their own structural characterization data in efforts to write a full scientific manuscript while the remaining students prepare to critically review the “submitted” manuscripts by searching the chemical literature. Both groups are expected to maintain a professional laboratory notebook, adhere to the principles of modern lab safety and invoke the principles of green chemistry (esp. atom economy calculations) in their writing and reviewing. Weekly projects range from multistep preparations and microwave syntheses to cross-coupling chemistry, click reactions and guided-inquiry transformations. Additionally, students perform these tasks with one random coworker every week, and grade each other with a rubric involving marks for punctuality, willingness to learn/teach and safety. Assessment of learning outcomes shows students are excited to be placed into a controlled, but professional scientific arena for their learning.

CHED 610

Electrocatalytic activity of metal-centered porphyrin thin films
Nature’s water oxidation catalyst’s (WOC) play a very important role in the conversion of solar energy into usable chemical energy for higher plants and photosynthetic bacteria. Here we present artificial WOCs consisting of water insoluble porphyrins that are drop-cast onto ITO coated PET electrodes, similar to previous research, which showed Co(II) porphyrin films on ITO coated glass slides had the capability of electrocatalytic water oxidation. Further investigation proceeded to test Mn(III) centered porphyrins for WOC capabilities. The synthesized metal centered porphyrins were characterized via UV-Vis while the catalytic activity of the drop cast thin films was determined by electrochemical techniques.

1) Han, A; Jia, H.; Ma, H.; Ye, S.; Wu, H; Lei, H; Han, Y; Cao, R; Du, P PCCP, 2014, 16, 11209.

CHED 611

Versatile lecture demonstration and laboratory exercise illustrating steric hindrance, electron induction, and catalyst nucleophilicity effects on catalyzed ester hydrolysis

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The aim of the project is to pinpoint a series of reactions based on the classic ester hydrolysis experiment which can serve both as a convenient visual demonstration in the lecture classroom and be extended into a full undergraduate organic and/or physical chemistry laboratory exercise. In the classic experiment, the progress of the imidazole catalyzed hydrolysis of p-nitrophenyl acetate (NPA) is tracked by monitoring the product’s UV-Vis absorption at 400 nm. We extend this to demonstrate the role catalysts, steric hindrance and/or electron induction play in the reaction rates. The role of steric hindrance is easily seen when the NPA analog 4-nitrophenyl trimethylacetate, whose bulky groups restrict access to the cleavage site, substantially slows the reaction. The significance of the inductive effect is illustrated with the NPA analog 4-nitrophenyl trifluoroacetate, whose strong electron withdrawing group dramatically enhances the reaction rate. To demonstrate the importance of catalyst nucleophilicity, the rates of reaction with imidazole and with 4-dimethylaminopyridine (DMAP) are compared. While the difference in rates are dramatic enough to be observed with the naked eye, a simple pseudo-first order kinetic treatment allows the extraction of rate constants of the catalyzed and the uncatalyzed reactions. Additionally, Eyring plot analysis of the observed rate constants’ temperature dependence can provide the change in entropy, enthalpy and Gibbs free energy of the transitions states. The simplicity of the reaction series renders it suitable as a qualitative lecture demonstration.
while the flexibility of the experiment allows the lab to focus on a wide range of concepts with essentially identical preparation each term.

CHED 612

**Lipid raft TNF-α pathway analysis of cytochrome C with methylparaben and UVB treatment**

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The parabens are antimicrobials used in cosmetics as a preservative that prevents fungal and microbial growth. However, the side effects of parabens include: endocrine disruptive effects, increased activity of estrogenic receptors, sensitization with broken skin, and adverse reproductive effects. Methylparaben is the most commonly used paraben in topical skin products. UVB radiation is known to increase the risk of skin cancer and is the most prevalent factor in skin cancer patients. In this study, M624 human melanoma cells were treated with methylparaben and UVB light. It is shown that expression of the apoptotic TNF- receptor is increased in the lipid rafts of the M624 cells treated with 5mM of methylparaben, but not in M624 cells treated with 5mM methylparaben and 25mJ/cm² UVB light. Expression of the Cytochrome C protein that is downstream in the TNF- pathway will also be analyzed via western blot after mitochondrial isolation in this study.

CHED 613

**Investigation of student understanding in spectroscopy labs**

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Most general chemistry laboratory curricula at the undergraduate level include at least one experiment that utilizes spectroscopy, most often UV-Vis spectrophotometry. These laboratory experiments target student understanding of how matter and light interact, how the color of a solution relates to the wavelength of light it absorbs, how absorbance and concentration are related (Beer’s Law), how to construct and analyze calibration curves, and how to determine the concentration of an unknown solution from a calibration curve. However, the research literature is sparse on what students actually learn from these experiments and what misconceptions students have about the related concepts. This poster will present our research on student learning for a variety of general chemistry spectroscopy labs at two different institutions, an undergraduate institution and a community college. Historical exam data, instructor goals for spectroscopy labs, and in-depth analyses of student conceptions will be presented.
**CHED 614**

**Novel regulation of p27 by transglutaminase**

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P27kip1 acts as a tumor suppressor protein in normal cells, and its deregulation correlates with development of aggressive cancers. Unlike most tumor suppressors, however, p27 function is compromised at the protein rather than gene level. This makes identification and characterization of p27 regulatory mechanisms essential to developing more effective therapies to treat these type of aggressive cancers. P27 protein is unique because it is mainly unstructured, existing in an extended conformation that allows extensive interaction with binding targets. Based on this information we hypothesized that imparting structure to p27 might compromise its tumor suppressing ability. We therefore investigated the possibility of p27 regulation by an enzyme called transglutaminase (TG), which typically crosslinks proteins by catalyzing the formation of amide linkages between lysine and glutamine amino acids. TG is responsible for many of the cross links found within the extracellular matrix of cells. Using a system of purified proteins, we found that the structure of p27 can be significantly altered by bacterial TG, suggesting a potentially novel mechanism of p27 deregulation. This study describes a kinetic analysis of p27 modification by TG, and provides evidence that structural changes in p27 alter its function.

**CHED 615**

**Development of histone deacetylase inhibitors**

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Histones are proteins used by cell components to coil and condense DNA. Acetylation of histones is a post-translational modification that makes the promoter regions more accessible, allowing for transcription. Deacetylation does the exact opposite, making DNA less accessible to cellular machinery and causing a decrease in the transcription rate. When chromosomes are condensed, transcription of the DNA is very difficult because access to promoter regions is blocked, making it impossible to transcribe. Histone deacetylases (HDAC) are enzymes that remove acetyl groups from histones that alter transcription and several signaling pathways involved in cancer development to enhance tumor survival/growth. HDAC inhibitors are used to prevent the enzyme from deacetylating histones, causing induction of apoptosis, cell cycle arrest, and inhibition of angiogenesis and metastasis, leading to a decreased rate of tumor
development. In this presentation, four carbamates and two benzamides were synthesized and evaluated for their enzymatic and cellular activities.

CHED 616

Progress toward synthesis of a novel trifluoromethyl substituted aurone as a potential cyclooxygenase-2 inhibitor

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Naturally occurring flavonoid compounds have shown great biological potential, in particular the subclass of flavonoids known as aurones. Previous studies have shown that aurones exhibit anti-cancer activity as well as a variety of other pharmacological activities, including anti-inflammatory and anti-viral properties. More specifically, these studies indicate that aurones show potential in inhibiting cyclooxygenase-2 activity (COX-2), which plays an integral part in inflammation and its associated diseases, such as cancer. Mills, et. al. recently performed molecular docking studies of several novel aurones at the COX-2 active site. As a continuation of this research, a synthetic pathway for one of the most promising aurone derivatives, a novel trifluoromethyl-substituted aurone, has been proposed. The final target molecule will be synthesized using this route and the novel compound will be characterized.

CHED 617

Modification of the p27 tumor suppressor by the transglutaminase enzyme

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P27 is a tumor-suppressor protein involved in cell cycle regulation. It functions by binding and inhibiting activity of cyclin-dependent kinases (CDKs). Surprisingly, the p27 gene is seldom mutated or deleted. Instead, p27 is deregulated at the protein level such that its tumor suppressing ability is compromised, thereby contributing to development of many types of aggressive cancer. For this reason understanding the molecular mechanisms controlling p27 function is essential. The p27 protein is unique in that it lacks significant tertiary structure and is heat stable. Thus, we hypothesized that compromising p27 function might involve imparding structure to the polypeptide. A search for enzymes having the ability to alter protein structure identified transglutaminase, which catalyzes protein cross-linking via formation of an isopeptide bond between lysine and glutamine groups. Interestingly, altered levels of nuclear and cellular transglutaminase have been observed in cancer cells. We therefore incubated purified p27 and transglutaminase, followed by analysis of p27 mobility on a denaturing
polyacrylamide gel. Surprisingly, p27 monomers were not crosslinked. Instead, p27 migrated faster, suggesting a conformational change due to intramolecular isopeptide bond formation. The kinetics, inhibition, and specificity of this novel reaction have been evaluated. Our results identify a possible link between transglutaminase modification of P27 and proliferation of aggressive cancers.

CHED 618

Analysis of organic compounds isolated from particulate matter produced by biodiesel and diesel fuel

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Particulate matter from fuel exhaust can contain potentially toxic and hazardous organic compounds. Airborne particulate matter was collected over a ten day period for both diesel and biodiesel fuels at two occupational workspace locations within the Keene Recycling Center (Keene, NH). Airborne particulate matter produced from biodiesel and petroleum diesel engine exhaust was chemically characterized using gas chromatography-mass spectrometry. Organic compounds were extracted from quartz filter field samples using sonication, and concentrations of polycyclic aromatic hydrocarbons, fatty acid methyl esters, hopanes, and steranes were determined using optimized separation methods. Filters were analyzed for the presence of 61 different standard compounds using class specific internal standards and selected ion monitoring detection, which resulted in low part per billion limits of detection. Extraction recovery efficiencies for standards spiked on filters were 106.3 ± 4.4% for polycyclic aromatic hydrocarbons, 97.6 ± 5.7% for fatty acid methyl esters, and 97.9 ± 8.1% for hopanes and steranes. Results will be presented that compare changes in chemical concentrations for the two fuels at the two locations. As expected for biodiesel samples fatty acid methyl esters showed the greatest mass as compared to other compounds classes, and the most abundant fatty acid methyl ester detected for biodiesel samples was methyl laurate. The variability in organic chemical composition of particulate matter as a function of size will also be investigated, as the Sioutas impactor used for filter collection separates content into discrete size ranges. The analysis of locally collected samples using analytical instrumentation will provide new data on the chemical composition of particulate matter produced from two different fuel types.

CHED 619

Synthetic studies toward Corynanthe indole alkaloid derivatives

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Monoterpenoid indole alkaloid natural products have been shown to exhibit promising biological activity, making their total synthesis of great significance across many disciplines. These syntheses have been challenging to organic chemists due to the complexity of the heterocyclic ring core present in many Corynanthe indole alkaloid natural products. The goal of this study is to develop a cost-effective route towards the synthesis of natural products containing the heterocyclic indole motif and to increase natural product efficacy through further derivatization. We report the effective synthesis of polycyclic intermediates in the synthesis of Corynanthe indole alkaloid natural products.

CHED 620

Free radical effect on the quantum yield of silicon nanoparticles

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Silicon nanoparticles (Si NPs) have band gaps that can be tuned to be in the red-to-near-infrared energy region, making them important for several practical applications. Efficient emissions are desired for these applications, and as such measuring and optimizing the quantum yield is necessary. Freshly etched hydrogen-terminated Si NPs are highly susceptible to non-radiative recombination as a result of free radicals present on the surface of the nanoparticle. This process results in a diminished quantum yield. The Si NPs studied herein were treated with TEMPO, a free radical scavenger, to remove surface radicals. A method for measuring fluorescence quantum yield was developed, which utilized a common fluorophore as a standard for comparison. A calibration curve was constructed using Coumarin-153 as a standard. The quantum yield of the Si NPs was measured before and after the addition of TEMPO, which was found to increase with free radical removal.

CHED 621

Determining the rate of oxidation of promethazine to its sulfoxide and sulfone in atmospheric O₂ using HPLC-MS and UV-VIS spectrophotometric analysis

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Analysis has been performed on the pharmaceutical compound promethazine in saline solution under various temperatures, to determine percent conversion of promethazine to its sulfoxide and sulfone upon exposure to oxygen in the atmosphere. Measurements were taken to determine the percent oxidation of promethazine as a function of time by
HPLC-MS analysis and UV-VIS spectrophotometric analysis with Beer's law correlations. Kinetic data established by these analyses were used to determine rate constants ($k_r$) calculated from the known rate expressions.

CHED 622

Detection of organic pollutants using EVA with GC-MS and AFM analysis

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In this research experiment Ethylene Vinyl Acetate (EVA) is used to analyze organic pollutants in the environment. EVA is an effective polymer for analyzing pollutants due to its high affinity towards organic compounds and its ability to be spread to sub-micron film thickness on various materials. Various indoor and outdoor environments were studied using EVA on glass substrates and silicon wafers substrates. After the EVA samples were exposed to environmental pollutants for several weeks. Gas Chromatography Mass Spectrometry (GC-MS) was used to analyze the EVA on glass substrates by first extracting the chemical pollutants with methanol and then direct injection into the GC-MS. The surface characterization of the silicon wafers were studied using Atomic Force Microscopy (AFM).

CHED 623

Analysis of University of Utah Fine Arts Museum Egyptian sarcophagus by scanning electron microscopy

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This project analyzed the elemental composition of pigment samples from an Egyptian sarcophagus in the collection of the University of Utah Fine Arts Museum. Scanning Electron Microscopy was used for Elemental Mapping and Quantitative Analysis to determine the elements present in the samples as well as the identity and quality of the
wood. The elements present within the pigments give a good representation of what materials the family members of the deceased had access to. The results of this study were used to give an indication as to the socioeconomic level of the deceased.

CHED 624

Determining source of discoloration in renaissance fresco using infrared spectrophotometry

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This project analyzed two samples from renaissance era frescoes. One sample was taken from a section that shows distinct coloration, while the other sample was taken from a section with the same pigmentation but without discoloration. Infrared Spectrophotometry was used to determine the compounds present in these samples. The chemicals present within the discolored sample were further analyzed to determine which organic compounds are the source of the discoloration by comparative analysis with spectra from various commonly used surface coatings.

CHED 625

1,3-Dipolar cycloaddition reaction

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The chemistry of heterocyclic compounds is used in almost all aspects of organic chemistry, medicinal chemistry, and biochemistry. Methods that can generate these compounds at milder conditions and lower costs are of utmost value. A 1,3-dipolar cycloaddition reaction is a common reaction to synthesize heterocyclic compounds. The current method for this reaction requires reacting a diazo compound with a rhodium catalyst. Rhodium is one of the most expensive and least abundant metals used for catalysis. Ruthenium is a cheaper solution that can be utilized. The goal of this project is to synthesize diazo compounds (1) that can be reacted with two different ruthenium catalysts (3 & 4) in order to produce a ruthenacarbene intermediate (2) which can then react with a dipolarophile (DMAD)(7) to generate a heterocycle (5). The two catalysts that will be screened are the Grubbs Generation-I catalyst (3) and the tris(triphenylphosphine)ruthenium(II)dichloride catalyst (4). The optimal conditions at which these two catalysts generate the ruthenacarbene intermediate will also be determined. Not only does this reaction provide a more economical process for the
synthesis of heterocycles, it also has the potential to impact the discovery of pharmaceutical drugs, insecticides, and various other chemicals.

CHED 626

Solvation equilibria of proximally-substituted copper bis-phenanthroline derivatives

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Copper phenanthroline complexes have been widely studied for many reasons, such as their use as reagents in molecular biology, and interesting photophysical behavior. Typically, the bis-phenanthroline complexes exhibit a five-coordinate geometry for the cupric complexes, with one donor being derived from solvent or counterion. Conversely, the cuprous state is invariably observed to have a four-coordinated geometry. Cupric complexes bearing substituents at the 2- and 9-positions of the ligands, which impose steric congestion close to the copper centers, have long been known to show facilitated reduction to afford the less congested cuprous forms. More recent studies of complexes of this type, however, have shown that the steric strain can also be alleviated by loss of the solvent ligand from the cupric centers, affording four-coordinate Cu(II) complexes. We will report on the influence of proximal substituents in determining the extent of formation of the four-coordinate cupric complexes both in solution and in the solid state, and the competition between the desolvation and reduction processes.

CHED 627

Aromatization of fragrant monoterpenes via palladium-catalyzed dehydrogenation

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Terpenes are a diverse class of naturally occurring compounds. We have developed an experiment for an organic chemistry laboratory course in which familiar monoterpenes are aromatized via dehydrogenation to give familiar monoterpenic products. Specifically, limonene (from lemon oil), carvone (from spearmint oil) and pulegone (from catnip) are aromatized to \( p \)-cymene (from oregano and thyme), carvacrol (from oregano) and thymol (from thyme) respectively.

The starting monoterpenes were dissolved in ethanol and heated via conventional reflux or microwave irradiation in the presence of Pd/C as a catalyst. The products were isolated after filtration and evaporation of solvent and then characterized using \(^1\)H-NMR and GC-MS. Thus, carvone was converted to carvacrol with excellent purity and a 90% yield. Limonene was converted to a 3:1 mixture of \( p \)-cymene and menthane with a total yield of 52%. Pulegone was converted to a 1:1 mixture of thymol and menthone which could be separated via acid-base extraction to give thymol in 46% yield.

\[
\text{limonene} \quad \xrightarrow{\text{Pd/C, } \Delta} \quad \text{\( p \)-cymene}
\]

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The world is searching for renewable energy sources in the face of a global energy crisis. Biodiesel has proven to be a successful alternative to fossil fuels, and there is current research into the most sustainable and effective feedstocks. With fast growth rates and exceptional oil yields, microalgae are a viable feedstock option. This project investigated the ideal laboratory-growing conditions of \textit{Chlamydomonas reinhardtii} algal colonies and their synthesis into biodiesel through acid-catalyzed transesterification. The results were integrated into Beloit College’s chemistry curriculum.
Forensic analysis of commercial color and black inkjet printer inks by micellar electrokinetic chromatography

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A critical priority for forensic analysis of fraudulent documents is determination of the ink source. With high resolution and low cost, inkjet printers have become an easy platform to create such fraudulent documents. In this study, micellar electrokinetic chromatography (MEKC) with ultraviolet-visible photodiode array detection was applied to the characterization of commercial inkjet printer inks. Although a destructive technique, MEKC with its high resolution, low sample volume requirements, and ease of sample preparation allowed for minimal damage to the analyzed document. Photodiode array detection permitted inks to be characterized not only by their electrophoretic mobility, but also ultraviolet-visible spectrum. A searchable database was created of color and black inkjet printer inks for a broad range of commercial inkjet printers.

CHED 630

Enzymatic reduction of a ketone for a college-level organic chemistry course using alcohol dehydrogenase

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The reduction of a ketone to an alcohol is a common laboratory experiment in college organic chemistry courses. In some variations of this experiment, baker's yeast is used to catalyze the stereoselective reduction of a ketone. In a separate reaction, a reducing agent, borohydride is used, which yields a racemic mixture of products. Students can then compare the specific rotation of the products from each reaction and observe the difference in stereoselectivity between the two methods. The disadvantage of using baker's yeast is that there is no clearly defined mechanism by which the ketone is reduced since the reaction is performed by whole yeast cells. This ambiguity impedes the opportunity to teach students about the stereoselective nature of enzymatic reactions. Here we demonstrate that the enzyme alcohol dehydrogenase can be used in vitro to catalyze the stereoselective reduction of methyl isobutyl ketone to a single enantiomer of 4-methyl-penta-2ol. The enzymatic reduction was performed using alcohol dehydrogenase with NADH as the reducing agent. The NADH was recycled using glucose dehydrogenase. Products were extracted with ethyl acetate and the enantiomeric excess of the products was determined from measurement of their specific rotation. While reduction with borohydride produces a racemic mixture, the enzymatic reduction yields a high enantiomer excess. Our experiment demonstrates the feasibility of using a purified enzyme for ketone reduction reactions in college organic chemistry courses. The recycling of NADH in the reaction also reduces laboratory costs of the enzymatic reaction because glucose dehydrogenase is less expensive that NADH. This
experiment also is well suited to teach organic students about the stereoselective nature of enzymatic reactions and the concept of enantiomeric excess.

CHED 631

Synthesis of the SRS and SSR isomers of lentiginosine from D-glucopyranoside and D-galactopyranoside

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The purpose of this project was to synthesize two of the eight stereoisomers, SSR and SRS, of the natural product, Lentiginosine. Lentiginosine is a natural product and has been isolated from the plant Astragalus lentiginosus. The polyhydroxylated alkaloids extracted from this plant, swainsonine and lentiginosine, have been found to inhibit enzymes called glycosidases. These glycosidase enzymes are responsible for the processing of carbohydrates. Lentiginosine and its stereoisomers are members of a class of compounds called iminosugars. Iminosugars are sugar analogs with a nitrogen atom replacing the natural oxygen atom within the heterocyclic ring. As a result, iminosugars mimic the structure of sugars and bind to sugar processing enzymes such as glycosidases. If the iminosugars could be used to inhibit these enzymes, then the processing and degradation of sugars into their monomers would be prevented. These compounds are of interest in bioorganic and medicinal chemistry for the treatment of numerous diseases including cancer, Gaucher disease, viruses, and diabetes, among others.

The goal is to synthesize all of the stereoisomers of lentiginosine, test their potency as inhibitors against glycosidases, and compare their potency to computer models of their binding in the active site of different glycosidases. Once their inhibitory properties are known, there is potential for pharmaceutical development. Therefore, in order to test these models, all eight stereoisomers of lentiginosine must be obtained for testing.

CHED 632

Team-based assessment of introductory organic chemistry lecture

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Introductory organic chemistry is often considered a difficult course for undergraduate students, with every student having a different set of strengths and weaknesses. Through promoting an environment that encourages teamwork, however, students can support and teach each other while building a “community of knowledge” in the class. In order to gauge the effectiveness of these cooperative efforts, students were divided into groups of four and asked to complete a written assessment involving conformational analysis, stereochemistry analysis, total synthesis completion, spectroscopic analysis of functional groups, and reaction mechanism proposal. Results of the individual teams
were evaluated and compared to past data. We determined such an approach is effective and provides a unique learning opportunity that students enjoyed.

CHED 633

Team-based assessment of a two-semester introductory organic chemistry laboratory course

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Introductory organic chemistry laboratory courses set the foundation for future chemistry laboratory classes and chemical research. Because research requires collaboration, we used a team-based assessment to demonstrate overall teaching efficacy of a two-semester introductory organic chemistry laboratory class, specifically testing mastery of experimental and analytical techniques. Students were divided into teams to complete the reduction of a ketone with a chiral auxiliary catalyst or with a yeast enzyme. To complete and verify this transformation, thin-layer-chromatography, IR spectroscopy, NMR, column chromatography purification, chiral shift reagent analysis, and chiral HPLC were used. The results of this assessment were compared between teams and years of classes. Overall, we found the assessment to be effective while also providing a unique learning experience to the students.

CHED 634

Initial investigation of pyrrolizidine alkaloids in Psacalium decompositum

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Pyrrolizidine alkaloids (PA’s) are potentially toxic, naturally occurring secondary products, typically found in the plant family Asteraceae. As part of an alkaloid analysis of the Asteraceae family, Psacalium decompositum from Cochise County, Arizona, was analyzed to establish a GC-MS PA profile. Preliminary analysis of the sample showed nine resolved PA’s: three were identified as retronecine based, and six were otonecine based. Many of the compounds appear to match, or were isomeric with, PA’s from closely related genera Arnoglossum and Yerimo. Chromatographic PA comparisons will be made with these allied genera to establish structural identities. Further elucidation of isolated PA compounds through 1D and 2D NMR experiments will help to determine the stereochemistry of Psacalium PA’s.

CHED 635
Cost effective ion selective electrodes from metal-azo complexes

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Ion Selective Electrodes (ISE) are used regularly in analytical chemistry to determine concentration of ions in solutions. These electrodes however, are either too expensive ($300+ per unit) or too complex to develop for a classroom level laboratory experiment. We have developed techniques reducing the cost and complexity for designing and performing classroom laboratory ISE experiments. These experiments involved, not only reducing costs of the electrodes themselves, but also reducing the costs of the metering equipment required in a classroom setting. The ISEs created were a membrane type using Ca²⁺, Mg²⁺ and Cu²⁺ ions complexed with either 2,2′-(Ethanediylidenedinitrilo)diphenol (GBHA) or 4-(4-Nitrophenylazo)resorcinol (Azo Violet), then homogeneously mixed into a thin layer of plasticized PVC. The success of each electrode was determined first by calibration, then by measurement of a separate “unknown” standardized solution. The electrode was also tested for interference by taking measurements of solutions with possible interfering ions. Measurements were also taken on different meters to verify accuracy of less expensive meters.

CHED 636

Burning truth about sunscreens: Zinc oxide nanoparticle growth kinetics


In the United States, more than 3.5 million cases of skin cancer are diagnosed every year. Of these cases, it is estimated that more than 3 million could be prevented by protecting the skin from excessive sun exposure. This protection can be achieved through broad spectrum sunscreen. Broad spectrum sunscreen relies on inorganic chemicals to reflect sunlight and organic materials are used to absorb the UV radiation. Zinc oxide and titanium oxide are the two primary inorganic compounds that are used to reflect UV radiation. This study focused on parameters affecting particle size and growth kinetics of colloidal zinc oxide nanoparticles as monitored by UV spectroscopy.

CHED 637

Small angle X-ray scattering (SAXS) of β₂-glycoprotein I suggests an alternative mechanism for antibody interaction in antiphospholipid syndrome

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Antiphospholipid syndrome (APS) is a systemic autoimmune disorder characterized clinically by vascular thrombosis and pregnancy morbidity and serologically by the presence of antiphospholipid antibodies (aPL). Despite their name, aPLs do not target phospholipids but recognize two circulating plasma proteins, prothrombin and β2-glycoprotein-I (β2GPI), only after adsorption onto anionic surfaces such as phospholipids. Why this interaction requires the support of the membranes in vivo and a molecular mechanism for it remain unknown. As the idea of molecular plasticity starts to find structural evidence in the literature, a new mechanism has emerged in the field and predicts that protein binding to the phospholipids induces a conformational change leading to the exposure of antigenic epitopes. Recent results obtained with cryo-electron microscopy seem to support this model and have shown that β2GPI may exist in at least two conformations, open and closed. The closed-inactive conformation of the protein circulates in the plasma and is converted to the active-open form upon binding to the membranes, a transition that was found to be reversible through changing salt and pH. To gain insights on the structural properties of this molecule in solution, we collected small angle X-ray scattering (SAXS) data for the plasma purified and recombinant β2GPI under solution conditions that are reported to stabilize the open (pH 11.5, 1.15M NaCl) and closed (pH 3.4, 0.15M NaCl) conformations and also under physiological conditions (pH 7.4, 150 mM NaCl, 5 mM CaCl2). To our surprise, SAXS experiments failed to reveal major differences between the samples and the molecule seems to acquire similar elongated shapes. Indeed, after background subtraction and necessary corrections for inter-particle interactions the scattering profiles were superimposable up to a q-value of 0.15Å⁻¹, and the radius of gyration (Rg), estimated via the Guinier approximation, was 41±1.9Å and 40.9±1.1Å for the closed and open conformations, respectively. Small but significant differences were observed in the higher-resolution region of the curve and were amplified in the Kratky plot, suggesting intrinsic flexibility of the molecule in solution. In conclusion, the lack of evidence of the closed form of β2GPI under these conditions suggests that binding of this protein to the autoantibodies requires alternative yet unidentified conformational changes, perhaps enabled by the plasticity of the linker domains.

CHED 638

Dynamics study of the resorcin[4]arene supramolecular assembly

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Six resorcin[4]arene monomers, when dissolved in water-saturated chloroform, combine with eight water molecules to spontaneously form a supramolecular assembly held together by sixty hydrogen bonds. This assembly can host molecules in its ~1400 Å³ interior volume and represents an exciting approach to controlling chemistry. Indeed, it has previously been demonstrated that encapsulating a catalyst inside the resorcin[4]arene assembly significantly affects the reaction selectivity. Despite extensive experimental studies, there are many open questions about the molecular-level
properties and thermodynamic driving forces that govern the host-guest dynamics of these assemblies. Key examples are: How does a guest molecule enter or leave the assembly? and How can the host-guest dynamics be modified to enhance the rates of intra-assembly reactions? Molecular dynamics simulations have been used to address these questions. The approach is to modify the assembly, by removal of water molecules, to probe the effect on the dynamics. Simulations were run at multiple temperatures to estimate the rate-constant of assembly dissociation and obtain the corresponding activation energy. For a resorcin[4]arene hexameric assembly in pure chloroform (no additional waters), the activation energy was found to be the same for an assembly with eight waters and one with no waters. In water-saturated chloroform, where waters in the assembly can be replaced by those in the solvent, the activation energy was also independent of the initial number of waters in the assembly. These surprising results suggest that the favorable enthalpy of the water hydrogen bonds in the assembly may not be as important as previously thought in preventing dissociation. Instead it indicates that entropic effects may be key or that reassembly dynamics may be more strongly affected by the presence of water.

CHED 639

Synthesis and luminescence studies of rhenium(I) tricarbonyl complexes using LabQuest 2

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Rhenium (I) tricarbonyl complexes have attracted considerable interest due to their potential use in anion sensing and recognition owing to their rich spectroscopic and luminescent properties. The unique properties of these complexes can be fine-tuned by varying the structure of the coordinated ligands as well as the anion binding subunit. Incorporating such rich and interesting chemistry experiments in the regular inorganic chemistry college curriculum has been very limited, this is partly due to the high cost of rhenium compounds, as well as the lack of or limited access to the requisite analytical instruments such as a fluorimeter for luminescence studies. Here, we will report the synthesis of various rhenium (I) tricarbonyl complexes based on various diimine ligands and their emission studies using a hand-held LabQuest 2 device. Luminescence studies of these rhenium (I) tricarbonyl complexes exhibited strong emissions at ~530 nm with slight variations depending on the nature of the ligands. The rhenium-complexes synthesized were used for advanced development of anion sensors, where they serve as luminescent signaling subunits.

CHED 640

Attachment inhibition of invasive species
Invasive marine and freshwater species have a detrimental impact on aquatic ecosystems and are easily transferred between bodies of water as a result of unregulated settlement and attachment on commercial and recreational watercraft. This results in infestation of waterways and disruption of native organisms throughout an ecosystem. The quagga mussel (*Dreissena rostriformis bugensis*) is one example of such invasive species that has called for a focus on cross-contamination prevention. Our goal is to develop an aquatic paint suitable for watercraft that prevents the settlement and/or attachment of various aquatic species such as algae, snails (*Physa* sp.), anemones (*Aiptasia* sp.), and quagga mussels. The paint will be integrated with newly developed surfactants that will inhibit the adherence ability of invasive aquatic species. The surfactants are added to provide a barrier between the paint surface and the organisms creating an undesirable surface area for the organisms to attach. The most innovative characteristic of the surfactant-based paint is its effectiveness on adherence inhibition without degradation, dissociation, or toxicity to the environment. Preventing adherence of pests to surfaces could have dramatic positive effects on the efficiency and costs of operations in marine environments and waterways.

**CHED 641**

**Writing exam questions that elicit evidence of process skills**

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As instructors adopt more student-centered instructional strategies that place more emphasis on process skills such as problem solving, information processing, and critical thinking, there is a need to assess these skills as well. For the ANAPOGIL project, exam questions were designed to elicit evidence of process skills in students’ responses. These questions covered the broad topic areas of analytical chemistry and were embedded in regular course exams at several institutions and over a period of years. Student responses were analyzed and coded to document evidence of process skills. The data was examined to look for trends among individual students in the same semester, for the patterns in individual schools across multiple years, and across institutions. Codes were generated for information processing, critical thinking, problem solving, and content knowledge. Insights from the analysis will help instructors write exam questions to elicit evidence of process skills and to evaluate student responses to assess and provide feedback on chemistry content knowledge and process skills.

**CHED 642**

**Understanding the cognitive load generated by constructing Lewis structures**
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To understand chemical reactions, it is essential to visualize the molecules involved in the reaction. To help with this process, G. N. Lewis introduced Lewis structures in 1916 to represent the elements and their bonding sequence in a compound. Since that time, Lewis structures have become a foundational idea for understanding chemistry. Given their role, it is important to understand the aspects of Lewis structure creation that students struggle with, and in particular, the cognitive load that their generation induce. To explore these concepts, we conducted paper and electronic test that asked students to create a series of Lewis structures; simultaneously, the load on the subject was determined by measuring heart rate changes. Data were collected from students enrolled in general chemistry, organic chemistry, and senior chemistry classes. This poster will present our results and discuss future directions.

CHED 643

Synthesis of 2'-phenoxy-4-hydroxyacetophenone

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Photoremovable protecting groups (PPGs), when bound covalently to compounds, provide spatial and temporal control of the release from the protecting groups. PPGs enable researchers to control the release of bioactive compounds, such as neurotransmitters, in living tissue. Like their name states, PPGs are removed by the action of absorbed light. The PPG used in this study is p-hydroxyphenacyl (pHP) because of its unique properties such as high quantum yields, a biologically inert byproduct, and quantitative yield of deprotected product. Most molecules protected by the pHP ligand have an acidic moiety such as a carboxylic, phosphoric or sulfonic acid functional group. Many biological compounds of interest, however, lack this sort of relatively acid moiety, and caging of much less acidic moieties such as phenols is currently under study. The main goal of the study is to develop a method to synthesize and deprotect caged phenols. Once the phenols are synthesized, their photochemical properties are measured in order to determine the viability of the chemistry. A three-step procedure was employed to synthesize 2'-phenoxy-4-hydroxyacetophenone. A solid-state organic reaction using the organic base 1,4-diazabicyclo[2.2.2]octane (DABCO) was studied as an alternative method for the final step.

CHED 644
Longitudinal study of the effects of a professional development program on the content knowledge and teaching practices of middle and high school science teachers

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The study examines the effects of multidisciplinary sciences higher education-based professional development programs funded by the Teacher Quality Grant Program (TQGP) designed for middle and high school science teachers in physical, life, earth and environmental sciences. The study focuses on assessing the different aspects of professional development and its effects on the changes in the content knowledge and teaching practices of 146 science teachers from 65 campuses in 13 school districts over a period of ten years from 2004-2014. The professional development program emphasized science content aligned with state and national science education standards, inquiry activities, technology application, implementation strategies of inquiry activities in teachers’ classrooms and building a Community of Practice of science teachers. Assessment instruments include pre-post test scores, modified lesson plans, teachers’ reflections, portfolios, artifacts, classroom observations, focus group interactions and survey responses. Analysis of data over time demonstrated increase in teachers’ practices in their classrooms and indicated gradual advancement in the use of inquiry-based instruction, active learning opportunities, instructional technology, and teacher networking.

CHED 645

Southern Utah University general chemistry case study: Identification of curriculum obstacles

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Teachers are expected to create a solid foundation for students as they scientifically explore their world. This research focused on identifying curriculum challenges students encountered in the General Chemistry courses provided at Southern Utah University by doing an evaluation of online homework and test scores. The analysis of the students’ online homework, provided by Sapling Learning during the 2013-14 academic year, qualitatively evaluated obstacles within the course by considering Bloom’s Taxonomy, logical reasoning, and question format. Difficulty was assessed by the correlation made between these qualitative parameters and the students’ performance on questions.
using a multivariable regression. The same analysis was done on tests given by some of the faculty during the 2012-13 and 2013-14 academic years. The multivariable regression identified statistically significant correlations for some of the components of logical reasoning and question format. These correlations support that it is possible to evaluate not only students understanding of curriculum, but also identify which forms of logical reasoning that hinder students’ success. This provide teachers a means by which they may be able to generate better questions that cater to developmental needs of novice chemist.

CHED 646

Research on surface modification of zinc oxide nanoparticles and incorporation into fibers

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The goal of the research performed over the summer was to modify the surface of zinc oxide nanorods and incorporate them into a fiber. The surface of zinc oxide was modified with dodecanethiol. FTIR data showed that dodecanethiol was adhered to the rods, which were then compounded with polypropylene through melt extrusion to form fibers. Photoluminescence data showed that the bimodal spectrum of zinc oxide was maintained in fiber form and that is potential for more work with these nanorods.

CHED 647

Newly established documentation and imaging system detecting DNA hybridization serves as a potential point of care device to further distinguish genetic susceptibility to diseases

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The need for point of care devices, or POC’s, has been high for medical purposes. With the need of ease of access tools within the medical field, more efficient and cost effective ways to diagnose and treat people has been a main priority. A multi-application imaging and documentation system has been recently developed for imaging multiple biochemical techniques with varying needs including bioluminescence, chemiluminescence, fluorescence, and transluminescence. This documentation system is cost effective and can be stored easily while being transported. Recognizing this documentation system as a potential POC device for detecting genetic susceptibility to diseases such as chronic myelogenic leukemia, its ability to detect DNA hybridization via fluorescent labelling was evaluated. The detection limits for fluorescein and
fluorescent labelled DNA probes were found to be 2.94× and 4.68× probes/mm² respectively. This demonstrates that the imager would be able to detect DNA hybridization used in techniques such as fluorescent in situ hybridization, or FISH, and would be particularly powerful if coupled with microfluidic based hybridization protocols.

CHED 648

Analytical techniques in environmental chemistry: Detection and quantification of common herbicides in surface water

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The prolific usage of atrazine and related herbicides poses a significant risk to water supplies, especially areas with high agricultural activity. Versatile methods of detection and quantification of these compounds via enzyme linked immunosorbent assay (ELISA) provide expedient results with low detection limits. However, ELISA is non-specific technique, causing substantial error and necessitating comparison with laboratory-based analysis. We have adapted a standard protocol using LC/MS-MS (Liquid Chromatography/ Tandem Mass Spectrometry) as a means of comparative analysis with ELISA field tests. Water samples were gathered from local surface water in an agricultural setting. Using the LC/MS-MS method, samples were probed for three common herbicides (atrazine, simazine, and propazine). Multiple samples contained relatively high concentrations of atrazine. This instructional laboratory will expose students to the capabilities and shortcomings of both ELISA and LC/MS-MS in the context of a “hot topic” in environmental chemistry. The developed LC/MS-MS analysis is fast with low detection limits and demonstrates the efficacy of instrumental features for the purposes of education.

CHED 649

Determination of mercury levels in living and nonliving systems of southwest Arkansas

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Cinnabar mining for the acquisition of mercury was one of the leading industries in Arkansas from 1931 into the mid-1940s. Mercury is a persistent bioaccumulative toxin, thus the focus of this project is to assess the regional impact of historic mining upon waters, soils, and organisms of southwest Arkansas by evaluating mercury content. Cold-vapor atomic absorption spectrometry is the method used to determine mercury levels in samples, which are treated in accordance with EPA-established protocols.

CHED 650
Physiological effects of massage therapy in college students and the elderly

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Massage therapy is experiencing resurgence as a valid form of alternative treatment. The aim of this research group is to quantify the changes in physiological and psychological state brought about by massage therapy in college students and the elderly. Psychologically, college students are evaluated for stress and anxiety, while depression levels in the elderly are compared. Physiologically, the hormone cortisol and the neurotransmitter oxytocin are studied as stress biomarkers. Analysis of the biomarkers is carried out using enzyme-linked immunosorbent assaying of saliva samples taken before and after treatment administration. In the interest of undergraduate education, the protocol is incorporated into a senior level biochemistry laboratory for students.

CHED 651

Continued study in Facebook™ as a collaborative learning platform for sophomore organic chemistry students

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The use of a Facebook™ group as a collaborative learning platform for sophomore organic chemistry students will be presented. Fall semester 2014 Organic Chemistry I students at Clayton State University were encouraged to post pictures of their answers for assigned practice problems and to offer feedback to other students regarding their posted answers. Pros and cons of this platform versus other available platforms will be discussed. Also, student opinions collected via an end-of-semester survey will also be presented.

CHED 652

Isolation and characteristics of flavonoids from ash tree leaves

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The ash tree (Fraxinus Velutina) is a plant which long has been used in southwestern American ethnobotany to relieve the symptoms of inflammation, especially that of the
Typically, the leaves of this tree are ground and boiled to yield a nontoxic tea. We chose to study the flavonoids of this plant because these compounds are known to be anti-inflammatory agents. We have isolated flavonoids from ash tree leaves. Starting with a simple comminution of the plant leaves, we have through a series of steps separated the plant material. These involve water/methanol fractions to separate the glycerides, and then subsequent washings of the methanol extract with dichloromethane to separate the fraction with flavonoids. Finally, we used thin-layer chromatography to separate the flavonoids from the chlorophylls. In this part of the work we used a mixture of the solvents hexane, methanol, and ethyl acetate to perform the TLC separation. We identified the fractions containing the flavonoids by UV light and then collected them. We have worked to characterize the flavonoids by infrared spectroscopy, nuclear magnetic spectroscopy, and mass spectroscopy. We then propose to use this general method to study flavonoids from other plants.

CHED 653

Kinetics of the reduction of nitrobenzene using hydrazine hydrate and cobalt (II) sulfide

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Hydrazine in the presence of Co$_3$S$_4$ was successful as an alternative hydrogen source for the conversion of nitrobenzene to aniline. The reaction observed does have a slower rate compared to that of sodium borohydride, but the slower rate provided the opportunity to analyze the kinetics of the reaction. GC and $^1$H-NMR spectra demonstrated the formation of PHA, a known intermediate for this reaction. The reaction showed a change in reaction order at ca. 150 minutes. At this time, the concentration of nitrobenzene was low while the concentration of PHA was relatively high. The conversions observed using GC suggest that the reaction follows a zero order mechanism (typical of catalyzed reactions) and then it changes to a second order mechanism in later stages of the reaction. The reaction kinetics was followed using $^1$H-NMR, which showed evidence of the formation of N-phenylhydroxyl amine (PHA) in relatively high concentrations. The presence of PHA in high concentration suggests that the initial step is a four-electron process. The reaction conditions can be manipulated to stop the reduction selectively at the PHA stage. It was demonstrated through $^1$H-NMR that the catalyst promotes of nitrobenzene to PHA and it also affects the reduction of PHA into aniline.

CHED 654

Biophysical analysis of CDK5R2 DNA secondary structures

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In addition to the classic DNA double helix structure, certain guanine rich DNA sequences can form secondary structures known as G-quadruplexes, and their complementary cytosine rich strand can form i-motif structures. G-quadruplexes can be formed by the stacking of multiple G-quartets which are formed by the Hoogsteen base pairing of several guanine residues. The i-motif structures are formed by the stacking of cytosine- cytosine base pairs and are stabilized at low pH values. The CDK5R2 DNA contains multiple guanine and cytosine base pairs and has the capability to form both a G-quadruplex and an i-motif secondary structure. These secondary structures are important because being aware of the structure of the DNA allows a person to understand the function of the protein within the cell. To characterize the different secondary structures of these DNA strands, many biophysical techniques were utilized including circular dichroism spectroscopy, $^1$H nuclear magnetic resonance spectroscopy, UV spectroscopy, and native polyacrylamide gel electrophoresis (PAGE).

CHED 655

Histone deacetylase (HDAC) inhibitors containing thioamide: Synthesis and biological evaluation

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Histone deacetylase (HDAC) is a type of metalloenzymes that removes acetyl groups from histone proteins found within DNA, therefore making DNA inaccessible for transcription. Research has shown that inhibition of HDAC triggers growth arrest, differentiation, and/or apoptosis in many types of tumor cells. HDAC (except class III) are known as Zn-dependent enzyme, therefore it is expected that inhibition of HDAC catalytic activity will be enhanced with the presence of a sulfur-containing group in an appropriate position. Herein we describe our recent findings in the identification and optimization of thioamide HDAC inhibitors. These compounds were synthesized through a three-step route, and computer modeling predicted stronger coordination between sulfur and zinc atom compared to their amide counterparts. These thioamides are undergoing biological assays to assess their effectiveness in cancer cells.

CHED 656

Synthesis of (2R,3S,4S)-2-(hydroxymethyl)pyrrolidine-3,4-diol from α-methyl-D-galactopyranoside

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Iminosugars, also known as azasugars, have been proposed as competitive inhibitors of glycosyl hydrolases by computational analysis. The potential inhibitory affects of these compounds can be applied medicinally to cancer, diabetes, infections, and other
metabolic processes. One of the research group’s primary goal is to synthesize all eight stereoisomers of the iminosugar, 2-hydroxymethyl-pyrrlolidine-3,4-diol. A number of these pyrrolidine diols are natural products known to inhibit glycosidases. In particular, the synthetic approach to (2R,3S,4S)-2-(hydroxymethyl)pyrrolidine-3,4-diol from α-methyl-D-galactopyranoside will be reported.

CHED 657

Development of a novel serotonin synthesis and derivatives for possible neuro-rehabilitation to treat neurodegenerative conditions

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The 5-HT receptors (5-Hydroxytryptamine) are serotonin receptors within the brain which have partial or total control over many autonomic neurological processes such as cognition, anxiety, mood, and thermoregulation. Regulation of these processes comes from the release of critical hormones including norepinephrine, dopamine, and acetylcholine; as a result these receptors are the targets for many species of pharmaceuticals. Antidepressants and antipsychotics are among the most populous and are often administered for conditions such as Parkinson’s, Alzheimer’s, and Huntington’s disease. The purpose of this research project is to use a gramine initiated, six-step synthesis to synthesize serotonin. At the current stage, the research focuses on increasing the percent yield of the reduction step to the indoline. Derivatives of serotonin will be created and specific functional groups will be analyzed according to their ability to stimulate the 5-HT1A receptors using a Structure-Activity relationship. Spectroscopic methods including IR and NMR spectroscopy will be employed for product verification.

CHED 658

Synthesis and characterization of sol-gel monoliths as glucose biosensors

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Silica sol-gels are porous materials formed through a series of chemical reactions: hydrolysis, condensation, and polymerization using a silicon alkoxide starting material such as tetramethoxysilane (TMOS) or tetraethoxysilane (TEOS). Sol-gels are often used to protect heat and humidity sensitive biomolecules in order to maintain maximum functionality. This project focuses on encapsulating glucose oxidase and horseradish peroxidase in the pores of the silica network to develop a biosensor capable of detecting glucose. Enzymatic activity of glucose oxidase will be monitored by the oxidation of 3,3’,5,5’-tetramethylbenzidine (TMB). Absorbance data will be analyzed
through Michaelis-Menten and Lineweaver-Burk plots to determine the enzymatic kinetics and the functionality of the sol-gel glucose biosensors.

CHED 659

Synthesis and characterization of potential TNR hairpin formation inhibitors

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Several neurological disorders, including Huntington’s disease, result from the expansion of (CAG)ₙ/(CTG)ₙ trinucleotide repeat (TNR) microsatellite sequences in the human genome. As part of the expansion process, the formation of non-B DNA hairpin conformations has been proposed in the base excision repair mechanism. As part of that proposed mechanism, an oxidized guanine residue is excised by 7,8-dihydro-8-oxoguanine glycosylase (OGG1) and repaired by β-polymerase (Pol-b). It is at this stage in repair that DNA slippage can occur, forming the hairpin conformations, leading to the addition of extra bases in the sequence. We propose that developing small molecules that have high binding affinity to the CAG/CTG sequence can be used to “clamp” the DNA duplex, preventing such slippage. We’ve constructed a model DNA system with a (CAG)₂₀/(CTG)₂₀ unit in a 100-mer duplex, with an abasic site at the first 5’-CAG repeat site. We have also synthesized naphthrydine/azaquinoline analogs of Nakatani [Curr. Prot. Nucl. Acid Chem., 2008]. The work presented here will focus on the synthesis and characterization of these analogs, along with the design of the model DNA duplex.

CHED 660

Effect of pH in sulflactoperoxidase formation

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For many years, hydrogen sulfide (H₂S) has been known as a toxic gas that is harmful to health, specifically at elevated concentrations. However, it has been discovered that H₂S is produced endogenously in mammalian tissue, at low concentrations. This has changed its reputation to an important biological molecule with potential therapeutic effects, such as neuromodulation, cytoprotection, vasodilatation, and angiogenesis. Additionally, H₂S interacts with heme proteins such as lactoperoxidase (LPO). Interaction of hydrogen peroxide (H₂O₂) and H₂S with LPO forms a sulflheme derivative. The aim of this research is to perform LPO interactions with H₂O₂ and H₂S at different pH values to monitor the formation of sulflactoperoxidase. It is expected that at lower pH values, the concentration of the H₂S specie increases; resulting in a greater intensity of
the 638 nm band. Consequently, there should be a higher amount of sulfLPO. In order to prove this, we will monitor the interactions of a native LPO (2.5µM) with H₂O₂ (9 µM) and H₂S (50µM), at varying pH values, using UV-Vis spectroscopy. This will provide more information regarding the mechanism of sulfheme derivative formation in other hemeperoxidases.

CHED 661

Investigating the effects of steric bulk on γ-silyl bridging by variation of the γ-electron-donating and α-substituent

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Phenyldimethylsilyl and trimethylsilyl groups are effective electron-donors for facilitating bridging and the synthesis of trifluoromethylbicyclobutane. We are currently investigating effects of steric bulk on both the γ-electron-donating and the α-substituent. One of the systems being prepared will contain a γ-triethylsilyl and an α-CF₃ group. Another substrate, whose preparation is in progress, will contain an γ-SiMe₃ group with an α tert-butyl group in place of the electron-withdrawing CF₃ group. Both compounds, as well as several other potential candidates, will be solvolyzed to determine the extent of silyl bridging to yield the corresponding bicyclobutanes. As well as the corresponding dependence on steric bulk.

CHED 662

Synthesis of 9-fluoro-9H-fluoren-1-ol

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The goal of this portion of the research project was to synthesize 9-fluoro-9H-fluoren-1-ol from 9-oxo-9H-fluorene-1-carboxylic acid. This scheme was tested in a model reaction. Here, the initial reagent was benzoic acid, and through various reactions, it went to benzamide, then aniline, and finally into phenol. Benzoic acid was treated with thionyl chloride to yield benzamide. Benzamide was treated with bleach to yield aniline. Aniline was then treated with sulfuric acid and sodium nitrite to yield phenol. Ultimately, this scheme can be applied in the process of synthesizing 9-oxo-9H-fluorene-1-carboxylic acid from 9-oxo-9H-fluorene-1-carboxylic acid.

CHED 663

Synthesis of polyhydroxylated pyrrolidine from a D-glucose derivative
Carbohydrates are used in a number of different biological processes, which allows carbohydrate processing to be the target of therapeutic agents. Glycosidases, are enzymes that catalyze the degradation of carbohydrates by hydrolyzing the glycosidic linkage. Iminosugars are homologues of carbohydrates in which the endocyclic oxygen of the sugar has been replaced by a nitrogen. Iminosugars are often useful therapeutic agents because of their ability to inhibit glycosidases. The ongoing conversion of commercially-available methyl 4,6-O-benzylidene-α-D-glucopyranoside into the iminosugar (2S,3S,4S)-2-(hydroxymethyl)pyrrolidine-3,4-diol is described.

CHED 664

**Synthesis of lentiginosine form D-glucose**

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Iminosugars have gained popularity as potential inhibitors for an array of cellular processes. Lentiginosine is a naturally occurring iminosugar that was first isolated from the leaves of _Astragalus lentiginosus_. Lentiginosine has been shown to be an effective fungal amylogucosidase inhibitor. Lentiginosine has also been shown to be an α-glycosidase inhibitor. Herein we report the synthesis of Lentiginosine from commercially available methyl-4,6-O-benzylidene-a-D glucopyranoside. Through a multistep synthesis, the desired naturally occurring isomer of Lentiginosine was synthesized and characterized by NMR.

CHED 665

**Computational investigation of the surface tension of supercooled water**

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It has been debated whether or not a second inflection point (SIP) exists in the surface tension of water as its temperature drops below the freezing point. Prior experimental and computational analysis pointed toward the existence of the SIP; while recent data suggest a linear relationship. We employ the accurate WAIL potential for water [E. R. Pinnick, S. Erramilli, and F. Wang, J. Chem. Phys. 137, 014510 (2012)], which was derived purely from electronic structure information, to determine the surface tension of water in the temperature range from 223K (-50°C) to 298K (25°C). Preliminary results
could either be fit with or without a SIP with the linear fit giving slightly better weighted sum of square residuals. The fit with a SIP gives its location at -13°C, also in agreement with prior experimental estimate. The WAIL model agrees better with experimental extrapolation at lower temperatures.

\[
\begin{align*}
\gamma &= aT + b \\
a &= -0.0663 \\
b &= 96.7 \\
WSSR (\chi^2) &= 1.00547
\end{align*}
\]

\[
\begin{align*}
\gamma &= hT^2 + jT + k \\
h &= 7.06 \times 10^{-5} \\
j &= -0.0287 \\
k &= 91.7 \\
WSSR (\chi^2) &= 1.05617
\end{align*}
\]

**CHED 666**

**DFT analysis of copper-based chemotherapeutics**

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A wide range of inorganic compounds are used in the development of chemotherapeutics. While the biological interactions of some of these compounds is well-understood, it is often difficult to predict whether or not an inorganic compound will be an effective agent against cancer. Some of the cancer drugs currently in use are also quite hazardous to the patient so that improving efficacy while minimizing harm to the patient is an important goal. While some research has found that copper-based inorganics show promise, the activity of these compounds is not well-understood. Computational chemistry is an important tool that can be used to predict the mechanism and activity of potential cancer-fighting compounds, such as the inorganic compounds examined in this work. We use B3LYP DFT with the 6-31G basis set to predict the three-dimensional structures, partial charges, and the electrostatic potential energy.
surfaces of known copper-containing molecules\(^1\) both in vacuum and in water. We examine the effect that certain ligands have on the charge distribution in the molecule. Further studies will model interactions of these compounds with DNA.


**CHED 667**

Peptide sequencing using gas-phase peptide carbocations

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Tandem mass spectrometry (MS\(^n\)) and collision induced dissociation (CID) are among the most important tools used to identify peptides and proteins in proteomics. Fragmentation of gas-phase, protonated peptides creates product ions that reveal amino acid sequence. Recently we found that conversion of peptides to N-terminal imines (as Schiff bases) enhances the sequence information revealed by the MS\(^n\) approach. More remarkably, we found that dissociation of Ag\(^+\) cationized versions of these peptide-imines creates never-before seen (M-H\(^+\)) ions (essentially peptide carbocations) by loss of AgH. The MS\(^n\) fragmentation of these ions provides important sequence information as well. In this presentation, the preparation of the peptide-imines will be described, as well as the generation of the carbocations and their CID behavior. Of particular importance is the comparison of the fragmentation of the carbocations to protonated peptide imines and to protonated peptides that lack the imine group.

**CHED 668**

Maximizing the extraction efficiency of arsenic in solid matrices followed by graphite furnace atomic absorption spectrometric analysis

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Arsenic is an element of concern due to its toxicity even at low levels and it is a known human carcinogen. Research studies have been done on arsenic content of rice and chicken, two most commonly consumed food products. The levels of arsenic found varied depending on the variety of rice and chicken, with some brands having alarmingly high levels of arsenic. Previous studies done in our lab involving rice and standard reference rice material showed that the extraction efficiency of arsenic is very low (40 % or less) using sample digestion on a hot block. Thus, we need to modify our
sample digestion method in order to increase the extraction efficiency of arsenic in rice, chicken and seafood using hot block digestion since we do not have a more efficient microwave digester. SRM 1568b rice flour and a few brands of ground white and brown rice were digested in 0.28 M HNO₃ in a closed vessel at 95 °C following FDA EAM Section 4.1, then analyzed for arsenic using graphite furnace atomic absorption spectrometry. SRM1566b oyster tissue and ground red and white chicken meat were digested in concentrated HNO₃ followed by the addition of 30 % H₂O₂. Our preliminary data indicates very low arsenic recoveries for rice (30 % or less). None of the chicken meat tested showed detectable levels of arsenic, however, only a 63 % recovery of arsenic in SRM1566b oyster tissue was achieved. We plan on finding a more effective hot block digestion procedure for both rice and chicken meat to improve our % recoveries.

CHED 669

Curriculum development for BSU's outreach program geared to spark interest in chemistry

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The field of chemistry is important and essential to everyday life but can be an intimidating subject to tackle for young students. Generating interest in the Science, Technology Engineering and Math, or STEM, fields is important to begin at a young age. Through interactive and hands on experience young students can be introduced to, and learn, the fundamental role of chemistry in everyday life. The CityLab at BSU is a science outreach program for grades 4-12 teachers and students, providing a biotechnology learning experience that supplements classroom curriculum for hundreds of local school students who visit the CityLab each year. During the Summer 2014 and through funding by BSU's Adrian Tinsley Program for Undergraduate Research, the first chemistry-gearied module for the CityLab was developed for Grades 7-8 using engaging everyday-life chemistry experiments. Various experiments centered on the analysis of freshwater quality were tried for adaptability to Grades 7-8 students, including pH testing using red cabbage extract, determination of dissolved oxygen by titration, and determination of total residual chlorine by colorimetric reaction using a benchtop spectrophotometer. One trial of the 3-hour module has been run by volunteer BSU science majors who provided great feedback on the clarity of the procedure within the module. Once the module has been rewritten, it will be offered to BSU CityLab for testing by visiting Grades 7-8 students. The module will be assessed for its effectiveness in engaging students in the field of chemistry using current CityLab assessment procedure.

CHED 670

Microwave synthesized succinimides purified by flash chromatography
The research that has occurred in our laboratory is utilizing microwave synthesis to generate different combinations of amines and anhydrides to form imides. The actual synthesis of the amine and anhydride takes around 8-10 minutes rather than the 8 plus hours as other methods found in the literature. The resulted product from the microwave synthesis is removed from the microwave and then heated in a mixture of 50% ethanol and 50% water until it dissolves. Then, the filtered and dried product was purified by flash chromatography by using 40% hexane 60% ethyl acetate solvent. The collected samples were tested by TLC analysis to determine if the desired product was isolated. The wanted products were concentrated by rotovaping. Since there is little to no solvent usage in creating our desired product, the microwave method is cheaper and faster than more traditional synthesis techniques. This method is great for classroom use and allows students to grasp a better understanding of basic organic concepts by generating many products and looking at percent yields and which will help students determine which aniline/anhydride combination gives the best and worst results. These combinations can be used outside of the academic lab as well and can serve a purpose in our everyday lives. For example, some succinimide derivatives can be used as insecticides, while other compounds are used for agriculture agents, drugs, or dyes. Therefore, generating and isolating these compounds by a method at faster times and lower costs can be beneficial to the scientific community.

CHED 671

Transesterification of hypophosphorous esters: Elucidating the synthetic scheme of phosphorous-based surfactants

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Large oil spills in the ocean are catastrophic events, which pose a great threat to marine life and the environment. For the BP Deep Water Horizon oil spill of April 2010, the response at sea was mostly done by releasing dispersants (solvent/surfactants mixture) in the ocean to encourage bioremediation and the decomposition of the toxic compounds found in oil. Our objective is to synthesize innovative phosphorous-based surfactants to simultaneously remediate the oil and serve as a natural resource for marine organisms. The synthesis of long chain hypophosphorous esters is conducted through a silicon-based esterification with tetraethyl orthosilicate (TEOS) followed by a transesterification with a long chain alcohol (long C-C chain silicon ethers are unstable compounds and/or expensive, thus, unusable). A one pot one-step (all reagents reacting at once) methodology was established after conducting multiple equivalence, solvent and time studies that led us to our routine reaction conditions of: 4 equivalence of alcohol in acetonitrile at reflux, under nitrogen for 2 hours. Moderate results for the transesters were obtained with a range of 63 to 65% yield. We consequently studied the
reaction sequence of one pot two-steps, where the esterification occurs first, followed by the addition of the alcohol for transesterification. This change in procedure was extremely successful in which our percent yield range increased to 83-84%, in the exception of cyclohexanol remaining at 64% due to steric hindrance in the reaction. We are currently investigating the second step of our synthesis, which involves a palladium catalyzed hydrophosphinylation reaction of the esters with bromoalkenes. Preliminary results show encouraging data with percent yields that range from 40-75%. Our next area of focus will be to isolate the compounds synthesized and optimize our yields in order to conclude the synthesis of innovative phosphorous-based surfactants.

CHED 672

Accessing vinyl fluoroalkyl-substituted cyclopropanes from homoallyl mesylates via a destabilized cation-mediated electron cascade

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Solvolysis of 3⁰ mesylates with an α-electron withdrawing group (EWG), a γ-π system, and an ε-silyl group gives rise to 3⁰ fluoroalkyl-substituted vinyl cyclopropanes. Cation destabilization by the α-electron withdrawing fluoroalkyl group facilitates strong neighboring group participation of olefin, inducing cationic ring closure (CRC). Rapid β-silyl elimination of the resulting β-silyl carbocation drives the process, making the CRC irreversible. The scope of the reaction and the influence of groups at the α-position on the stereochemical outcome are currently under examination.

CHED 673

Chemistry laboratory safety: Misconceptions among first- and second-semester general chemistry students

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The general chemistry laboratory can be a dangerous place, and the possible danger is amplified by the fact that general chemistry is frequently a student's first chemistry laboratory experience. College students come from a variety of backgrounds with only some having had chemistry in high school, and therefore many students will not know beforehand what kind of precautions to take or what kind of action to take in case of an accident in the lab. Safety information is given briefly at the beginning of the semester, but the efficacy of this is uncertain. An online survey was conducted to gauge first- and second-semester general chemistry students' knowledge about chemistry laboratory
safety and the data gathered was analyzed. This survey was conducted at two secondary schools in two different countries. Statistical analysis will be presented. Results will allow discernment of misconceptions held by students over two semesters and between countries, and conclusions can be made about the effectiveness of current laboratory safety instruction methods.

CHED 674

Chemical and biochemical stability of guanine lysine cross-links formed by guanine oxidation

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Mutations in DNA are caused by oxidative stress and can lead to aging and various cancers. Guanine is susceptible to oxidation because it has the lowest oxidation potential of the DNA bases, and guanine oxidation leads to DNA-protein cross-links. Here, we examined whether such cross-links are stable under various conditions. Poly-L-lysine was used as a model protein to examine the stability of the crosslink at room temperature, high temperature, and high temperature with hot alkali. We also tested the stability of the cross-link to digestion with Fpg, a bifunctional DNA glycosylase that is capable of excising the damaged base and cleaving the phosphodiester bonds.

Samples containing DNA, lysine, Ru(phen)$_2$dpdz$^{2+}$ [phen = 1,10-phenanthroline, dppz = dipyridophenazine] and Co(NH$_3$)$_5$Cl$^{2+}$ were irradiated with the 442 nm output of a HeCd laser to oxidize the DNA by the flash quench method. The samples were then analyzed for cross-linking using both the chloroform extraction assay and the gel shift assay. By the chloroform extraction assay, the cross-link was found to be stable at room temperature. In contrast, incubation at 100°C with piperidine cleaved nearly all the cross-links whereas the 100°C treatment without alkali or digestion with Fpg cleaved only some of the cross-links. Lastly, agarose gel electrophoreses with irradiated samples of pUC19 plasmid showed a band of free DNA that shifted toward the wells upon irradiation. Treatment of irradiated samples with Fpg gave rise to different behavior. At lower irradiation times, a band of slightly lower mobility, probably nicked DNA, is observed, consistent with cleavage of the cross-link. At the highest irradiation time, the DNA runs as a smear, indicating it was heavily fragmented by the enzyme. Thus, since high temperatures and Fpg enzyme are not fully efficient in cleaving the cross-links, it appears that guanine-lysine cross-links could persist in vivo.

CHED 675

Comparisons of Synaptotagmin 1 and Synaptotagmin 7 C2A domains in membrane associations by molecular dynamic simulations
Synaptotagmins (Syt) are membrane binding proteins that regulate the release of hormones and neurotransmitters through exocytosis. Previous works suggest that the C2A domains of Syt1 and Syt7, two members of the Syt protein family, have different membrane-docking mechanisms despite their structural similarity. Here, we report the MD simulations of both Syt1 and Syt7 C2A domains associated with membrane of mixed POPC and POPS (3:1) to identify the origin of the differences. We also analyze how the simulation results depend on the initial orientations of the C2A domains with respect to the membrane.

CHED 676

Computational modeling of STAT3 SH2 domain inhibition

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Signal Transducer and Activator of Transcription 3 (STAT3) plays a significant role in the regulation of important cellular processes. Phosphorylation of Tyr705 and Ser727 activates STAT3 dimerization and translocation to the nucleus. Here, the dimer promotes transcription of targeted genes by binding to specific regions of DNA. In various cancer cell lines, STAT3 is overexpressed leading to cell proliferation and inhibition of apoptosis. In this way, STAT3 activation is a viable target for treating cancer. XZH-5, a small molecule inhibitor of STAT3, works on the principle of interrupting dimerization by disrupting the interactions between the pTyr705 peptide and its associated pocket on the SH2 domain. In an attempt to optimize the binding of the inhibitor to the pTyr705 pocket, several derivatives of XZH-5 have been developed. This computational study seeks to investigate the structural aspects of the binding of these XZH-5 analogues to the pTyr705 pocket of the STAT3 SH2 domain using the RosettaLigand docking application. Docking results are compared to in vitro activity assays against multiple human cancer cell lines with the goal of identifying optimal XZH-5 analogues.

CHED 677

Computational modeling of temporary anion states in the field of dipole or quadrupole moment

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It has long been known that electrons can be bound by either the dipole or quadrupole moment of a molecule. Of course, in real molecular situations there are always other attractive and repulsive forces present as well. Previous workers have used model systems to demonstrate that for sufficiently large moments, an electron can be bound to the permanent moments. The present work investigates temporary anions, sometimes called shape resonances, in which the electron is temporarily bound to the permanent moment. Typically in shape resonances the electron is pictured as trapped in the attractive region of the potential by an angular momentum barrier. Thus, the resonance parameters can be strongly dependent on the nodal characteristics of the wave function. The electron attraction to the moment is damped at short-range and a short-range repulsive potential is also added to make model more realistic. The energy and the lifetime of the anion state are investigated as a function of the model parameters.

CHED 678

Computational modeling of resonant vibrational excitation of CO by electron impact

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Vibrational excitation of carbon monoxide, CO, by electron impact is greatly enhanced near incident electron energies of 2 eV by temporary electron capture and formation of the $^2\Pi$ anion state. Previous studies have demonstrated that in order to correctly model the experimental angular distribution of electrons emitted upon vibrational excitation of CO, two partial waves must be considered: p and d. Previous work used experimental data to estimate the relative contribution of each partial wave in terms of a single mixing parameter. The present study uses the stabilization method in conjunction with the Equation-of-Motion Coupled-Cluster Singles and Doubles (EOM-CCSD) with a quadruple zeta basis set to calculate the complex potential energy curve of the $^2\Pi$ state of CO, restricting the electron at large distances from the molecule to be having either a p-like or d-like distribution. Vibrational excitation cross sections and angular distributions are calculated from this complex potential using a time-dependent wave packet approach and compared to experimental data. Further refinements of the complex energy surface are obtained by fitting to the experimental data.

CHED 679

Cyclic voltammetric and computational structure-electrochemistry relationship studies of the reduction of a series of 9,10-anthraquinone derivatives

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The electrochemical behavior of 9,10-anthraquinone (AQ) derivatives was experimentally and theoretically studied to determine a linear relationship that allows for a calculated prediction of AQ reduction potentials that have not been experimentally determined. The b3lyp method of DFT to analyze the electrochemical potential of several sets of anthraquinones. The calculations were performed at the 6-31+G* level of theory. In addition to the electronic structure methods, the integral equation formalism variant of the Polarizable Continuum Model (IEFPCM) was used with DMF as a solvent. Preliminary calculations indicate similar single (double) reduction potentials Q/Q− (Q/Q2−).

Calculations were carried out on a series of amino, alkyl, hydroxyl and chloro substituted anthraquinones. The data were corroborated linearly with CV data obtained experimentally. Preliminary results suggest that the a roughly linear correlation of CV determined reduction potentials to in silico calculated energies may be dependent upon the substituted moieties. The amino, alkyl, and chloro substituted anthraquinones appear to correlate well (R² = 0.78). While the hydroxyl and alkoxy substituted anthraquinones are not well described. The correlations and advanced analysis will be discussed in detail.

CHED 680

Effect of unequal strand length on DNA hybridization in a model microarray system via Monte Carlo simulation

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DNA microarrays are systems consisting of single stranded DNA that is bound to a surface, the probe strand, which hybridizes with its complement that is free to move in solution, the target strand. For this study Monte Carlo molecular simulations were done to look at the effects of target and probe length as well as sequence on hybridization of DNA microarrays for a 25-base strand with a complementary 10-base strand. Four alternate surface bindings were used – either the long strand at the 3’ or 5’ end, or the short strand at its 3’ or 5’ end. Compared to hybridization with both strands being free to move, duplex destabilization occurred with setups having non-complementary bases on the target directed towards the surface as well as those having non-complementary bases on the probe directed away from the surface.

CHED 681

Journey of 4-HNE: How biochemistry became computational

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The chemical 4-hydroxy-2-nonenal (4-HNE), a major end product of lipid peroxidation, is an inducer and mediator of oxidative stress. It is thought to be involved in the pathogenesis of a number of degenerative diseases including: Alzheimer's,
atherosclerosis, cataracts and certain types of cancer. The normal cellular concentration of 4-HNE in humans ranges from 0.1 mM-0.3 mM; however, under conditions of oxidative stress, this concentration increases to 5 mM-10 mM. The mechanism and reason this occurs, although, is unknown. 4-HNE, an α,β-unsaturated aldehyde, can likely react, via Michael addition, across its carbon-carbon double bond with many cellular components, including DNA and proteins. This mechanism was studied by synthesizing 4-HNE and reacting the synthesized product with the functional groups of histidine and cysteine. After analysis by nuclear magnetic resonance (NMR) these two reactions were then studied by computational chemistry using the density functional M05-2X.

CHED 682

Predicting the function of structural genomics proteins of unknown function in the crotonase superfamily

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Structural Genomics (SG) efforts have given rise to the need for better methods to predict protein function. Protein structures are often correlated with their function, but this relationship is complex. Proteins with the same function may have different structural folds. Proteins within a superfamily can have different biochemical functions although the structures are highly similar. Members of the Crotonase Superfamily have the common feature of recognizing an acyl-CoA substrate and stabilizing an enolate anion intermediate. However, this superfamily includes diverse biochemical functions, including hydrolase, isomerase, and dehalogenase activities. This project focuses on the functional characterization of proteins within the Crotonase Superfamily through computational and experimental methods. The computational methods, THEMATICS, POOL, and SALSA, are used to analyze the local structures at predicted active sites and are employed to predict the functions of the SG proteins of unknown function within the superfamily. Functional assignment is based on the predicted sets of catalytically active amino acid residues for the proteins of known function within the superfamily. Predicted sets of active residues for the SG proteins are compared with the local structural signatures obtained from the previously characterized proteins. Biochemical assays serve to validate the computational predictions. Thirty-four SG proteins were analyzed and 13 aligned with known members of the Crotonase Superfamily. Twenty-one SG proteins in the Crotonase Superfamily did not align with the consensus signatures of the known functional subfamilies. Several of the proteins were expressed recombinantly and purified to be used for functional assays to validate predictions. Accurate functional annotation by computational methods facilitates practical application of SG data.

CHED 683
Conformational sampling of glucose oxidase for bio-fuel cell applications

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Glucose Oxidase (GOX) is a redox enzyme that uses flavin adenine dinucleotide (FAD) as a cofactor to reduce β-D-glucose into δ-gluconolactone via a ping-pong steady-state kinetic mechanism. While it remains a candidate for developing alternative fuel cells, instability of the dimeric interface remains a concern. Electrochemistry experiments have determined that enzymatic efficiency depends upon the orientation of FAD to a carbon nanotube. Our hypothesis is that the orientation of FAD effects the conformational space sampled by the protein. Towards this we have applied computational chemistry methods to identify the way in which glycolysis reaction impacts the various oligomeric states of GOX. In close agreement with literature, molecular dynamics simulations of apo-GOX find that the protein undergoes large conformational changes that have been implicated in the modulating the glycosylation reaction. Our long-term goal is to develop computational chemistry methods in order to simulate the entire protein and electrode assembly in order to provide a means to stabilize GOX for applications in a bio-battery.

CHED 684

Role of glycosylation in protein structure: A bioinformatics-based computational study

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Proteins can be engineered with improved or novel functions by altering primary sequence. Covalent modifications offer an additional tool for protein design since they enhance the diversity of protein structure and function given by the 20 amino acids. Glycosylation is a common covalent modification that occurs on more than half of all polypeptides. Glycans function as recognition sites, mediate immune responses to pathogens, and regulate protein folding and turnover. N-linked glycosylation to asparagine occurs co-translationally in the endoplasmic reticulum potentially facilitating proper protein folding and stabilization of secondary structure. It has been suggested that specific interactions between the sugars and amino acids contribute to structural stabilization. This study characterizes protein-glycan interactions that enhance protein secondary structure. A bioinformatics analysis of the Protein Data Bank identified amino acids with the potential to stabilize specific secondary structures through such interactions. Computational methods were used to further analyze the effects of the identified constructs on secondary structures at the molecular level.

CHED 685

Effect of motor protein binding on microtubule depolymerization
Our study focused on the role of kinesin-1 motors in depolymerization of curved microtubule (MT) protofilaments (PFs). In particular, we determined the effect of kinesin-1 on the mechanical behavior of PFs. We compared and contrasted this behavior with the mechanical response of apo PFs and PFs decorated with kinesin-13, a known efficient MT depolymerizing motor.

Set up used for course grain pulling simulations of kinesin-1 loaded protofilaments.
Curved Protofilament-Interdimer Bending Angle
Interdimer bending angle propagation for a 6 dimer curved microtubule protofilament under application of simulated pulling force. Results achieved via molecular dynamics simulation.

CHED 686

Solid-state NMR chemical shift peak matching of geometry optimized organic crystals by computational methods

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Solid-state NMR (SSNMR) spectra hold chemical and structural information, however the spectral peaks must be assigned to atomic sites to utilize this information. Computationally calculated chemical shifts can be assigned to experimental peaks if an accurate crystal structure is first determined. Triphenylsilanol, representative of reactive sites of important silica materials, has a challenging $^{29}$Si SSNMR spectrum (Figure 1) to assign because it contains 8 chemically identical, but crystallographically unique, Si positions in the crystal resulting in 40,320 possible assignments. The size of the triphenylsilanol unit cell (Figure 2) containing 588 atoms makes quantum mechanical geometry optimizations prohibitive. We have optimized the diffraction structure using molecular mechanics with FORCITE and assigned peaks using a least-squares fit of the chemical shielding tensors calculated with CASTEP. CASTEP makes use of the Perdew-Burke-Ernzerhof generalized gradient approximation functional and a plane wave basis set. We report chemical structures and shift assignments for 1,4-dimethoxybenzene and triphenylsilanol.

Figure 1. $^{29}$Si SSNMR spectrum of Triphenylsilanol
CHED 687

Theoretical study of the factors that contribute to the conformational energy of six-membered rings

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Various studies have shown that 2-hydroxyltetrahydro-2H-pyran has a negative conformational energy and is said to manifest an anomeric effect. The cause of the anomeric effect is not well understood and by computationally studying the energies and geometries of a series of compounds in a series of solvent systems, the contributions of steric factors, of hyperconjugation effects, of stereoelectronic interactions and solvent interactions to the relative stability of axial and equatorial conformers were investigated. A series of monosubstituted cyclohexanes with minimal electronic interactions were studied followed by a series of monosubstituted tetrahydro-2H-pyrans. The relaxed scans of energy as a function of the orientation of the ring substituent of the tetrahydro-2H-pyran series show the combination of the electronic effects and the steric effects and comparison to the scans of the cyclohexane series to the allowed separation of the electronic effects from the steric effects. Natural Bond Orbital analysis of the full sequence of both sets of compounds is used to establish the extent of any hyperconjugative effects. To study the solute-solvent interactions, the
energy and geometry studies were repeated using a continuum solvent model with water ($\varepsilon = \sim 80$), acetone ($\varepsilon = \sim 20$) and cyclohexane ($\varepsilon = \sim 2$) selected as the solvent.

CHED 688

Computational study of the contributions to the relative stability of the $\alpha$ and $\beta$ conformers of D-glucopyranose

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In order to better evaluate the contributors to the conformational energy of D-glucopyranose, the geometry-energy relationships for a sequence of model compounds were determined. The conformational energies of 1-hydroxy 3-hydroxymethylcyclohexane and 2-hydroxy 6-hydroxymethyltetrahydro-2$H$-pyran were used to model D-glucopyranose. The conformational energies were determined at the B3LYP/6-311G++(d,p) and MP2/6-311++(d,p) levels in the gas phase and solution. The relative B3LYP energy as a function of the orientation of the substituents were determined by relaxed scans as the –CH$_2$-OH at C5 was rotated about the OCCO and HOCC dihedrals and the –OH at C1 was rotated about the HOCO dihedral. The lowest energy rotamers for the axial ($\alpha$) and equatorial ($\beta$) conformers were used to calculate the conformational energy. Because solute-solvent interactions have significant effects on the relative stability of the axial and equatorial conformers, the energy versus dihedral scans were repeated using a continuum solvent model with water ($\varepsilon = \sim 80$), acetone ($\varepsilon = \sim 20$) and cyclohexane ($\varepsilon = \sim 2$) selected as the solvent.

CHED 689

Solid-phase heats of formation of energetic compounds using computational methods

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Computational investigations of high energy density materials (HEDMs) are being conducted in order to determine solid-phase heats of formation. HEDMs are compounds that detonate rapidly to evolve large volumes of gas and have a wide range of uses including mining, airbag design, and military applications. These compounds have a number of important structural considerations including ring strain and steric interactions as well as nitro, nitroso, and azido functionalities. Our research is primarily focused on finding appropriate and time-efficient methods for determining accurate gas-phase heats of formation for a set of twenty compounds. In order to determine solid-phase heats of formation, experimental heats of sublimation are subtracted from our calculated gas-phase heats of formation. Methods currently being evaluated involve Hartree-Fock (HF) theory and density functional theory (DFT) using the B3LYP functional with at least
6-31G as the basis set. Our analysis examines the relationship between the connectivity of the atoms and the accuracy of the calculated energetic parameters when compared to available empirical parameters.

CHED 690

Computational studies of the hyperpolarizability of halogenated saccharins and their anions and salts

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We have continued and expanded our research calculating the hyperpolarizability of organic molecules related to saccharin. Synthetic interest in metal-organic framework materials that contain fluorosaccharin and that may have the possibility of second-harmonic generation has created an interest in identifying both ligands and metal complexes with a large hyperpolarizability. This project has extended the molecules surveyed to include all of the isomeric fluoro-, chloro-, bromo-, and iodo-saccharins as well as their anions and main group metal salts. Additional preliminary results with extremely electronegative substituent groups are also reported. We also summarize our survey of levels of theory, basis sets, and solvation for the calculation of hyperpolarizability of several reference organic molecules.

CHED 691

Electronic structure calculations of Li₂-II-IV-VI₄ diamond-like semiconductors

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Diamond-like semiconductors (DLSs) are compounds whose structures are derived from either the cubic or hexagonal form of a diamond. DLSs are versatile and have many potential technological applications. Several DLSs are commercially available for photovoltaic and nonlinear optic applications. DLSs are also of interest for their potential use in thermoelectric materials. Through the use of the WIEN2k computational software package, the electronic structures of various quaternary DLSs were determined, most notably density of states (DOS) and band structure. This program utilizes the full-potential linearized augmented plane wave (FP-LAPW) method of density functional theory (DFT) to perform electronic structure calculations on extended solids, such as DLSs. It has been hypothesized that a change in the tetravalent metal of the compound will affect the band gap accordingly. This is due to a rationale surrounding the impact of crystal radius and orbital overlap on the valence/conduction band of extended solids.
Coarse-grained modeling of reverse micelles

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Though often unnoticed, confined water molecules are ubiquitous in chemical and biological systems, such as within protein pockets, and exhibit non-bulklike behavior in these crowded environments. The non-bulklike behavior of water in the confined environment of a reverse micelle is studied in order to better understand the behavior of water in important biological systems. A one dimensional simulation of a line and a two dimensional simulation of the reverse micelle were produced using a Monte Carlo algorithm with the Glauber acceptance criteria. Overall spin polarization was calculated for the one dimensional model, and a rotational correlation function was employed to study the behavior of each individual water molecule in the two dimensional simulation.

CHED 693

Computational study of the visible spectrum of curcumin's protonation states

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Curcumin, the main dye in the important Indian spice turmeric, has received much attention in the literature recently for its potential anti-cancer and anti-Alzheimer properties. Other research interests include curcumin's stability, degradation, radical activity, chelation with metals, and bioavailability. From an educational standpoint, curcumin is a good example of important chemical concepts like the relationship between pH and protonation state, spectroscopy, and thermodynamics. As a part of a summer research experience, one project was to study the thermodynamics and UV-vis absorptions of curcumin’s various protonation states theoretically using Gaussian 09 to determine which computational method gives results that best agree with experimental results. M06/3-21G* gave the best thermodynamic results, while M06 with 3-21G* and 6-31G* gave good spectroscopic results for the neutral and dianionic forms of curcumin. However, applying diffuse functions appears to be necessary for the trianionic form. Interestingly, M06 and B3LYP with 6-31+G* gave good spectroscopic results for the singly anionic form. Other conclusions include that the formation of dimers and trimers was supported theoretically, that unusually short H-bonding between dimers and trimers was observed, that there was good agreement with theoretical results and the particle-in-a-box method, and that B3LYP also gave relatively good agreement with experimental spectroscopy results.
In silico insight into mechanism for the formation of C8 products from the reactions of guanine with substituted aniline

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It is thought that most arylamines can be oxidized to hydroxylamine and are further activated to carboxyl and sulfate esters. However, only some arylamines are mutagenic, reacting with purine bases resulting in modified DNA, primarily at the C8 position of guanine. To study the mechanisms of the reaction of the activated arylamines and guanine, we examined the mechanism using theoretical calculations at the B3LYP/6-31+G(d) level with the aqueous CPCM solvation model. We modeled guanine as imidazole, 1-methylimidazole, guanine, and 1-methylguanine. The arylamines modeled in this study were aniline, 2,6-dimethylaniline, 2-methylaniline, and 2,4-dimethylaniline. Our study suggests that the mechanism is a tandem addition-cyclization-elimination reaction that starts with guanine N7 reacting with the activated arylamine in an $S_{N}2'$ or $S_{N}1'$ fashion. A five-membered ring intermediate is generated, followed by deprotonation at C8, resulting in a ring cleavage to the final product of the modified
purine base. For all the systems, the greatest energy barrier after the initial rate limiting $S_N^2$ or $S_N^1'$ reaction is around 14 kcal/mol, and the acid constants leading to the final products are predicted to be very acidic around -27 $pK_a$ units.

CHED 695

Computationally simulating the metabolic enantiospecificity of CYP2C9 using molecular dynamics

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It is estimated that about half of the pharmaceutical drugs currently available on the market are chiral. CYP2C9 is a relatively abundant cytochrome P450 enzyme located in the liver that is involved in the oxidative metabolism of many drugs. CYP2C9 has been known to exhibit enantiospecificity among its substrates, metabolizing one enantiomer of a specific chiral drug more efficiently than the other enantiomer. This selective metabolic characteristic is thought to arise from the interaction of the ligand with certain specific amino acid residues near the enzyme active site. Enzyme-ligand interactions with various drugs during metabolism were examined computationally through a molecular modeling suite (Sybyl-X). Utilizing molecular dynamics to simulate the oxidation reaction made it possible to determine which residues were involved in stabilizing the enzyme-ligand complex. By comparing the energy differences contributed by the interacting residues between each enantiomer, LEU208, THR301, and PHE476 in particular appeared to selectively stabilize either the R or S enantiomer of the wide range of drugs tested in this experiment: Bortezomib (antineoplastic agent), Carvedilol (beta-blocker), Clopidogrel (antiplatelet medication), Pioglitazone (thiazolidinedione), and Valsartan (angiotensin II receptor antagonist).

CHED 696

Elbow room: How surfactant proportions modify interfacial properties

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In this study, computational chemistry modeling tools are used to simulate oil-water systems containing one of two structurally related surfactants, sodium dodecyl sulfonate (SDS) and sodium dodecylbenzene sulfonate (SBS). The objective of this study is to understand how the addition of a benzene ring near the head group (hydrophilic end) of SBS will change its behavior relative to SDS at the interface between water and an immiscible organic solvent. The modeling tool used is Amber MD, a chemical simulation tool suite based on classical molecular dynamics. In addition to Amber MD, various analysis tools have been developed to perform secondary analytics on the resultant
molecular trajectory files. We seek to elucidate the structural differences of SBS and SDS at the interface and the consequent changes to the interface properties using various metrics, including interfacial tension and molecular ordering.

Sodium dodecyl sulfonate at water hexane interface

CHED 697

Computational docking to analyze substrate metabolism in CYP2E1

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CYP2E1 is a protein of the cytochrome P450 family that is vital in the metabolism of many foreign substances in the human body, including styrene and acetaminophen. Human exposure to these substrates has persisted for years, yet the exact mechanisms by which they react are still unknown. Although these drugs are both metabolized by CYP2E1, they each have a different non-hyperbolic kinetic profiles that make them unique to CYP2E1. This observation has led to increased examination of these molecules as they bind alone and in combination to investigate interactions with key amino acid residues along the channel of the protein and near the active site. Using molecular dynamics of computational software Sybyl-X, the mechanism of action and kinetic profile by which each of these drugs interacts is studied. Important residues of the protein structure and fundamental energy differences are determined to examine the toxicological effects of these complexes and their cooperative properties.

CHED 698
Computational investigations on ligand isoform selectivity in the liver X receptors

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The LXRα are a nuclear receptor, exhibiting two isoforms (LXRα and LXRβ), that have been demonstrated to be important mediators in a number of human diseases, including atherosclerosis, diabetes, cardiovascular disease, autoimmune disorders, Alzheimer’s disease, and several types of cancer. It has been observed that nonselective agonists lower serum cholesterol levels and also tend to raise triglyceride levels in the liver, which can lead to serious medical issues, while LXRβ-selective agonists tend to lower cholesterol levels without affecting triglyceride levels; thus, there is a strong drive to develop selective liver X receptor modulators (SLiMs) whose action is different in various tissues. Here we use computational chemistry methods to investigate the binding of four ligands, 2 α-selective, 1 β-selective, and one non-selective, to both LXRα and LXRβ. Molecular dynamics techniques are used to generate an ensemble of protein-ligand structures for each of the systems and protein-ligand scoring methods are used to generate estimates of binding free energies. Glycin scanning methods are used to investigate the particular ligand-residue contacts that are responsible for ligand binding and LXRα/β selectivity.

**CHED 699**

Studies of factors affecting the reaction mechanism of formation of the levoglucosan

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Formation of levoglucosan is an important step in the fast pyrolysis of renewable cellulosic biomass to producing carbon-neutral, drop-in transportation fuel. Many experimental and theoretical efforts have been made and a variety of mechanisms have been proposed, yet none agrees with each other. Previous theoretical studies based on a relatively small model (cellobiose) generate two different mechanisms. In this study, several factors that may affect the reaction mechanism are investigated. This includes: the size of theoretical model, the medium that the reaction occurs, and the position of the reaction sites. A hybrid QM/MM approach is used where M06 is used for the QM part and UFF is used for MM part. PCM model is used for the solvation. All calculations are performed by using Gaussian 09.

CHED 700

Mechanistic insights into the alkylation reactions of quinone methide precursors: Studies towards the realkylation of aged acetylcholinesterase

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Acetylcholinesterase (AChE) is an essential enzyme in the human body. It hydrolyzes the neurotransmitter acetylcholine into choline and acetate at neurosynaptic junctions. Organophosphorus (OP) nerve agents such as Sarin and Soman are covalent inhibitors of AChE. Following exposure to OPs, AChE is inhibited and undergoes a subsequent irreversible aging process in which the OP-AChE adduct is de-alkylated, resulting in the accumulation of excess acetylcholine in the central nervous system. Current oxime-based pharmaceuticals can only be used to treat the inhibited AChE and are ineffective on the aged AChE. Our research focuses on re-activation of the aged AChE. Quinone methides (QM) have been shown to react with model phosphates to alkylate them, and therefore may potentially reverse the damage done to the active site on aged AChE through a kinetically favored alkylation of the phosphorylated serine residue in aged AChE. Computational methods were used to analyze the potential reaction pathways and docking poses in AChE of a variety of quinone methide precursors (QMPs). Snapshots of human aged-AChE were used for our docking calculations, in which the QMPs were allowed to interact with the enzyme active site. Certain poses were further investigated using molecular dynamics simulations to better understand the interaction between ligand and enzyme. The analysis of these results has provided guidance to which potential therapeutics should be investigated further.
The acetylcholinesterase (AChE) active site

CHED 701

Unpaired electron density in retinal model compounds

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Determining radical character of molecules is often of interest to chemists. Experimental methods, like ESR (electron spin resonance), can be used to locate unpaired electron density in molecules, and several computational methods are available that calculate electron spin densities. But most high-level computational methods yield the spin-averaged density only so that characterizing unpaired electrons is problematic. For this study we have implemented, in the natural bond orbital (NBO) program, a novel approach proposed by Head-Gordon that yields a measure of radical character from the spin-averaged density matrix. We use this approach together with CAS/cc-pVDZ calculations to examine the distribution of unpaired electrons in several retinal model compounds as they undergo cis-trans isomerization. Our calculations show that the \( p \) electrons remain largely paired at most angles as the retinal model compounds undergo cis-trans rotation. Significant radical character is only revealed at angles within 10-15° of the fully twisted 90° transition states.

CHED 702

Computational study on the formation of hexamethylene triperoxide diamine

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The first steps in the mechanism for the formation of hexamethylenetriperoxidediamine (HMTD) from hexamine and hydrogen peroxide with acid catalyst were investigated using ab initio quantum chemical methods. Determining the possible intermediates involved in the synthesis of this peroxide explosive may lead to the development of better detection methods. Preliminary results using the MP2/cc-pVTZ method indicate an exergonic process for the net reaction of -26 and -32 kJ/mol for the \( C_2 \) and \( D_3 \) HMTD
conformers, respectively. The first step in the mechanism is presumed to be proton addition to a basic nitrogen site in a nearly barrier-less process. Then steps consisting of alternating C-N bond scission, peroxide addition, and ring formation continue until all three peroxides are added; during which one of the two product ammonias is formed. Intramolecular rearrangement then leads to the loss of a second ammonia and final ring closure. Possible alternate pathways will also be discussed.

CHED 703

ARGOS: A rigid geometry optimizer for supramolecular complexes

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The computational study of supramolecular complexes is often difficult due to the weak nature of the noncovalent interactions that hold these complexes together. In particular, the flat potential energy surfaces associated with these interactions are problematic for more general geometry optimization schemes. Additionally, the motions of atoms in the individual monomers in such complexes are highly correlated, contributing to the inefficiency of algorithms that treat each atom separately. To address these demands, we have developed ARGOS (A Rigidbody Geometry Optimizer for Supramolecular complexes). ARGOS parameterizes the space of rigidmonomer pairs using Euler angles and enables optimizations using either cubic spline curve fitting or a finite difference based Newton method. We assess the performance of ARGOS on a set of non-bonded dimers and discuss possible extensions of the algorithm to systems containing more than two monomers.

CHED 704

Group 13 chiral Lewis acid stereoselective control of enal Diels-Alder reactions

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Group 13 chiral Lewis acids MCl₂OR (M = B, Al, Ga) complexed with substituted enal dieneophiles have been used in asymmetric Diels-Alder reactions; however, the factors that influence stereochemical control are not yet well understood. A “formyl hydrogen bond” between a boron Lewis acid and the formyl hydrogen of an enal has been proposed to explain selectivity. New competing interactions between the enal vinylic alpha- and beta-hydrogens and the Group 13 chiral Lewis acids have been investigated. Second-order Möller-Plesset theory and M06-2X density functional with Dunning basis sets have been used to study these three bidentate complexes. It is found that the previously unconsidered, alpha-hydrogen effectively competes for complexation in the
chiral Lewis acid complexes. Evidence is found for competition between the formyl and alpha-hydrogen interactions in aluminum and gallium chiral Lewis acid complexes, but not with boron. These two organizing elements explain experimental selectivity reported by Koga.

CHED 705

Solvation effects in bimolecular Diels Alder cycloaddition of cyclopentadiene: A tool for benchmarking expected errors in more sophisticated Diels Alder reactions

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The bimolecular Diels Alder cycloaddition of cyclopentadiene occurs with minimal charge separation and dispersion, thus follows a non-ionic gas-phase mechanism when in solution. The challenge for theory and computation is to compute the gas-phase parameters accurately, and differentiate the subtle effects of solvent upon computed activation energies in cycloadditions. Second-order Moller-Plesset theory (MP2) and Truhlar’s M06-2X density functional with Dunning’s cc-pV[D,T,Q]Z correlation consistent basis sets, and AM1, PM3, PM6, and PDDG semiempirical methods have been used with two different solvent schemes. The Gaussian09 and TeraChem programs were used. Semiempirical methods greatly overestimate, and DFT and MP2 are within 15% of the experimental activation energies. Tomasi’s polarizable continuum model was used to estimate solvation effects and compared to an all-atom explicit-solvent approach. The effect of solvation is generally accounted for in the implicit solvation scheme. The preliminary results for the explicit solvent approach will be discussed.

CHED 706

Computational modeling of fluorescent probes to understand how lithium treats manic depression

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Lithium carbonate has been prescribed as the gold-standard treatment for bipolar disorder for over fifty years, continuing to outperform newer, alternative mood stabilizers. Despite this, the pharmacological mode of action for Li⁺ in treating bipolar disorder is still speculative. A lithium-specific fluorescent probe for use in the cells would aid researchers in fully understanding how lithium salts work to treat the disease and help design more effective drugs. Potential probes were modeled in WebMO using Density Functional Theory with Gaussian09 as the computational engine and using mixed basis sets of 6-31G(d) for C and H and 6-311+G(d) for N, O, and metal cations.
Geometry was optimized in an aqueous solution and molecular orbitals were calculated for two coumarin-based proposed sensors that are functionalized with a 1-aza-9-crown-3 ion-bonding moiety. The ability of these sensors to selectively bind $Li^+$ was estimated by comparing free energies of the molecule with and without a metal ion present. Molecules that appear to exclude competing ions (e.g., $Mg^{2+}$, $Na^+$, $K^+$) and yield reasonable complexes with $Li^+$ will be targeted for synthesis in the laboratory.

CHED 707

**Using the relativistic particle in a box to model conjugated dyes**

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Current studies of conjugated dyes in the undergraduate physical chemistry laboratory employ the nonrelativistic particle in a box as the model for calculating electronic energies. We will compare the results of experiment with the current model, and with a model based on the relativistic particle in a box. While the later is often thought to apply only to heavier atoms in chemistry, its has been employed to accurately model systems with lighter atomic masses such as the SCF MO calculations for water.

CHED 708

**Using molecular dynamics to computationally simulate metabolic enantiospecificity of CYP2C9**

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Approximately 50% of pharmaceutical drugs currently available on the market are chiral. Cytochrome P450 is a well-known superfamily of enzymes involved in the oxidative metabolism of vast ranges of pharmaceutical drugs. Specifically, the liver enzyme CYP2C9 has been known to be the main metabolite contributor for at least forty drugs and to metabolize one enantiomer better than the other. Warfarin is a classic example of an enantiospecific drug where the S-enantiomer metabolizes 1000 times better than the R-enantiomer. Crystallized protein structures provide the medium to run molecular dynamics and analyze intermolecular forces. Using molecular dynamics through a molecular modeling suite Sybyl-X, computational approaches were performed to simulate the oxidation reaction and to determine which interacting amino acid residues had stabilizing effects on the enzyme-ligand complex. Jointly, thermodynamics and kinetics work to guide the favorability of interactions between drugs and enzymes. Residues present in CYP2C9 such as ARG108, ILE205, LEU208, PHE476, and THR301, in particular, interact strongly with the drug enantiomers by means of Van der Waals forces, hydrogen bonding, and π-stacking. Significant residue energy differences
between R and S enantiomers were identified for multiple chiral drugs used in the treatment of acid reflux, type 2 diabetes, and cancer.

CHED 709

Folding of meta-poly-phenylene ethynylene

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The folding process is essential for many cellular functions, but not completely understood due to the complexity of biomolecules. Foldamers are synthetic polymers that mimic biological folding and can help us understand the fundamental nature of the folding process. The foldamer, met-poly-Phenylene Ethynylene (mPPE), folds into a helical shape, which mPPE was studied via computational molecular dynamics. These computer simulations allow an atomic level perspective of the mPPE dynamics and were performed with the CHARMM and NAMD packages. mPPE foldamers of 12 monomers were generated in linear and helical conformations in pure water solutions. Videos of simulations progress were created to observe the folding and unfolding process.
Further computational investigation on the conformationally-restricted allenyl cope rearrangement of Syn-7-allenynorbornene

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This computational study investigates the conformationally restricted allenyl cope rearrangement of syn-7-allenynorbornene using recently developed density functional theory (DFT) functionals and compares the results to past DFT and complete active space self-consistent field (CASSCF) calculations performed on the same reaction. The results from these calculations were compared to the experimental research done on the same reaction, which produced multiple stereoisomers, suggesting the reaction proceeded through a non-concerted mechanism. The CASSCF level calculations reported that the mechanism for this rearrangement followed two non-concerted pathways with a common biradical intermediate. These pathways accurately reproduced the stereoselectivity of products found in the experimental results of this reaction. Therefore it was concluded that CASSCF calculations predicted the correct mechanism for this rearrangement. Past investigation of this mechanism with DFT functionals B3LYP, BLYP, and BPW91 were unable to model the experimental stereoselectivity but were able to reproduce portions of the mechanism found by CASSCF calculations, including the biradical intermediate essential for the formation of the products. In this study, the Minnesota series of DFT functionals were used in an attempt to improve upon the B3LYP functional. However, the newer functionals found a concerted mechanism in all cases and were unable to reproduce the needed stereoselectivity. Therefore it was concluded that the newer Minnesota series of DFT functionals do not improve upon past DFT calculations and instead find less accurate mechanistic pathways than B3LYP.

CHED 711

Possible explanation for the formation of trans-Whiskey lactone: A computational approach

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Computational modeling is used to explore the energy barriers to the formation of cis- and trans-whiskey lactone from the glycoside of the corresponding open chain cis hydroxyacids. Two mechanisms are probed: a conventional nucleophilic attack by the hydroxyl on the protonated carbonyl group, and an attack of the acid group on an activated glycosidic bond. The former pathway proceeds with retention while the latter inverts the stereochemistry and provides a mechanism for potential interconversion of these isomers, an area of historical interest.

CHED 712
Investigation of biological anion effects on phospholipid structure and oxygen diffusion free energy

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Biological membranes experience environments with significant ionic compositions. Interactions with these ions are known to stimulate subtle structural and behavior changes. Monatomic ions have previously been shown to alter membrane stability and ordering. The divalent cation calcium can interact with lipid headgroups and form “bridges” between neighboring lipids. Previous work in our group has indicated that the transbilayer diffusional free energy profile of oxygen was more significantly impacted by divalent calcium than by monovalent sodium and potassium. As calcium concentrations are typically low in biological systems, the relatively high calcium concentration used in our study are unlikely to be biologically relevant. However, the influence of calcium on bilayer structure and permeability suggests that other divalent ions may affect membrane mechanics and permeability to small molecules such as oxygen. The intracellular and extracellular leaflets of biological membranes experience distinctly different ionic environments, with the monobasic anion bicarbonate predominant extracellularly and dibasic phosphate predominant intracellularly. We suspect that the singly charged bicarbonate and the doubley charged phosphate may differently alter the heights of the leaflet energy barriers to oxygen transport. Thus, we have initiated a molecular mechanics simulation study to investigate bilayer structure and oxygen diffusional free energy in the presence of a bicarbonate/dibasic-phosphate gradient.

CHED 713

First principle calculations of optical properties of platinum(II) diimine complexes

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The effect of the aromatic group N-Methylnaphthalimide on optical properties of platinum(II) diimine complexes bearing 7-benzothiazolylfluoren-2-yl motif on the bipyridine and acetylide ligands are theoretically investigated using time-dependent density functional theory (TDDFT) calculations. Substitution of benzothiazolyl groups by N-Methylnaphthalimide in all ligands results in wider and redshifted absorption band with a longer lower-energy shoulder. For all complexes, the lower energy optically weak shoulder of the absorption spectra is dominated by metal-to ligand (singlet MLCT) and ligand-to-ligand (singlet LLCT) charger transfer character. The first highly intense band originates from 1\pi,\pi* transitions associated with bipyridine ligands. For emission,
substitute N-Methyl-naphthalimide groups in acetylide ligands result in blue-shifted triplet transitions with dominating triplet π,π* character, while while its substitution of benzothiazolyl in fluorene motif have significant contribution from triplet MLCT/triplet LLCT transitions. Our calculated spectra demonstrate good agreement with experimental data validating feasibility of applied computational approaches.

CHED 714

Conformational distribution of cysteine and selenocysteine dyads in biological redox processes

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Thioredoxin reductase (TrxR) is an enzyme that belongs to a class of selenium-containing pyridine nucleotide-disulfide oxidoreductases and is utilized by all known living organisms.[1] Although TrxR is primarily responsible for the reduction of thioredoxin, a small peptide,[2] its primary substrate specificity is relatively low making it a key drug target against several diseases such as cancer[3] and rheumatoid arthritis.[4] The active site dyad in mammalian TrxR contains vicinal cysteine (C)-selenocysteine (U) while in non-mammalian systems it consists of two vicinal cysteine residues. These dyads form a flexible eight-membered ring, which is not resolved in any available crystal structures.[5] This investigation is intended to understand the conformational equilibrium of these eight-membered rings using chemical computations. Monte Carlo simulations were performed to generate an initial set of conformations for the dyad ring (UU/CC/CU/UC dyads), followed by more accurate energetic evaluation using Density Functional Theory (DFT) methods. Obtained free energies of various local minima were utilized to acquire Boltzmann distributions of dyads at physiological temperature. Further, we calculated the NMR shifts of these conformers for future experiments. We will present the differences in conformational equilibrium of the aforesaid truncated dyads. These dyads will be utilized along with previously reported crystal structures of TrxR to prepare a full-scale enzyme model for subsequent studies.

Evaluating oil dispersant systems via emulsion stability and optical microscopy

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Though chemical dispersants are employed to minimize the deleterious effects of oil spills, their diverse composition of organic solvents, surfactants, and additives may bestow further detrimental effects on marine environments. This study is part of a larger effort to engineer a novel dispersant that replaces surfactant molecules with mineral particles, thus allowing surfactants and particles to work in tandem to optimize oil slick degradation and emulsion stabilization efficacy.

Core shell vs. alloy iron/nickel nanoparticles for water treatment

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With current water filtration techniques lagging behind the rate of newly emerging organic contaminants and disinfection by-products, many researchers are interested in using metal-based nanoparticles as a water treatment solution. Nanoparticles could be deposited on or immobilized in a water filtration membrane or carbon-based filtration media and impart additional water contaminant removal capability to the filter material. Nanoparticles made from precious materials such as palladium, ruthenium, and platinum have been demonstrated to successfully remove and/or degrade organic water contaminants, but these nanoparticle materials are expensive and not cost effective for general use. A less expensive solution is needed if nanoparticles are to be used practically in the future. This study looks at the effectiveness of zero-valent iron/nickel nanoparticles in degrading water-borne contaminants. Specifically, this study will be focusing on the effect of core-shell (iron core with nickel shell) versus alloy (homogeneous mixture of nickel and iron) synthesized nanoparticles, to determine which type of nanoparticle is the most effective in eliminating contaminants. Batch experiments will be used to evaluate the decrease in the concentration of the azo dye Orange G over time in aqueous solution with iron-nickel nanoparticles. Parameters including Orange G dye concentration, nanoparticle concentration, nickel to iron molar ratio and core-shell versus alloy morphology will be varied to determine the removal efficiency of the nanoparticles for Orange G dye, as well as the effect of each parameter on removal efficiency. Electron microscopy will be performed on the nanoparticles.
before and after batch experiments to determine initial nanoparticle morphology and changes to morphology that occur as a result of Orange G dye water treatment.

CHED 717

Orange G dye degradation using iron-nickel nanoparticles: Effect of iron to nickel ratio, concentration and pH

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As the demand for fresh water increases and resources dwindle, the search for new water purification methods has become an increasingly urgent effort. Currently, some of the most common water pollutants are dyes, which oftentimes go untreated and are released into rivers and streams by establishments that deal with textiles, inks, papers, and plastics. Azo dyes, characterized by a double nitrogen bond, constitute a large portion of these wastes, and are often toxic. This study examines the ability of bimetallic iron-nickel nanoparticles to degrade a nontoxic model azo dye, Orange G, through breaking this bond. The ratio of iron to nickel in the nanoparticles, the initial ratio of nanoparticles to dye in the test solution, and the pH at which the experiment is conducted will all be tested. Bimetallic nanoparticles of 1:50, 1:100, 1:500, and 1:1000 mol Fe:mmol Ni ratios as well as zero-valent iron nanoparticles were synthesized using a sodium borohydride reduction, core-shell method. These were then tested in aqueous batch reactions with Orange G Dye, and samples of the dye-nanoparticle solution were taken at intervals throughout test. Samples were then read using a UV-Vis plate reader in order to determine the dye concentration at each time point. This process will be repeated at various solution pH levels. The process was most effective using greater ratios of nanoparticles to dye as well as greater ratios of nickel to iron. Both resulted in a greater rate and degree of degradation. It is expected that pH will also have an effect on dye degradation, and that a range of pH’s at which the process is most effective will be found. Optimum conditions for azo dye degradation using iron-nickel nanoparticles will be determined, as a step towards potential industrial applications in the future.

CHED 718

Electrochemical characterization of iron nanoparticle–clay interaction for groundwater remediation

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Iron nanoparticles (FeNPs) have great potential in groundwater remediation applications based on their ability to reduce a range of contaminants. One issue that arises in
considering their use in the field is rapid passivation of the surface; one possible way to prevent passivation is with exposure to clays. Previous work in our lab has used electrochemistry to study the effect of smectite clays on the electrochemical behavior of passivated iron electrodes. Potentiodynamic potential scans and cyclic voltammograms were taken using clay-modified iron electrodes, which suggested that the clay removed the passive layer of the underlying iron electrode and limited any further growth. These results were attributed to the Brønsted acidity of the clay as well as its ability to sorb iron cations. In this poster we extend this work to iron powders (FePs) and FeNPs. Preparation of electrodes, however, is more difficult with FePs and FeNPs than bulk iron. Two approaches were taken to prepare them. In the first, we adhered a layer of FeP or FeNP to an ITO electrode. In the second, a packed powder electrode was prepared with FeP or FeNP. Both electrodes were either immersed in a borate buffer to which clay was added or a layer of clay was dried on the electrode surface. The shifts in corrosion potential and changes in the passivation current were studied with these two electrodes as the ratio of iron powder to clay was varied to show that the clay was able to depassivate the FePs and FeNPs as it did the bulk iron. The results suggest ways to use iron nanoparticles in remediation applications as well as how to interpret the kinetics of remediation reactions with FeNPs prepared using clay templates.

CHED 719

Analysis of mineral content in MWSU parking lot runoff water using PXRF, FAA, and EDTA titration

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Urban runoff is a contributing factor to poor water quality and can cause damaging effects if the level of pollution is not closely monitored. This particular issue has been a question of some interest due to the high level of deicing road treatment that occurs on campus at MWSU. The treatment involves usual salting techniques, thus, this project sought to examine mineral content such as sodium and calcium that might be the result of that practice, as well as overall hardness of the runoff water in question. Two particular elements that contribute to water hardness are calcium and magnesium. Water hardness of samples obtained from MWSU parking lots during spring runoff periods was measured using commercial indicator strips, PXRF (which was inconclusive), and EDTA titration. Collections were made from the perimeters of the stream and ponds on campus over a period of five years. The results showed an increase of calcium and decrease of magnesium over time. Other minerals of environmental interest, such as sodium and potassium, were also examined using PXRF and FAA.

CHED 720

Drugged wildlife: The potential impacts of environmental endocrine disruptors on reproductive development
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The growing use of oral contraceptives and hormone therapeutics prompts concerns that estrogenic and progestogenic compounds are present in wastewater at concentrations that may affect the reproductive health of aquatic animals as well as humans who consume affected animals. In this study, potential endocrine active compounds were extracted from effluent produced by the Charleston Water System wastewater facility at Plum Island according to EPA method 1694. The extract, when concentrated 100 times, activated the human nuclear estrogen and progesterone receptors in an in vitro transactivation assay. This provides a mechanism for the alterations in secondary sex characteristics that have been reported in fishes exposed to effluent at other locations. Bioaccumulation of some synthetic hormones has also been reported in teleost fishes. There is, therefore, potential for humans to be exposed to endocrine active compounds through consumption of these fishes. To explore the potential biological consequences of human exposure to these endocrine active compounds during sensitive windows of development, we also evaluated the effects of neonatal exposure to progestogens on the reproductive development of mice. Quantitative RT-PCR analysis of target genes from adult mice treated with the synthetic progesterone 17α-hydroxyprogesterone caproate (17PC) as neonates suggested that developmental exposure to progestogens decreases sensitivity to E₂ at the uterine transcriptome level. These data indicate a need for further exploration of the long-term impacts of neonatal progestogen exposure on reproductive development.

CHED 721

Monitoring the long term effects of fracturing in Western Pennsylvania, Butler County: How long is long enough?

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Over the last decade, horizontal hydraulic fracturing of the Marcellus shale bed which expands across portions Pennsylvania, New York, Ohio, and West Virginia has become a heated issue. This unit of sedimentary rock is estimated to contain up to 500 trillion cubic feet of natural gas which would be able to power the United States for decades. In order to extract the natural gas, a well is drilled 5,000 to 9,000 feet vertically and then up to 10,000 feet horizontally. The well is then encased by a steel pipe and cement in order to prevent natural gas and flowback from entering the groundwater supply. Once the drilling is completed, three to five million gallons of water, per frack, are injected into the well at high pressure to fracture the shale and allows the natural gas to flow back up the well to the surface. The frack water that is injected into the well contains sand and other proppants which help with the fracturing of the shale. Only about 30% of this frack
water returns to the surface. The purpose of this research was to analyze surface water that was collected near hydraulic fracturing sites in Butler County, Pennsylvania for contamination as a direct result of drilling. The samples that were collected were tested with the use of a handheld multiparameter meter, Ion Chromatography, Gas Chromatography Headspace, Atomic Absorption Spectroscopy and other techniques. The research showed that there is no significant surface water contamination as a direct result of the hydraulic fracturing process. However, contamination is likely to occur from negligence, such as inadequate water disposal and surface spills. Continued monitoring of water quality over time is crucial to fully observe and determine the environmental impact of horizontal hydraulic fracturing.

CHED 722

Development of 2-component surrogate mixtures for alcohol-to-jet fuel

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Alcohol-to-jet (ATJ) fuel is a new alternative fuel produced from bioderived isobutanol. The combustion of this type of fuel is being tested using various engines and simulated using numerical models. As with many fuels, modeling and combustion efforts can be simplified if a surrogate mixture containing fewer components can be found that matches the fuel's properties. In this work, various 2-component mixtures containing 2,2,4,4,6,8,8-heptamethylnonane and 2,2,4,6,6-pentamethylheptane were prepared, and their physical properties were compared with those of ATJ to determine the best match. The physical properties tested were those that impact the transport and combustion of fuels in engines and safety: density, viscosity, surface tension, flash point, speed of sound, and bulk modulus. This poster will present results that show that 2-component mixtures containing between 15% and 30% 2,2,4,4,6,8,8-heptamethylnonane in 2,2,4,6,6-pentamethylheptane best matched the properties of ATJ.

CHED 723

Analytical identification of polycyclic aromatic hydrocarbons: The bio-monitoring of Cyprus trees in Los Angeles

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Polycyclic aromatic hydrocarbons (PAHs) are potent pollutants produced from the incomplete combustion of organic materials such as octane and may accumulate in areas of high population and pollution. These compounds are of major concern to our health due to their carcinogenic, mutagenic, and teratogenic biological properties; thus,
our focus is to create a demographic of PAH concentrations in the Los Angeles area through the bio-monitoring of Cyprus trees. Three distinct locations were chosen for examination: a secluded mountainside, a busy main street, and alongside the I-405 freeway. The methodology included extraction, concentration, and analysis. The resulting samples were analyzed through gas chromatography mass spectrometry (GCMS). Prior data analysis technique required the evaluation of individual chromatographic peaks manually matched against an NIST (National Institute of Standards and Technology) compound library stored in the GCMS software. Currently, a SIM (Selected Ion Monitoring) table is being utilized for a more thorough analysis of the previously collected data allowing for PAH identification as well as quantification of relative peak height and average retention time. We have successfully identified all 16 PAHs in the I-405 area and hillside location. Analysis of relative peak height indicated a 93% greater PAH concentration near the I-405 freeway. The data also revealed retention times with average standard deviation of ± 8.9 s whereas our previous analysis technique failed to find an average retention time for any of the 16 PAHs. We are currently working towards the quantification of the PAHs, using a calibration curve to precisely quantify the pollutants’ concentrations in the chosen locations. From the data gathered a statistical demographic model of PAH concentrations in Los Angeles will be established.

CHED 724

Potential heavy metal water remediation using 5-formylfuran-2-sulfonic acid thiosemicarbazone (DIFANEX) chelating resins

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In the literature, thiosemicarbazones have demonstrated an array of uses, including analytical applications and separation of metals. This is in part due to their ability to form chelates with metals efficiently. In this study, resins were separately loaded with three new 5-formylfuran-2-sulfonic acid thiosemicarbazone (FFSA-TSC) ligands and were tested to determine if they could be utilized for heavy metal water remediation. Strong anion exchange resins used in the study were loaded with one percent by weight of each ligand, and then they were exposed to Co-57, Ni-63, or Cd-109. Using batch techniques for these radiotracers, the resins were placed under various environmental pH levels at different time intervals. The adsorption values of the metals to the resin beads were calculated as dry-weight distribution (Dw) values. The metals, specifically the Cd-109, were extracted at very high levels in these conditions. These materials which we call DIFANEX could potentially be used to extract heavy metals from water sources under environmental conditions, or they could be used to separate mixtures of metals for analytical purposes.

CHED 725
**Novel method for the extraction of lead ions from bulk water supplies using chelation chemistry**

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Since the introduction of industry, the amount of naturally occurring safe drinking water has drastically decreased because of an increase in toxic heavy metals such as lead, arsenic, and cadmium from industrial waste. Currently, there are approximately 500,000 children ages 1-5 years in America diagnosed with blood lead levels above those recommended by the Centers for Disease Control and prevention (CDC). Chronic lead poisoning can lead to malfunctioning organs, damaged tissues, encephalopathy, anemia, nervous disorders, and even death. The objective of this project is to develop a lead removal technique that is environmentally friendly, effective, and cost-efficient.

Here, we describe the construction of a novel apparatus that utilizes coordination chemistry to extract lead from a bulk water supply. In addition, we present preliminary results on its efficacy. The apparatus consists of a simple PVC pipe capped with a semi-permeable, organic membrane separating the source phase, containing lead ions, from the lead-trapping reservoir inside the PVC pipe, which contains the metal chelator, ethylenediaminetetraacetic acid (EDTA). Lead is drawn into the device through the membrane via an ionophore (dicyclohexano-18-crown-6) that allows the lead ions to be passed though the hydrophobic membrane into the trapping reservoir, where it forms a stable complex with EDTA. Data presented here demonstrate that the apparatus can be used to remove lead from a contaminated water source to concentrations below 15 ppb, which is the “action level” set by the Environmental Protection Agency (EPA). The reusable device consistently reduces lead concentrations below 15 ppb with the most common final lead concentrations remaining between 6 ppm and 8 ppm. Additional experiments show that the device can be reused without changing the membrane or lead trapping solution within the reservoir. Reusing the device showed a gradual decrease in efficiency that corresponds to a decrease in free EDTA available for metal chelation in the trapping solution.

**CHED 726**

**Metal-sequestration from water using a polysulfide synthesized from sulfur and limonene**

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Removal of metals from contaminated water is an important environmental issue. In this presentation we introduce a novel polysulfide material synthesized from sulfur and limonene--waste products of the petroleum and citrus industries, respectively. This polysulfide can be processed into a coating or mold and used to remove soft metals such as mercury and palladium from water. Benefits of this novel material include its
inexpensive starting materials, facile synthesis and processing, and high affinity for soft metals. An additional useful feature of this material is that it changes color upon binding to inorganic mercury, and can therefore be considered a sensor for this toxic salt. Prospects in remediating natural waterways contaminated with inorganic mercury are discussed.

**CHED 727**

**Determination of total mercury in the top three consumed seafood products of the United States**

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In contrast to other toxic heavy metals, the amount of mercury entering the environment has been rising in recent decades, due in large part to expanding use of fossil fuels. Airborne elemental mercury gets deposited into the oceans where microbial processes oxidize it to methylmercury, which bioaccumulates in fish. Mercury is known to be harmful to human health and consumption of fish is the primary source of human exposure. This study presents mercury concentration measurements of the top three seafoods consumed in the United States: shrimp, canned tuna (albacore), and salmon. Samples of cold and warm water shrimp varieties, solid white and chunk light canned tuna brands in both oil and water, and wild caught, as well as farm raised salmon were obtained from grocery stores. Samples were tested for total mercury content using Thermal Decomposition and Amalgamation coupled with Atomic Absorption Spectroscopy. Concentrations of mercury were found in μg/kg (ppb), and are reported as the mean ± error (1s) followed by the range in parentheses. Cold and warm water shrimp were found to be 9.5 ± 0.8 (5.0 – 18.3), and 8.3 ± 1.0 (4.5 – 21.8) respectively; solid white canned tuna in water and oil 305.0 ± 11.2 (250.7 – 388.7), and 313.8 ± 5.3 (224.7 – 428.6); chunk light canned tuna in water and oil 76.0 ± 3.4 (14.2 – 330.8), and 59.8 ± 4.2 (20.9 – 234.5); salmon, 7.3 ± 0.8 (4.4 – 12.5), and 47.5 ± 1.6 (32.5 – 75.6), for farmed and wild caught, respectively. Mean mercury is calculated per serving for each of the types of seafood studied, and compared to recommended daily limits. The environmental and health implications of this are discussed.

**CHED 728**

**Reactions of alcohol amines with atmospheric oxidants N₂O₅, H₂O₂ and O₃ analyzed through a Particle-into-Liquid Sampler coupled to dual ion chromatographs**

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Gaseous alcohol amines are emitted into the atmosphere through various sources, including carbon sequestration technologies from power plants. Yet, little is known about how gas-phase alcohol amines interact with atmospheric oxidants, such as N₂O₅, H₂O₂ and O₃, to form particulate matter. This study is important because particles formed from volatile organic compounds like alcohol amines, which include: monoethanolamine, 2-(methylamino) ethanol, 2-amino-2methyl-1-propanol, and N, N-dimethylethanolamine, may have short and or long term adverse health effects. In this study, Ion Chromatography separations of the potential reaction products of the target alcohol amines were performed with standards to make a calibration curve from which the concentrations of the target species could be calculated. Then a Particle-into-Liquid Sampler coupled to dual ion chromatographs (PILS-IC’s) was used to analyze the water-soluble ion component of the particulate matter formed. The experiments were conducted in an environmental chamber at the Center for Environmental Research and Technology, College of Engineering, University of California, Riverside (CE-CERT/UCR). The chamber is designed to emulate real environmental conditions allowing the reactions to proceed in a controlled environment. As of now there is little knowledge of how the alcohol amines will react. The experiment will provide data exposing products of alcohol amines reactions with atmospheric oxidants to better understand the consequences of current carbon sequestration technologies.

CHED 729

Analysis of the open limestone channel at the Swank 13 abandoned coal mine

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Open Limestone Channels (OLC) have been constructed as an inexpensive tool to remediate Acid Mine Drainage (AMD) from abandoned mines. In order to examine the efficacy of the Swank 13 Mine Reade Township, PA Open Limestone Channel that was constructed in 2011, the concentrations of iron, calcium, aluminum, and manganese were analyzed over a two year period along with pH and stream flow rate. Calcium concentration increased down the OLC, trending from \( \sim 10 \text{ppm} \) to \( \sim 20 \text{ppm} \). In the second year, the channel pH only increased from 3.5 at the top to 3.8 at the bottom site as a consequence of the armoring of the limestone rocks. While metal hydroxide precipitation is limited due to low pH, a high stream flow rate aids in metal precipitation.

CHED 730

Degradation of the layer of calcium carbonate (CaCO₃) on the Pyrodinium bahamense (dinoflagellates) from bioluminescent lagoons in Puerto Rico

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Pyrodinium bahamense are microorganisms that serve as a food source for other species that inhabit different bodies of water in Puerto Rico. These are responsible for producing bioluminescence in certain lagoons by a reaction between luciferin, oxygen and luciferase. A drastic decline in the population of these organisms has been observed due to the large amount of runoff water discharges bringing fertilizers used in the agricultural industry and household detergents into the lagoons waters. This causes a decrease in the bioluminescence of these water bodies. Using several analytical techniques to verify the pH levels and also the sulfates, nitrates, phosphates, zinc and copper levels on water samples from the lagoons "Las Cabezas de San Juan" (Fajardo), "Puerto Mosquito" (Vieques) and "La Parguera" (Lajas), it was determined that a degradation reaction occurred on the calcium carbonate layer of Pyrodinium bahamense causing a state of turgor and the instant death.

CHED 731

Separation of oil contaminates from oil-in-water emulsions using nylon 6,6 nonwoven fabric filters

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Inland industrial oil spills can have detrimental effects on the river and stream environments and may contaminate the groundwater. Nylon 6,6 nonwoven fabric bags and fences have been employed to separate spilled oil from contaminated water along the coast of the Gulf of Mexico and the southern United States. This work describes the laboratory scale analysis of the effectiveness of these nylon filters to remove light crude oil from fresh and saltwater. Small filters (38 mm in diameter) were tested at varying flow rates of water passing through the filter and varying concentrations of oil-in-water emulsions. Samples were taken before and after the filter and analyzed by gas chromatography/flame ionization detection to determine the oil levels in the water. The filters were effective at removing the oil with concentrations of 70 and 140 ppm. The filters trapped oil better at the lower flow rates.

CHED 732

Synthesis of water filtration composites for use against microorganisms and heavy metal in water

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The application of composite materials has been useful in the development of water filters. Here, silver nanoparticle-carbon microsphere composites were formed for examination in water filtration applications. Carbon microparticles were synthesized using various biological materials, including excess byproducts such as corn husks and sawdust through the process of hydrothermal carbonization. Silver nanoparticles were synthesized on the surface of the carbon microparticles by a three-step process that includes coffee as the reducing agent. The carbon microparticles were characterized by FTIR spectroscopy and imaged using Scanning Electron Microscopy. Bacterial viability tests were conducted to examine the success of the silver nanoparticles against E. coli and Bacillus cereus. Characterization of the filtration capacity is ongoing. Our most recent results will be presented.

CHED 733

Bioremediation of nickel and cobalt by **Bacopa monnieri**

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There has been a strong interest in the use of aquatic plants as a potentially useful group for pollutant uptake, like heavy metals, in aquatic systems. *Bacopa monnieri* is an excellent candidate because its heavy metal accumulating potential has been tested with the ions cadmium, iron and chromium. *B. monnieri* was also chosen because it is a medicinal herb used to treat anxiety, improve focus and memory. These aquatic plants were collected at the *Caño Tiburones* wetland and transported to the research laboratory for sample treatment and analysis. In this study we investigated the uptake of nickel (Ni) and cobalt (Co) by *B. monnieri* after being treated with different concentrations of the ions (1 ppm, 2 ppm, 4 ppm and 6 ppm) individually in separate containers. Plant tissue was sampled weekly and water was sampled every two days. Plant samples were treated with wet digestion method using 5 mL of concentrated nitric acid (70% w/w) and 10 mL of hydrogen peroxide (30% w/w). Also, by applying mass balance, an analytical equation was developed to estimate how fast is the heavy metal uptake by *B. monnieri*. Analysis was performed by means of an atomic absorption spectrophotometer, using a flame atomizer (PE Analyst 200). Preliminary results showed that, after 12 days, a decrease in Ni concentration was obtained in water samples treated by plants. Further research will allow us to study the capability of this aquatic plant to uptake other heavy metals.

CHED 734

**Influence of cation charge density, ionic strength, and pH on NOM particle size distributions in aqueous solution**
In this study, we attempt to quantify the roles of pH and cation charge density on the size and polydispersity of Suwannee River NOM aggregates suspended in water using Dynamic Light Scattering (DLS). Unraveling the details of NOM-NOM interactions in solution are a critical precursor to understanding the mechanisms of NOM-mineral interactions and how NOM-mineral composites influence the transport of organic and inorganic contaminants in the environment or the role of organo-mineral interactions in the global carbon cycle. Recent molecular dynamics computer simulations have suggested that cation bridging amongst NOM molecules and between NOM molecules and mineral surfaces are an important interaction mechanism in water-rich systems under basic conditions. They also suggest that such bridging is more important for systems bearing Ca$^{2+}$ than for other alkaline earth metals and alkali metals. We tested these ideas in the laboratory by performing systematic DLS studies of NOM suspensions as a function of pH and time in the presence of Cs$^+$, K$^+$, Na$^+$, Ca$^{2+}$, Mg$^{2+}$, and Sr$^{2+}$. Our DLS instrument showed no statistically significant variation in mean equivalent hydrodynamic radius of suspended NOM aggregates with the cation charge density or time among the metals examined here with the exception of the Cs$^+$ solution at pH 2. In this sample, we observe an increase in the mean aggregate size with increasing time over one month of observations. However, we do see trends in the number of unique hydrodynamic radii observed in the DLS results. Alkali metals at pH 2 tend to be monodisperse, single-maxima while increasing pH leads to increasing number of maxima, with mean hydrodynamic radii appearing between 100 nm and 1.5 mm. In contrast, the alkaline earth metal-NOM solutions exhibit multiple unique maxima at pH 2 and decrease in number of maxima with increasing pH. In alkaline earth metal-NOM solutions, the protonation state of NOM seems to be the dominant feature in determining the number of maxima with more deprotonation leading to increasingly monodisperse NOM aggregates. In contrast, charge density seems to be the dominant feature controlling the number of maxima among the alkali metals. From our data set, we hypothesize a model in which the percent saturation of available ion bridges between NOM molecules affects the degree of polydispersity and number of unique particle sizes.

**CHED 735**

**Three years of full scale testing an enhanced bioswale**

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Green infrastructure is to manage stormwater through on-site capture and infiltration. The ability of low impact designs to manage chemical contaminants was characterized to provide data for engineering calculations. BioMix Osorb® was evaluated has a soil amendment. A dual-chamber bioswale allowed for comparison of standard and
amended soil. A dual chamber full-scale bioswales were constructed in June 2011 at the College of Wooster retrofitting an existing drainage basin. The bioswale accepts water from 1.9 acres including 2 parking lots, 3 housing units, and the spillage from a roof of a large multi-purpose building. The dual chamber design allows comparison testing of soil amended with Iron-Osorb sorbent. Various parameters were measured including influent and effluent water quality, infiltration rate, plant growth, microbial populations, and maintenance requirements. Input stormwater was spiked with contaminants at intervals to measure effectiveness of treatment. Gas chromatography is used to measure volatile and semi-volatile compounds. Nutrients and plant mass was measured by the STAR laboratory at The Ohio State University. Infiltration of stormwater was high for the bioswales exceeding 99% in all rainfall events. Input water was spiked atrazine, nitrate, and phosphate and was reduced on average 99%, 85%, and 95%, respectively. Above ground plant growth was 15% greater in the Fe-Osorb chamber of the bioswale. Over the past three years, a relatively compact bioswale has effectively managed stormwater inputs from 1.9 acres of campus grounds without an incident of overflow. Maintenance involved annual removal of plant mass in the late Fall and general mowing. Augmenting the soil with amendments specifically designed to treat chemical contaminants improves performances and promotes a larger above ground plant biomass, presumably by removing bioinhibitory compounds.

CHED 736

Catalysis in chromic acid oxidations: A co-oxidation model for the detoxification of hexavalent chromium in water

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Hexavalent chromium compounds are lung carcinogens and occupational hazards. The high levels of hexavalent chromium in ground water have been a public health issue since the case involving California Pacific Gas & Electric Company and the Hinkley ground water contamination. Past and current large-scale in-situ remediation efforts involve injection of lactate (milk sugar) or ethanol; the removal of Cr(VI) to safe levels has not been achieved over the last 5 years.

The chromic acid oxidation of alcohols has a second order dependence on \([H^+]\), and therefore, it is not surprising that chromium (VI) is still found in significantly high concentrations at pH levels (5.5 - 8.5) of contaminated ground water. Any meaningful approach to the detoxification of Cr(VI) has to take into account this second order dependence on acidity and the pH of chromium contaminated water in the soil environment. Earlier work had demonstrated catalysis in the cooxidation of a mixture of 2-propanol and co-substrates such as oxalic and hydroxy acids (Rocek, Mahapatro and Krumploc; J. Am. Chem. Soc., 1980, 102, 3799-3806; and references therein). In the present work we have investigated the cooxidation of ethanol with substrates such as oxalic and citric acids in an extended concentration range of substrates(s) and pH.

The cooxidation of a mixture of ethanol (1.0 M) and oxalic acid (0.01 – 0.1 M) was
extremely rapid. The observed first-order rate constant for the co-oxidation reaction is faster than the individual oxidation of alcohol, oxalic acid, citric acids. The observed catalysis may serve as a model for the detoxification of Cr(VI) contaminated water. Oxalic acid is a renewable resource and its oxidation to CO$_2$ and its conversion to benign Cr(III)-oxalato complexes make the co-oxidation strategy an attractive model for the detoxification of hexavalent chromium in water. We are currently extending our studies to possible co-oxidation of ethanol with humic and gallic acids. This work was supported by an undergraduate research grant from the Western Alliance to Expand Student Opportunities (WAESO; Hispanic Research Center, Arizona State University, Tempe, Arizona)

CHED 737

Studying reactivity and leaving group effects in aryl chloroformate esters

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Chloroformate esters are used to study substitution reactions and serve as stable intermediates in chemical synthesis. This undergraduate project focuses on the reaction rates of 4-methoxyphenyl chloroformate (4-MeOPhOCOCl) and 4-methoxyphenyl p-toluenesulfonate (4-MeOPhOCOOTs). 4-MeOPhOCOCl is beneficial in environmental science because of its ability to be recycled to create new chemicals. Equimolar amounts of analytical grade 4-methoxyphenyl chloroformate and silver p-toluenesulfonate were allowed to react at room temperature. The silver chloride quickly precipitated out and the resultant (filtrate) 4-methoxyphenyl p-toluenesulfonate solution was used as a substrate. The solvolysis of 4-MeOPhOCOCl and 4-MeOPhOCOOTs were followed in ethanol (EtOH), methanol (MeOH) acetone, 2,2,2-trifluoroethanol (TFE), 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP), and in TFE-EtOH mixtures. This study was completed at 25.0 °C using the acid-base titration method. Here we show that the leaving group has no significant effect.

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CHED 738

Correlation analyses of solvent reactions of 2-fluoroethyl chloroformate and 2-benzyloxyethyl chloroformate

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There are several patent applications describing the use of substituted ethyl chloroformates in design and synthesis of diverse libraries of small molecules for agricultural products and chemical biology. Recent mechanistic work using substituent effects, solvent effects, and product studies, has suggested that a number of these esters solvolyze by competing reaction channels, involving association-dissociation (addition-elimination) and ionization. Here we report on results obtained from a study of the influence of substrate variation in aqueous binary mixtures of ethanol, methanol, acetone, 2,2,2-trifluoroethanol (TFE), 1,1,1,3,3,3-hexafluoro-2-propanol (HFIP), and TFE-ethanol mixtures. The substrates involved in this study are: 2-fluoroethyl chloroformate and 2-benzyloxyethyl chloroformate.

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CHED 739

Confirming the use of phenyl chloroformate as an appropriate addition-elimination standard in LFER analyses

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Background: Two decades ago, phenyl chloroformate (PhOCOCI) was extensively studied 49 solvent mixtures and an addition-elimination (A-E) mechanism was proposed (Kevill, D.N. and D'Souza, M.J., 1997). Since then, it has served as a reference compound in linear free energy relationship studies (LFERs). In this project, Phenyoxy carbonyl tosylate (PhOCOOTs) was first synthesized and its specific rates were determined in the same set of solvents as PhOCOCI at 25.0 °C. The principal goal of the project is to determine the presence or absence of any correlation trends between the rates of reaction (energy barriers) observed and the differences in anionic leaving group abilities (between the chloride and tosyl anions).

Methods: PhOCOOTs was synthesized from equimolar additions of silver tosylate to phenyl chloroformate. A rapid precipitation of silver chloride occurred and the resulting solution was used directly as the source of the substrate. The specific rates of reactions were determined by acid-base titrations and conductometry.

Results: The specific rates of PhOCOOTs in a wide range of solvents were found to be very similar to those observed for PhOCOCI (in the same set of solvents).

Conclusions: A tosyl leaving group is a sulfonic acid derivative which is a better leaving
group than the chloride anion as it considerably stabilizes the negative charge by resonance stabilization. If the leaving group played an important role in the rate-determining step, the rates of reaction of PhOCOOTs should have been much faster than those for PhOCOCl. We therefore conclude that the mechanism of reaction of PhOCOOTs is exactly the same as PhOCOCl, and hence, it is very appropriate to continue to use PhOCOCl as a standard for A-E reactions.

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CHED 740

Integrons and multiple-antibiotic resistant bacteria in Minnesota surface waters

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Prior research has demonstrated that the bacteria in untreated and in treated municipal wastewater frequently harbor Class 1 integrons, which are genetic elements capable of incorporating exogenous genetic material into the genome and modulating the expression of these gene cassettes. Integrons, therefore, are believed to play an important role in the evolution of multiple antibiotic resistant bacteria. In this study, more than 300 bacterial strains were isolated using tetracycline-amended LB agar plates from the effluent of a municipal wastewater treatment facility and from the river to which this effluent is discharged. PCR targeting the integrase gene of class 1 integrons confirmed that bacteria in treated wastewater were likely to harbor a class 1 integron (102 out of 124 isolates) whereas none of the bacteria isolated from the river harbored a class 1 integron (~250 strains). All of these bacterial isolates were then tested for resistance to eight different antibiotics or groups of antibiotics (ciprofloxacin, sulfonamides, tetracycline, streptomycin, ampicillin, polymixin B, rifampicin and trimethoprim-sulfamethoxazole) using the Kirby-Bauer disc diffusion assay. Bacterial isolates originating in the wastewater treatment plant were, on average, less susceptible to 6 of the 8 antibiotics than a control. Similar results were observed for bacterial isolates originating from the river. These results suggest that although bacteria isolated from wastewater effluents are more likely to harbor a Class 1 integron, these bacteria are not more likely to be resistant to multiple antibiotics.

CHED 741
Viability of ozonation as a water treatment method for the elimination of the antibiotic roxithromycin

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This study examined antibacterial activity of the products formed when the macrolide antibiotic roxithromycin was oxidized at a range of pH values (5-9) and while in the presence of filtered wastewater treatment plant effluent. Ozone-induced oxidation was used as the treatment method. Antibacterial activity assays using E. coli DH5 alpha were used to screen for products that exhibited antibacterial properties. To date, no products exhibiting significant antibacterial activity have been observed. Experiments were also performed to characterize the reaction products. Experiments using an LC-quadrupole/time-of-flight (QTOF) mass spectrometer determined that the main product of the reaction under all conditions tested had a mass at 852.5 amu (+16 amu from roxithromycin). Further experiments examining only the pH-adjusted samples using a triple-quadrupole LC-MS/MS instrument gave evidence that the main product is roxithromycin-N-oxide. Current work is focused on characterizing other products formed in the presence of effluent.

CHED 742

Aqueous photochemistry of altrenogest

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Altrenogest (17-alpha-allyl-17-beta-hydroxyestra-4,9,11-trien-3-one), a synthetic progestogen, is used for equine and swine livestock to maximize reproductive success rates. Unmetabolized altrenogest may enter the environment through excretion from these animals. With sunlight likely playing a vital role in the environmental degradation of this compound, it is important to determine photolysis rates of the parent compound. In addition, the process by which photoproducts may undergo thermal dehydration reactions that have been observed for other conjugated trienes must also be understood. In this research, the degradation rate of altrenogest was studied under different pH (3-9), temperature (30-45 °C), and oxygen conditions in aqueous environments. An Atlas Suntest CPS+ solar simulator was used to artificially mimic sunlight. Parent compound and photoproduct analysis was performed using an Agilent 1100 series High Performance Liquid Chromatograph with a UV-Vis diode array detector (Agilent Eclipse XDB-C18 4.6 X 150 mm, 5 µm particle size column). Findings suggest pH and temperature have no significant effect on altrenogest whereas the presence of oxygen has a strong effect. Photoproducts showed increased rates of dehydration under warmer (35°C) and acidic (pH 2) or basic (pH 12) conditions.
CHED 743

Analysis of San Antonio River water for metals using inductively coupled plasma-mass spectrometry

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The water source of the San Antonio River comes from Edward’s aquifer through wells beginning in Brackenridge Park. This river flow is augmented with recycled water from the City wastewater treatment plant. The purpose of this study is to analyze the metal content in the San Antonio River water by the use of Inductively Coupled Plasma- Mass Spectrometry (ICP-MS) following EPA methods in order to monitor the levels of toxic elements. Samples are collected beginning in Brackenridge Park and continuously taken from six different sites going south along the river’s flow. Weighed aliquots of the homogenized samples are first solubilized with concentrated nitric acid by gentle refluxing. After cooling, samples are made to volume and allowed to settle over-night prior to analysis. Twenty-seven metals are analyzed in the water samples by ICP-MS using Varian 820-MS model and compared to EPA limits for recreational water. Future studies will analyze organic contaminants for toxicity levels.

CHED 744

pH profile determination of the cation exchange capacity of heavy metals from estuarine sediment and its correlation with outer shell content of benthic organism Mercenaria mercenaria

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Industrialization and urbanization of Rhode Island and surrounding communities has resulted in a dramatic increase in heavy metal sediment loading into Narragansett Bay (NB). In a southerly transect of the West Passage NB eight sites were sampled to determine their heavy toxicity metal rating in benthic sediment, pore water and outer shell content of sedentary bivalves. The suite of heavy metals was determined by X-ray fluorescence spectroscopy in whole and dried sieved granular sized sediments and surface shell analysis. This research investigated the relationship of sediment particle size and heavy metal content with their elemental inorganic and organic carbon and HNS composition. Reflective Fourier transform infrared spectroscopy and HACH\textsuperscript{®} spot tests were used in the determination of common anions for each of the sedimentary particles and surrounding pore water. The cation exchange capacity and pH profile (1, 5 and 8) of whole sediment samples, sized particles and the outer surface shell of benthic
bivalves were determined to access heavy metal rerelease into the water column. These relationships have further aided in the understanding of the possible bioaccumulation of heavy metals and the health of benthic bivalves in sediments of a dynamic pH changing estuarine environment.

CHED 745

Characterization of metal cation binding to pyridine-based compounds in aqueous solution

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There is a need for novel techniques for removing metal cations from wastewater such as contaminated hydraulic fracturing flowback water. Certain small molecules have the ability to bind cations in aqueous solution. 2,6-dipicolinic acid (DPA) is a small molecule known to bind calcium cations in aqueous solution, but no documentation of DPA binding to other heavy metal cations in aqueous solution is reported. We have characterized the binding of DPA to calcium, magnesium, strontium, and barium using NMR titration in PBS buffer. In addition, we have shown a strong correlation of our binding experiments to the ability of DPA to successfully extract these cations from contaminated water.

CHED 746

Analysis of heavy metal leaching from motor oil into water

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In this experiment, the effects of heavy metal leaching from motor oil into water in the environment was examined. I analyzed six metals (chromium, copper, iron, nickel, lead, and tin) associated with human health concerns and their potential to harm the environment. The leaching of heavy metals has been examined through organic extractions, but there has not been much research with examining the leaching effects of metals into water from oil. I approached my research by using the ICP-AES to look at the concentrations of the six metals leaching into water by using a shaking method for one day. The results illustrate the ability of metals to leach out of the oil in small quantities. There is also the indication that changing water parameters (such as pH, ionic strength, and temperature) to mimic the environment, will influence the metal concentration in the water.

CHED 747
Photochemical reactive oxygen species production by petroleum water accommodated fractions

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Photochemically produced reactive oxygen species (ROS: hydrogen peroxide and superoxide) were detected in Water Accommodated Fractions (WAF). WAFs were prepared in sterile seawater in the dark. Samples containing the water fraction were exposed to simulated sunlight. ROS were determined using the fluorometric reagent method of Yocis et al. Superoxide dismutase was added to samples for superoxide production determination. Initial determinations made for Jay oil indicated nM/sec production rates of both hydrogen peroxide and superoxide. Additional studies will compare ROS production from WAFs made using Macondo Surrogate oil.

CHED 748

Did the Bastrop wildfire affect the phosphorus quantity in the soil?

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On September, 4 2011 the most destructive fire in the history of Texas hit the Bastrop County Park. Two people were killed by the fire while it destroyed 1,673 houses. The fire left $325 million in property damages. You can see many physical differences from before and after the fire. However, the chemical changes are much harder to see. Fires cause many chemical changes to soil but there hasn’t been much study over this subject and even less study done on specific chemical compounds effected by fires. Nitrogen, phosphorus, and potassium are essential nutrient elements obtained in soil. This research will compare how these nutrients have been effected by the Bastrop fire. The first nutrient that was studied on is phosphate. There will be a comparison of the phosphate concentration between different burn severities and horizons. With these and furthermore results, we can better understand the affect that the fire has on the nutrients and how it currently and will affect the nutrients’ cycles.

CHED 749

Cd, Ni, Zn and Cu concentrations in fish muscles collected from sites along the Ashley River

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The study of metal accumulation in animals centralizes on the risk that high metal concentrations could do great damage to the organism and those who consume it. Most metallic elements do not originate in the host carrier, although in small amounts they are essential to biological function. Metals arrive in the body over a length of time through a various and intricate food chain that differs for almost every species of animal. Examples of metal contamination include erosion of sediment along river banks, and industrial sources among others. This study focuses on four specific species of fish in the Ashley River. Metal concentrations will be determined in muscular tissue using Inductively Coupled Plasma–Optical Emission Spectroscopy (ICP-OES). The specific metals of concern are Cadmium, Zinc, Nickel, and Copper. An ANOVA test will be performed to examine statistical site and metal concentration differences.

CHED 750

Algal toxin dynamics in a eutrophic lake and indicators of toxins in raw drinking water

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Cyanobacterial toxin concentrations were determined weekly at six locations in eutrophic Lake Winnebago, Wisconsin and at two drinking water intakes (Appleton and Menasha). These concentrations were compared to 23 chemical, physical, and biological parameters to determine the strongest correlations to toxin presence in the raw water at each drinking water intake. Total microcystin concentrations were determined by carrying out a 70% methanol extraction of lyophilized biomass followed by LC/MS/MS analysis of four microcystins (MCLR, MCYR, MCLA, MCRR), nodularin, anatoxin-a, and six non-toxic bioactive peptides (NTBPs) including anabaenopeptins (B,F), cyanopeptolins (1007,1041,1020), and microginin-690. All microcystins and five out of the six NTBPs were detected in lake and raw drinking water. The average and max concentration of the sum of all microcystins in raw drinking water was 3.2 µg/L and 21.1 µg/L and in lake water was 10.2 µg/L and 87.0 µg/L. Significant (p<0.03) correlations were observed at both the Appleton and Menasha drinking water plants, between the concentration of microcystins in raw water and turbidity (R=0.6 for Appleton; R=0.8 for Menasha) and the concentration of microcystins in raw water and Microcystis cells/ml (R=0.6 for Appleton; R=0.7 for Menasha). Other parameters correlated with microcystins in raw water at one of the two plants including color (R=0.7) and silica concentration (R=-0.7). These results can be further utilized to develop a modeling program to predict when elevated toxin concentrations may be a concern based on specific environmental conditions.

CHED 751
Effects of woolly adelgid induced hemlock productivity decline on soil nutrient content

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Invasive insects continue to have a serious negative impact on our ecosystems. The hemlock woolly adelgid (HWA) is one of the species that is threatening our area in upstate New York as it is spreading at a rate of about 25 km per year on the eastern coast of the US. HWA extracts carbohydrates from the hemlock’s cells causing a slow death, usually about 4-5 years. Most of the studies have been conducted on the biological and ecological impacts of this species and less has been done to understand its chemical impact on soils, and on soil and surface waters. The goal of this study is to determine the effects of HWA induced hemlock productivity decline and death on nutrient content of the soil, and then correlate these results with surface and soil water results to determine how these nutrients mobilize in the infected hemlock ecosystems.

Two parks, the uninfected Robert V. Riddell and the infected Mine Kill State Parks in central NY, were chosen for this study. Three sites were selected within Mine Kill State Park; uninfected, infected and untreated, and infected and treated. One site was chosen in Robert V. Riddell State Park. Soil samples were collected using soil cores and pits at each site in three replicates. Soils were separated by horizons and analyzed for soil pH, moisture and organic carbon contents. Extractable nitrate, phosphate and sulfate concentrations were determined by using UV-vis spectrometry. At each site, the top horizon has the highest concentrations of both sulfate and phosphate that decrease below detection limit in the lower horizons. The highest sulfate and phosphate concentrations, 22.5 and 20 mg/L, respectively, are found in Robert V. Riddell State Park. At Mine Kill, the uninfected site has 6.6 mg/L phosphate and 21.2 mg/L sulfate, while the two infected sites only have 2.4 mg/L phosphate and 9 to 14 mg/L sulfate. The pH of the soils ranges between 3 and 5. Soil moisture and organic carbon content decreases from top to bottom in each soil profile. In soil and surface waters, sulfate (6 mg/L) and chloride (0.5 mg/L) are the dominant anions while nitrate and phosphate are below detection limit. Soil waters contain 6-7 times more total dissolved solids than the surface waters, both within neutral pH range. Data of the uninfected sites provide baseline conditions, and all data will be further analyzed to understand how the decreased productivity and death of hemlock can affect nutrient mobility in HWA infected ecosystems.

CHED 752

Analysis of heavy metals in Lutjanus griseus and Lutjanus campechanus at the natural reserve “La Parguera”, Puerto Rico

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The natural reserve “La Parguera”, located in the island of Puerto Rico, is one of the major tourist attractions due to the fact that this region is home to one of the of the seven bio-luminescent bays in the world. This reserve is supervised by the Department of Natural and Environmental Resources of Puerto Rico (DRNA) tasked with protecting and maintaining a balanced ecosystem. In this study we analyzed the concentrations of As and heavy metals Cd, Pb, and Cu in the edible part of three *Lutjanus Griseus* and the three *Lutjanus campechanus*. We took the samples from trees from different places in the Natural Reserve considering the habitat of each fish. In order to determine As and the heavy metals in each fish, they were subjected to a wet digestion with nitric acid and the resulting solution were then analyzed by flame atomic absorption spectroscopy. Preliminary results, showed a content of heavy metals in all the samples. Finally, we aim to study heavy metals content in the entire ecosystem.

![Map of La Parguera](image)

CHED 753

Detection of precursors to methamphetamine in city sewers lines

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Methamphetamine has been found in surface waters, wastewaters and sewers. In wastewater, because there is no known way to distinguish between methamphetamine discarded from clandestine laboratories and methamphetamine excreted in the urine of drug users, finding precursors used in methamphetamine production can provide that distinction. The ability to pinpoint the presence of clandestine laboratories may be used in the future as an environmental or forensic tool. This research focused on the detection of methamphetamine precursors, specifically ephedrine and pseudoephedrine, in city-owned sewer lines. Passive samples were obtained by deploying Polar Organic Chemical Integrative Sampler (POCIS) disks into city sewer lines for a period of two weeks in areas of the city suspected to house clandestine methamphetamine laboratories. POCIS disks were filtered, extracted, and analyzed by LC-MS/MS. The results of this research will be discussed.

CHED 754

Optimization of fly ash nanogeo polymer and its application in pervious concrete for bioremediation of fecal coliform-containing water

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Approximately 5% of current anthropogenic CO₂ emissions worldwide are attributed to the cement industry. Coal fly ash (FA), an industrial byproduct, can be used to synthesize geopolymer concrete pavement. Environmental benefits of FA utilization in cement and concrete include reductions in the consumption and production of Portland cement so that the amount of CO₂ released to the atmosphere is decreased. This study consisted of two main tasks. The first task was to obtain the optimum mix ratio of FA nanogeo polymer paste by a four-factor two-level central composite design with liquid-to-binder (L/B, 50-70%), FA-to-binder (FA/B, 60-100%), nanoSiO₂-to-binder (NS/B, 0-4%) and NaOH concentration (NaOH, 0-8M). The spread percentage of the fresh paste and the early age compressive strength of the hardened paste cured for 7 days at ambient temperature were tested. The second task was to evaluate FA nanogeo polymer pervious concrete made of the optimum mix ratio of the paste for its potential to remove fecal coliforms in the storm water runoff. Compressive strength and permeability of FA nanogeo polymer pervious concrete hardened for 7 days at ambient temperature were ~20 MPa and ~10 mm/s, respectively. Results from the first task generally showed that the lower L/B, FA/B or NaOH or the greater NS/B was, the greater compressive strength was achieved. Higher spread percentages were obtained with the greater L/B or the lower FA/B, NS/B or NaOH. All four factors had a significant impact on the spread percentage, whereas NaOH was the factor that made insignificant main and quadratic effects on the compressive strength although interactive effect of FA/B and NaOH was significant. The optimized mix ratio of the paste for the highest compressive strength of 22.2 MPa and the desired spread percentage of 110% was 50% L/B, 60% FA/B, 0.04% NS/B and 1.7M NaOH. Despite of the high volume FA utilization, neither alkali-activation with high NaOH concentration, large quantity of nanoSiO₂ addition, nor curing at an elevated temperature was necessary to produce FA nanogeo polymer paste having the
desired workability and gaining the structural strength in a short period time. FA nanogeopolymer pervious concrete showed a ~65% FC removal on average with a maximum 100% removal. Therefore, findings from this study imply potential sustainable use of FA nanogeopolymer pervious concrete pavement for storm water runoff control.

CHED 755

Extracting metal (II) cations from aqueous solution using dipicolinic acid

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Wastewater handling from hydraulic fracturing sites has become a large issue in Marcellus Shale. In order to recover natural gas buried underground, industry uses pressurized water to fracture shale rock and collect desired natural gas. The shale rock that is fractured during this process contains high concentrations of cations that are then dissolved in the millions of gallons of fresh water needed for the drilling process. Currently, wastewater treatment plants cannot handle the high levels of cations from the hydraulic fracturing wastewater. There is an urgent need to develop a new clean and efficient method for wastewater disposal. The purpose of this research is to explore the removal of metal (II) cations from aqueous solution by introducing dipicolinic acid derivatives that will aid in bioremediation of wastewater.

CHED 756

Pesticide analysis in Southeast Michigan waters by gas chromatography-mass spectrometry

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Pesticides have adverse health effects due to their action as endocrine-disrupting compounds. In this work, we analyzed pesticides in Southeast Michigan lake and river water by gas chromatography-mass spectrometry (GC-MS). Prior to analysis of environmental water samples, nine pesticides (alachlor, aldrin, atrazine, cyanazine, endosulfan I, endrin, metolachlor, methoxychlor, and pendimethalin) were dissolved in HPLC-grade acetone and analyzed by GC-MS to determine the retention time and the mass spectrum for each. Pesticides in water samples were concentrated by filtering the samples with a C18 solid-phase extraction disk in a glass-filtration apparatus. The pesticides on the disk were released using a mixture of acetone and n-hexane. The organic phase was dried with anhydrous sodium sulfate, concentrated with a rotary evaporator, and evaporated to dryness with a dry-bath incubator under nitrogen gas. The sample was dissolved in acetone and then analyzed by GC-MS. Our work to date
has primarily focused on analysis of atrazine, which is one of the most widely used pesticides in the United States. Various concentrations of atrazine were used to spike several water samples including distilled, tap, and river water to assess recovery through the solid-phase extraction procedure. Additionally, a method for separation and detection of atrazine metabolites was developed and was employed to investigate their presence in Southeast Michigan lake and river water.

CHED 757

Study of analyte recovery using headspace solid-phase microextraction

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Headspace Solid-Phase Microextraction (HS SPME) has been shown to effectively extract pesticides and PCBs from aqueous samples at the expected ultra-trace levels (parts per quadrillion) of alpine lakes. Several variables of the HS SPME technique have been adequately evaluated including water temperature and length of fiber exposure, but surprisingly, analyte recovery as a function of analyte concentration and storage time has not been included in previous studies. This investigation evaluates the recovery of chlorinated hydrocarbons, such as DDT, in concentrations from parts per quadrillion to parts per billion in lake water samples. The HS SPME technique was further used to determine the concentration of chlorinated pesticides in Pacific Northwest alpine lakes.

CHED 758

Scanning electron microscope analysis of Columbia River, Chesapeake Bay, Lake Hartwell, and Mississippi River sediment suspensions

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The release of hydrophobic pollutants during sediment resuspension events such as dredging, violent storms, or bioturbation, is today one of the largest sources of these pollutants in aquatic systems. While the equilibrium partitioning and kinetic rates of releases of pollutants such as DDT have been extensively investigated, information on the nature of the actual sediment particle releasing these pollutants is lacking. This investigation used manual inspection of SEM micrographs to determine the distribution of particle types in each suspension. Particles were divided into individual particles, particle aggregates, and “other” mostly consisting of organic matter (individual cells and organic detritus). The most important finding of this research was that organic detritus may dominate the total organic mass in typical sediment suspensions and may account for most of the pollutant sorption sites.
CHED 759

Quantification of epoxides from their carbamate derivatives: Environmental applications

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This project focuses on developing a method to quantify epoxides in atmospheric organic aerosol samples. In the atmosphere, there are copious environmental contaminants present that can affect people’s health as well as climate and one particular class of compounds of growing interest are epoxides. Epoxides are formed in the atmosphere through oxidations of volatile organic compounds, but there is little information on their ambient concentrations due to their high reactivity. Previous research has been done to quantify epoxides in biological and water samples, but there are few methods to quantify in atmospheric aerosol samples. Various model epoxide compounds are derivatized with sodium diethylcarbamodithioate (DTC) and the concentration of the resulting carbamate is measured at 276 nm. Calibration curves for 6 model epoxides have been measured with a linear dynamic range of 2.5-50 μM. An HPLC method has also been developed to separate derivatized epoxides from the aerosol mixture for identification using electrospray mass spectrometry. Finally, these methods are used to quantify epoxides formed from the reaction of m-xylene with hydroxyl radicals in an environmental chamber. These methods allow for quantification, identification, and structure elucidation of epoxide compounds in organic atmospheric aerosol.

CHED 760

Detection of amphetamine type substances in sewers using Polar Organic Chemical Integrative Samplers

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This research is a follow up to a pilot study on the qualitative detection of Amphetamine Type Stimulants (ATSs) in sanitary sewer systems using Polar Organic Chemical Integrative Samplers (POCIS). Because ATSs pass through the body unchanged, they can enter waste waters through excretion of urine or through manufacture from clandestine laboratories. This is a qualitative study using POCIS discs to collect samples from areas of suspected drug activity. Sewer samples were collected two weeks after samplers were deployed. ATSs were extracted from the POCIS sorbent and
analyzed using high performance liquid chromatography tandem mass spectrometry (HPLC-MS/MS). Results will be discussed at a later time.

CHED 761

**Mercenaria mercenaria** a potential bioindicator of heavy metal releases into Narragansett Bay, RI

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Though the release of pollutants into Narragansett Bay (NB), Rhode Island has been curbed, capped contaminated sediments can still reenter the ecosystem by natural perturbation or human activity. To continuously monitor the extent of these pollution events over a vast area would be cost prohibitive. To circumvent this problem this research investigated the ability of the native bivalve *Mercenaria mercenaria* (quahog) as a natural bioindicator. The quahog has ability to bioconcentrate heavy metals to levels that greatly exceed those present in surrounding pore/water and benthic sediments. The quahog has adapted its habitat from open ocean to freshwater environments and because of their abundance, sedentary long lifespan (>10yrs) make them ideal in-situ biomonitors. Eight sites in the West Passage of NB were assessed for quahogs, their heavy metal content and their relationship to benthic sediment metal concentrations. X-ray fluorescence spectrometry was used to analyze heavy metals in selected dry sieved benthic particles (4-20 µm), those normally selected during the quahogs’ siphon feeding. Dried dissected soft tissue was assessed for acute heavy metal exposure and the internal side of the shell for long-term depositions. The benthic sediment particles cation exchange capacity was also assessed for heavy metals perturbation from benthic pore water to open water as a concurrent route of exposure into the bivalve when siphon feeding.

CHED 762

**Study of the effects of two PPCPs on algal growth**

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The effects of Pharmaceuticals and Personal Care Products (PPCPs) on the environment, mainly through their presence in water, are largely unknown. These drugs, soaps, lotions, etc. are exposed to the environment through runoff water, flushing them down the toilet, human and animal excretions, and much more. Most water treatment plants are ill equipped to remove PPCPs out of the water, and they end up in rivers, streams, or lakes. This study focused on two common medications: phenazopyridine hydrochloride (HCl) and cetirizine hydrochloride (HCl). Phenazopyridine HCl is the active ingredient in AZO, the most common urinary tract pain reliever. Cetirizine HCl is the active ingredient in Zyrtec, a common antihistamine. These drugs were chosen
based on two factors: their popularity and the amount of unchanged drug in the urine. As much as 66% of phenazopyridine HCl is passed through the urinary system completely unchanged and flushed right down the toilet, providing an opportunity for the pure compound to be present in the environment. As much as 50% of cetirizine HCl is passed through the body unchanged, and it is used by an innumerable amount of people during pollen season, meaning there could be a lot of the drug in the environment. This study attempted to determine the effects of these drugs on the environment by using *Selenastrum capricornutum* as an analog for the environment.

**CHED 763**

**Exploring the interactions between citrate-stabilized silver nanoparticles and humic acid via fluorescence quenching**

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The fate of silver nanoparticles in the aquatic environment is a topic of interest due to their antibiotic properties and their use in various other applications. Fluorescence quenching was used to investigate the complex formation between humic acid and silver nanoparticles. Silver nanoparticles were synthesized by reduction of silver cation (from silver nitrate) with heat and stabilization by trisodium citrate; particles were purified by centrifugal ultrafiltration. The fluorescence intensity of humic acid with varying concentrations of quencher was measured to construct a Stern-Volmer plot. The quenching was investigated at five temperatures, and decreasing slopes with increasing temperature indicated static quenching. A Van’t Hoff plot was produced to determine $\Delta H = -4.02 \text{kJ/mol}$ for the binding reaction, suggesting an exothermic process. The small value of $\Delta H$ indicates that the nanoparticles are weakly bound to humic acid and as a result are likely to be more bioavailable than organic pollutants.

**CHED 764**

**Investigating the formation of thioarsenic species under sulfidic conditions**

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Arsenic is a carcinogenic toxin that has a maximum standard of 10 ug/L in drinking water, as established by the World Health Organization. In sulfidic environments, particularly sulfate-reducing groundwaters, arsenic readily forms a mixture of thioarsenite species and thioarsenate species (mono-, di-, tri-, and tetra- thio). Quantification of the thioarsenite species is difficult for aqueous samples at low arsenic concentration. Knowledge of groundwater arsenic speciation is important because the
species vary both in levels of toxicity and difficulty in removal. The specific formation mechanisms are poorly understood. Formation of dithioarsenate has been proposed to be by reaction of sulfide with monothioarsenate, however contradictory evidence exists for the importance of this mechanism. This reaction was investigated through the use of ion chromatography interfaced to inductively coupled plasma mass spectrometry (ICP-MS). Concentrations of thioarsenic species following reaction were determined and compared against a 350 ppb standard of monothioarsenate, prepared from solid form. This standard also contained about 12% each of arsenite and arsenate. Following reaction arsenite decreased by approximately 75% while monothioarsenate increased by 30%. The percent of dithioarsenate was slightly decreased. The decrease in arsenite suggests that the monothioarsenate was not the reactant, but rather, the arsenite combined with the sodium sulfide to produce more monothioarsenate. These results suggest a redox reaction mechanism to produce the monothioarsenate, as opposed to previous assumptions that monothioarsenate would undergo further substitution of sulfur to generate dithioarsenate. Results provide insights into arsenic behavior in reduced groundwaters as well as into treatment and impacts of arsenic toxicity.

CHED 765

Study on UV-Vis spectroscopic characteristics of soil humic substances

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Humic substances are important in environmental chemistry of soil and waters. They are naturally occurring organic substances ubiquitously present in aquatic and soil environments. They consist of large organic molecules with many aromatic rings, carbon double bonds, and various functional groups, acting as binding agents (ligands) to bind metal ions and thus control their speciation and fate in the environment. UV-Vis spectroscopy can provide information to understand the structures and behaviors of humic substances. A spectroscopic index was created to reflect the UV-Vis spectrum of a humic substance sample and thus link the index value to the properties and structures of humic substances. Experimentally, the index IS obtained by using the UV-Vis spectra of a humic substance sample in a series of dilutions. The index is given by the slope of the plot of the slopes of the calibrations (abs. vs. concentration) from the UV-Vis scans of the series dilutions of the humic substance sample vs. wavelength of the UV-VIS scan. A group of soil humic substance samples were extracted using NaOH solution. The index values of these samples ranged from 3.9 to 25.9, exhibiting a wide variation of the index values. These preliminary results show some potential for the use of this index. Further research will be carried out to test more humic substance samples from a variety of sources. A large pool of the index values will make it ready to further link the index to the properties and structures of the humic substance samples.

CHED 766

Rhodium catalyzed hydrodehalogenation of fluoroarenes in mild conditions
The fate of fluoroarenes in the environment has become a concern, in part because of the higher use of fluoroarenes in pharmaceuticals and industrial processes. One way to help alleviate this environmental concern is to explore ways in which fluoroarenes are degraded to benign compounds. Fluorinated aromatic compounds are hydrodefluorinated using a heterogeneous 5 wt % rhodium on alumina catalyst under mild conditions (1 atm. H$_2$, 25°C). The catalytic hydrodehalogenation mechanism and substrate scope were explored by looking at a variety of substituted fluoroarenes. The effects of electron-withdrawing and electron-donating substituents as well as the position of the substituents to the fluorine atom (ortho, meta, para) were examined. The substrate degradation, subsequent intermediate(s), and product formation rates were monitored using GC/MS. The fluorotoluenes are the quickest to undergo degradation with an average rate of 3.5 ± 2.1 x10$^{-3}$ min$^{-1}$mg$^{-1}$ Rh/Al$_2$O$_3$ and the fluoronitrobenzenes, with an average rate of 0.88 ± 0.79 x10$^{-3}$ min$^{-1}$mg$^{-1}$ Rh/Al$_2$O$_3$, are the slowest.

CHED 767

Removal of phosphate from aqueous media by adsorption onto humic acid-coated magnetite

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Eutrophication in natural aquatic systems is a serious problem for water utilities. The runoff of nitrogen and phosphate from fertilizers and sewage into lakes, river and streams has led to increases in harmful algal blooms which produce and contaminate drinking water sources with potent toxins. We report herein the application of environmentally compatible materials, humic acid-coated magnetite nanoparticles (HA-MNP), as potential adsorbents for the removal of phosphate from aquatic systems. This nanomaterial was synthesized by coating nano-sized iron oxides with natural humic acid. HA-MNPs readily adsorbed phosphate over a temperature range of 15°C – 65 °C. Under our experimental conditions the highest phosphate adsorption capacity was 8.31 mg/g observed at 25 °C. At elevated temperatures the humic acid coating may become flexible or porous thus facilitating desorption equilibrium processes. The adsorption capacity was also higher under acidic conditions than under neutral and basic conditions and fitted to the Langmuir adsorption isotherms assuming monolayer coverage on the adsorbent surface. The adsorption was modeled to the intra-particle diffusion model yielding K$_{id}$’s (ppm/g*min$^{1/2}$) of 0.031 to 0.2658 for 1 PPM solution to 50 PPM solution, respectively. This indicates that intraparticle diffusion within the pores of the adsorbent is significant during the adsorption process. The overall adsorption
process has been found to follow the second order reaction kinetics, with $K_p$'s (g/min*mg) ranging from 0.611 to 0.022 for 1 PPM and 50 PPM solution, respectively (with associated $R^2$ values of 0.9985 and 0.9966). The HA-MNP appear to be effective for the adsorption of phosphate, that can be later easily removed by using a magnetic field and offer a promising strategy to consider for the removal of phosphate from aquatic environments.

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CHED 768

Use of CYCLAM and other tetraamines to probe the mechanism of influence of surfaces on ligand exchange

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The role of surfaces in ligand exchange reactions is poorly understood. This research uses 1,4,8,11-tetraazacyclotetradecane (CYCLAM) and linear analogs (such as 2,3,2-tet) to probe the mechanism(s) by which surfaces affect ligand exchange reactions. The exchange of Ni from CYCLAM to a stronger chelating agent (Y) was monitored via capillary zone electrophoresis (CZE). The formation of NiY was monitored both with and without the presence of a metal oxide surface. Equilibrium calculations indicate that NiCYCLAM is present in two forms: an octahedral complex and a complex with planar coordination and electronic geometry. The octahedral complex forms initially and is kinetically stable, but the planar complex is thermodynamically favored. The octahedral complex has potential to allow additional inner sphere coordination to Ni by the surface, while the planar form does not. By exploring each of these variables, this research aims to identify pathways by which surfaces influence ligand exchange reactions.

CHED 769

Studying the reactions of alcohol amines with atmospheric oxidants

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Alcohol amines are becoming more prevalent in the atmosphere due to the increasing use of carbon capture and sequestration (CCS) by power plants, a process that commonly uses alcohol amines. The environmental and health effects of these alcohol amines are unknown. Experiments were carried out in an environmental chamber to see the products of certain alcohol amines (monoethanolamine [MEA], 2-amino-2-methyl-1-
propanol [AMP], N,N-dimethylethanolamine, and 2-(methylamino)ethanol [MAE]) and atmospheric pollutants (ozone, the nitrate radical, and the hydroxide radical). An aerosol mass spectrometer and a particle-into-liquid sampler coupled with dual ion chromatographs (PILS-IC) were utilized to determine the products formed and their concentrations. A method of separating the possible products, which include ammonium, methylamines, ethylamines, butylamine, and trimethylamine-n-oxide picrate, was developed using ion-chromatography, and will be used to determine the concentrations of the reactions carried out in a environmental chamber located at the University of California, Riverside, College of Engineering, Center for Environmental Research and Technology (UCR CE-CERT). A new chamber was constructed this summer and is designed to simulate a range of atmospheric conditions, and allows the reactions to proceed in a controlled environment. The experiments will offer results showing possible dangers created by the release of these alcohol amines.

CHED 770

Effects of "real world" biodiesel and petroleum diesel combustion on PM composition and production of ROS in BEAS-2B cells

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Due to the reduction in mass emissions of particulate matter (PM), biodiesel is considered a greener alternative to petroleum diesel fuel. Despite being considered environmentally friendly, there is little known regarding the toxicological responses to biodiesel PM relative to diesel PM, especially from PM generated in 'real world' combustion operations. The composition of 'real world' biodiesel and diesel PM can include transition metals, and polar and nonpolar organic species, all of which can induce production of Reactive Oxygen Species (ROS) in human lung cell lines. ROS is believed to be associated with a number of diseases including diabetes, neurodegenerative disorders, and is linked to aging. During the summer of 2014, we collected PM samples generated from a heavy duty front loader that operated on both biodiesel and diesel fuels at a rural recycling center. The PM was collected from the operator's breathing zone and ranged in sizes from 2.5-0.25µm. In this poster we will present results from our evaluation of the ROS production of PM from each fuel type in a BEAS-2B lung cell model. We will also measure the water soluble organic carbon (WSOC) from each PM type to investigate potential associations between WSOC and ROS. Understanding PM exposure levels, PM composition, and the link to toxicological endpoints are important in performing more comprehensive exposure assessments evaluating the impact of various fuels used in 'real world' conditions.

CHED 771

Impact of "real world" biodiesel and petroleum diesel combustion on particulate matter composition and oxidative potential
Biodiesel is considered an environmentally friendly alternative fuel to petroleum diesel. While it is well known that biodiesel blends reduce emissions of particulate matter (PM) mass compared to petroleum diesel, less is known regarding the impact of PM on toxicological responses, especially from PM generated in 'real world' operations using biodiesel fuel. The dithiothreitol (DTT) assay has been used by many researchers to approximate the oxidative potential of reactive species in ambient and fuel related PM. Oxidative potential is related to the ability of PM to generate reactive oxygen species \textit{in vitro} and is associated with adverse health effects. In this project, we collected fine PM from within the cabin of a heavy duty large front loader (John Deere 624K) operating on both B20 (20% biodiesel/80% diesel blend) and petroleum diesel at a rural recycling center. We performed the DTT assay on both diesel and B20 PM collected near the worker’s breathing zone to determine the PM’s oxidative potential; additionally we measured the water soluble organic carbon (WSOC) content of the PM to investigate any relationships between DTT consumption rates and WSOC content. This poster will present the results on PM collected over a 10 week field sampling period in the summer of 2014. Our goal is to better understand the impact of ‘real world’ combustion of biodiesel fuel on the PM’s composition and oxidative potential as a measure of toxicological response.

CHED 772

Enhancing the chemical mixture methodology: Revising the health code number assignments of hazardous chemicals to account for varying intensities of respiratory irritation

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The Chemical Mixture Methodology (CMM) is used by the Department of Energy, its contractors, and other private and public organizations for emergency response planning to ensure the safety of individuals exposed to airborne mixtures of hazardous chemicals. The CMM estimates the potential adverse health effect by calculating the hazard indices (HI) for each chemical present in the mixture at a given receptor point downwind of the release site. The CMM assigns health code numbers (HCNs) to each chemical based on the human organs that are impacted by chemical exposure. The HIs of the chemicals that target the same or similar organs are summed to determine their overall impact. In this work, we hypothesize that refining the HCNs for chemicals that are respiratory irritants according to the severity level of corresponding toxic effects will reduce over-conservatism in the CMM. Currently, the CMM has only one HCN that to cover all severities respiratory irritation. In our project, we are applying HCN values to respiratory irritants: mild irritants, moderate irritants, and severe irritants. When
calculating HIs, weighting factors are applied to account for the differences in severity of the respiratory irritation. We anticipate that the expanded set of HCNs for respiratory irritants will allow emergency planners more accurately assess the consequences of chemicals that present a hazard involving respiratory irritation.

CHED 773

Chemical analysis in the *Eryngium foetidum L.*

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The concentration of heavy metals (Pb, Hg, Cd) has been studied in *Eryngium Foetidum L.* ("recao"). Triplicated samples of *Eryngium Foetidum L.* were taken from a home garden, two different supermarkets and by the aquaponic system. The purpose of this research is to know which of the samples of the spice will present the highest concentration of contaminants. After preparing the samples by nitric acid dissolution, they were tested in two methods, the atomic absorption and the electrochemistry. In electrochemistry the current produced for each metal in the displacement is directly proportional to the concentration of each metal. In atomic absorption the amount of light absorbed after passing through the flame determines the amount of ions existing in the sample. No presence of mercury (Hg) or lead (Pb) was found in the *Eryngium Foetidum L.* analyzed samples. However, concentrations of cadmium (Cd) were detected in both methods. With the atomic absorption method, traces of cadmium (Cd) were found in the majority of samples. The obtained concentrations of cadmium (Cd) exceed the limits allowed in agricultural soils. Therefore, we can conclude that the given hypothesis was true; the highest concentrations of contaminants in the samples were from the supermarket.

CHED 774

Static quenching of acridine yellow G and norfloxacin by humic acid

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The ability of humic acid to bind to pollutants is important to determine their transport and bioavailability. Static quenching was observed by fluorescence and UV-Visible spectroscopy at 25, 30, 35, 40, and 45°C. Stern-Volmer plots allowed for determination of the equilibrium binding constants for a variety of temperatures that were averaged to construct a van’t Hoff plot. The enthalpy of binding between acridine yellow G (AYG) and humic acid and norfloxacin and humic acid were determined from van’t hoff plots to be -15.4±7.9 and -10.3±3.8 kJ/mol. Since the magnitude of the enthalpy of binding is
greater for AYG than norfloxacin, AYG will more readily join with soil and will have a lower level of bioavailability.

CHED 775

Correlation of nitrogen dioxide and ozone gas concentrations between Milwaukee and Chicago

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Concentrations of ozone and nitrogen dioxide gases in Milwaukee are high in the summer months, and they contribute to adverse health effects. The American Lung Association states that Milwaukee has a weighted average of 10.8 days during the summer with an unhealthy concentration of ozone. Palms-type passive diffusion tubes for nitrogen dioxide and ozone were placed at four different sites between Milwaukee and Chicago to measure the abundances of the gases over time. These tubes were exchanged regularly to gather five-day samples. The concentration of nitrogen dioxide and ozone gases between Milwaukee and Chicago during the summer was determined and analyzed for possible connections.

CHED 776

Extraction of barium from aqueous solution using pyradine based small molecules

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Wastewater treatment facilities cannot remove high levels of cations found in the millions of gallons of produced water from hydraulic fracturing drilling in the Marcellus Shale region. Other current disposal methods, including ion exchange and evaporation, are too costly or inefficient to address the quantity of produced water, thus a new purification method must be developed. This research explores the ability of pyridine based compounds to extract barium, and other cations commonly found in high levels of hydraulic fracturing produced water, from aqueous solution.

CHED 777

Design and characterization of a pulsed laser cavity ring-down spectrometer for use in the measurement of aerosol optical properties

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Accurate measurements of optical extinction coefficients and scattering parameters for atmospheric aerosols are needed in order to quantify the effects aerosols have on climate change. Although this field was once dominated by Fluorescence FAGE and long-path absorption spectroscopy DOAS, cavity ring-down spectroscopy (CRDS) has emerged as a cost-effective, accurate alternative technique that has numerous advantages. CRDS is an optical absorption technique based on Beer’s Law that allows for the characterization of extremely low concentration target samples by using two highly reflective mirrors to create an optical cavity with a pathlength thousands of times longer than its meter long laboratory footprint. System ring-down information has been monitored and collected using a LabView based program written in-house to collect, analyze, and store the relevant data. Polystyrene spheres were used to model scattering aerosols of various sizes so that the instrument could be characterized before its use in other aerosol measurements.

CHED 778

Size characterization and metals analysis of particulate matter generated by candle burning

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It is well known that poor indoor air quality is due to gas and particle emissions inside the home. In addition, ventilation that would dilute the pollutants with clean outside air is often inadequate causing the pollutants to concentrate even further. Household candles contribute to indoor air pollution as they emit particulate matter while they burn. Inhaling particulate matter can lead to lung cancer, cardiovascular disease, asthma, and other health problems. The particulate size is a concern as the detrimental health effects of particulates are more severe as the size of the particle decreases. In the present study, particulate matter emitted by various candles was coarsely size selected using a multi-stage impactor. Gravimetric analysis of the particulates collected in each size range allowed measurement of the size distribution of the particles formed in the burning process. Candles commonly also contain various metals including lead in their wicks which may be volatilized when the candle is burned. Atomic Absorption Spectroscopy was used to determine the concentration of several metals of interest in the collected particulates. By correlating the metal concentrations with the size range of the particles we were able to see if the metal concentration changed as the particle size range was varied.

CHED 779

Quantitative determination of antidepressants in wastewater effluents and biosolids

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Antidepressants are one of the most widely dispensed classes of pharmaceuticals in the United States. As a result, these drugs are commonly detected environmental contaminants in wastewater-impacted environments including in tissues of non-target organisms living in these impacted ecosystems. Liquid chromatography tandem mass spectrometry coupled with an extraction technique was used for quantitative determination of a suite of SSRI and SSNRI antidepressants and their respective metabolites in effluents and surface waters. This method was also used to measure the same suite of antidepressants in biosolids destined for land application. Venlafaxine and its metabolite were the most abundant antidepressant observed in the aqueous samples. Sertraline, fluoxetine, and citalopram and their metabolites were the most commonly detected antidepressants in the sludge samples. These results further confirm that discharges from wastewater treatment plants are a source of antidepressants in aquatic and terrestrial environments.

CHED 780

Closing the gap on secondary organic aerosol formation: Oligomerization of glyoxal

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The goal of this project is to determine both radical and non-radical mechanisms of aqueous phase secondary organic aerosol (SOA) formation. Aerosols affect public health with their atmospheric presence by increasing cardiopulmonary diseases. The climate is affected when solar radiation is absorbed or deflected, in addition aerosols can serve as cloud condensation nuclei. Atmospheric climate models underestimate SOA formation solely from gas phase chemistry as such the investigation into the mechanisms of oligomer formation from specific compounds can be compared to ambient data to identify potential aqueous SOA precursors. Understanding SOA formation in wet aerosols has the potential to eliminate the gap between predicted and measured SOA. Dialdehydes are known to form oligomers in wet aerosol and simulations of aqueous phase reactions in the laboratory can explicate the mechanisms responsible for oligomer formation in wet aerosols. Here we present our HPLC-UV/MS results of the formation of high molecular weight compounds from the glyoxal photolysis reaction and reaction with hydroxyl radicals. Hydroxyl radicals are formed via photolysis of H₂O₂ or via the Fenton reaction. Glyoxal was chosen as our model compound since it is the smallest, most prevalent dialdehyde in the atmosphere.

CHED 781

Submarine groundwater discharge as a potential hidden pathway for eelgrass decline in San Juan county

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Understanding recent eelgrass declines in San Juan County is of vital importance, as these eelgrass communities represent incredible ecological and economic value. The alarming magnitude of these losses and the unlikelihood of natural recolonization are additional reasons to continue exploring factors that may have contributed to decline. This project addressed one of the least studied vehicles for coastal pollution as a potential contributor to eelgrass loss: submarine groundwater discharge (SGD). SGD can introduce potent pollutants such as nutrients and herbicides directly to nearshore ecosystems. The goal of this project was to determine whether SGD is affecting eelgrass health in San Juan Island National Historical Park sites by adding excess nitrogen or phosphorous to waters at these sites. While no phosphate loading was detected, elevated nitrogen concentrations were observed both in seawater samples, at approximately 1 mg/L, as well as in SGD samples at 1-2 mg/L nitrogen. Roche Harbor, on the north side of the island showed the highest concentrations at 2.1 mg/L. Considering the harmful effects of nitrogen loading on eelgrass, it seems that SGD may have a negative effect on local eelgrass habitats.

CHED 782

Arsenic analysis and speciation of water samples from Chihuahua México, by HG-CT-AAS

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Arsenic is an ubiquitous element in the earth which species in water are very toxic to human health. Natural geochemical leaching is the primary source of dissolved arsenic in ground waters. Arsenic is a metalloid present in a very low concentration in soils, water and air. It presents a very high mobility and transformation capacity within the different environments, presenting an important capacity to adsorb, change in oxidation states and ability to react with oxygen, even mediated by microorganisms. The high arsenic concentration in water is related to its liberation from solid phase, transport phenomena and other dilution processes. The main arsenic species in water are the inorganic As³⁺, As⁵⁺ and the organic MMA and DMA. In our country, 75% of the water supplies relies in ground sources. For instance, many communities present an As concentration above the maximum concentration limit. There is evidence that As exceeding 50 ppm in water produces cancer in a high risk 1/100. In Chihuahua As concentration is reported as high as 0.05-0.5mg/L. Currently there are many quantification methods that could be used to analyze the different compounds of As,
such as CE-UV, LC-ICP-MS and HG-AAS. HG-AAS is the most used due to its sensivity, and lack of interferences. Cryogenic trapping has been employed to separate the different As species, allowing to differentiate among trivalent, pentavalent and organic compounds. In this work data obtained from well sampling is presented. Over 200 wells were monitored during one year and the concentration ranges from 1.83 - 172.9 ppb presenting the different As compounds, mainly pentavalent ones.

CHED 783

Photodegradation of organic dyes using quantum dots of Cd(Se,S) in aqueous solutions

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Several water pollution issues are frequently associated with the discharge of industries and municipal waste. Dyes from textile and paper manufacture can cause serious environmental problems because the toxic character of the compounds themselves and their corresponding byproducts. Quantum dots of Cd(Se,S), a fluorescent material, were used as photocatalytic agent in the degradation of methylene blue (MB) and Victoria blue (VB) under UV irradiation (302 nm) at pH 6.5. Quantum dots were characterized by X-ray diffraction (XRD), UV-Vis and photoluminescence techniques. The degradation of MB, VB and their photo-degradation products after 5 hours of UV irradiation were monitored using High Performance Liquid Chromatography (HPLC) at 600 nm. Titanium dioxide nanoparticles (Aeroxide P25), a well-known photocatalyst standard, were used to compare the efficiency of the QDs. The efficiency of the photodegradation process was strongly dependent on QDs concentration.

CHED 784

Photodegradation of antibiotics in aqueous solutions using quantum dots of Cd(Se,S)

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Drugs hormones and antibiotics found in municipal waste can cause a detriment effect on the ecosystems. Actual waste water treatment approaches fail to remove these new
contaminants when they are at low concentrations. Microwave-assisted synthesized quantum dots of CdSe(S) were used as photocatalyst in the photo-degradation of tetracycline (TC) and oxytetracycline (OTC) under UV irradiation (302 nm) in aqueous phase at pH 6.5. Quantum dots were characterized by X-ray diffraction (XRD), UV-Vis and photoluminescence. The degradation of TC and OTC were monitored using High Performance Liquid Chromatography (HPLC) at 355 nm. The photodegradation efficiency was dependent on the QDs concentration. Titanium dioxide (aeroxide P25) was used as a standard photocatalyst, for comparison purposes.

CHED 785

Cadmium phytoremediation of in vitro culture with micro-propagated clones of Spermacoce assurgens

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Spermacoce assurgens, known by the vernacular name of “Juana la Blanca”, has been selected as a target plant for the phytoremediation of Cd\(^{+2}\). Juana la Blanca is a medicinal plant native to Puerto Rico used mostly to disintegrate kidney stones. Phytochemistry of this plant suggests strongly that Juana can also be a potent phytoremediator. Preliminary work in our lab with Juana la Blanca as phytoremediator for the explosive TNT (trinitrotoluene) gave encouraging results. These bright preliminary results were shadowed by the suspicion of fungal contamination. To clarify this situation and ascertain the putative strong phytoremediation role of Juana la Blanca, we decided to isolate and identify the organism growing in symbiosis with this plant. The first objective of the research was to obtain a line of plant clones for experimentation using the technique of in vitro plant cell and tissue culture. Special attention was placed in detection of the focus of contamination, the identification of the organism and its eradication. It has being found that bacterial contamination of the genus Xanthomonas was the culprit of the contamination. Following multiple trials using proper aseptic techniques and controlled environmental conditions, clones of the available mother plant were successfully grown free of contamination. The second objective was to expose plants to Cd\(^{+2}\). Plant clones were re-cultured in vitro in media doped with Cd\(^{+2}\). A control group of clones was set aside to establish a basis for comparison. Plants were tested for Cd\(^{+2}\) resistance. We have found that Juana survive in media up to 50 ppm Cd\(^{+2}\). The third objective was to quantify Cd\(^{+2}\) in culture media. It is assumed that the quantity of cadmium ions missing from the medium has sequestered by the plants. A modified procedure of Hach Colorimetric Dithizone Method was used. Juana proved to be an excellent phytoremediator, accumulating 60% of the Cd\(^{+2}\) added. Experiments to confirm these results are in progress. The experiment were performed using the atomic absorption spectroscopy.

CHED 787

Selective synthesis of ribose via the formose reaction under prebiotic conditions
Since the beginning of time, humankind has sought the answer to the question of why we are here. There have been many theories postulated, with one such school of thought being that self-replicating ribonucleic acid (RNA) is a precursor to life. One of the main structural components of RNA is the sugar ribose. The primary goal of this experimental work is to selectively synthesize ribose via the Butlerov (also known as formose) reaction by refluxing formaldehyde, an initiator, and base together. Examples of bases that are being used are calcium hydroxide, calcium oxide, and thiazolium salts. Additional bases that resemble minerals present during prebiotic earth will also be examined. To identify the products of the reaction, mixtures are being reduced and benzoylated before being characterized via high performance liquid chromatography. Additional analytical techniques of ultraviolet/visible absorption spectroscopy, thin layer chromatography, nuclear magnetic resonance spectroscopy, and electrospray ionization mass spectrometry are being employed to further determine the composition of the reaction products.

CHED 788

Impact of methanotrophy on methane gas hydrate dissolution rates

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Methane is a potent greenhouse gas with approximately 20 times the global warming potential of CO\(_2\). The largest reservoirs of methane reside in gas hydrates, located in deep ocean sediments and arctic permafrost. Gas hydrates are structures of lattice ice that trap gas molecules, primarily methane. These gas hydrates form under high pressure and low temperature conditions. Fluctuations in these parameters impact the stability and dissolution rates of hydrates. In addition to temperature and pressure, microbial activity has the potential to impact hydrate dissolution rates. Methanotrophs colonize the area surrounding gas hydrates in nature, and have the potential to oxidize the hydrate containing methane to carbon dioxide. This study explores this potential link between methanotrophs and methane dissolution in gas hydrates. Initial experiments determine the capacity of two species of methanotrophs, *Methylococcus capsulatus* and *Methylosinus trichosporium*, to grow under hydrate formation conditions. Growth of these cultures is monitored by measuring concentrations of methane and CO\(_2\) present in the culture headspace using gas chromatography. We hypothesize that cultures of these species will grow at a reduced rate under hydrate formation conditions. Once growth under hydrate formation conditions is established, further experiments will monitor changes in carbon stable isotopic composition in an inoculated high pressure chamber containing gas hydrate, using cavity ring-down spectroscopy. We hypothesize that the presence of methanotrophs will increase the carbon stable isotopic composition
in the pressure chamber over time. Results of these experiments could provide
evidence to suggest that methanotrophs help to mediate the release of methane from
gas hydrates through the conversion of released methane to CO$_2$.

CHED 789

Formic acid uptake on montmorillonite clay: An FTIR study

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Formic acid is one of the most abundant organic acids in our atmosphere and has been shown to interact with mineral aerosol surfaces. Chemical reactions on the surface of mineral aerosol can alter the atmospheric gas phase budget as well as the chemical reactivity, water adsorptive properties and the chemical composition of the mineral aerosol. We have studied the uptake of formic acid on montmorillonite clay as a model mineral dust aerosol. Fourier transform infrared (FT-IR) spectrometry equipped with a dual-transmission reaction cell was used to probe the condensed and gas phases simultaneously during exposure of the clay to formic acid. The gas phase formic acid was generated and diluted using a five channel flow system. Ion chromatography was used to quantify surface-adsorbed formate and gas phase formic acid exposed to the sample and collected using a denuder during formic acid exposure. Results suggest significant and efficient reactive uptake of formic acid on montmorillonite clay.

CHED 790

Exploring the mechanism for iron uptake by phytoplankton: A biomarker study

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Oceanic phytoplankton produces half of Earth’s primary production, and as such is critical in the carbon cycle. In shallower seas, upwelling of deeper nutrient-rich water fuels growth, but in deeper waters their limiting nutrient is often iron. Deposition of iron-containing mineral dust can often be the main source of limited micronutrients. However, much of the iron in such dust is locked away as biounavailable Fe$^{3+}$. Little is known of the mechanism of how phytoplankton reduces Fe$^{3+}$ to Fe$^{2+}$, or how it sequesters iron. This study aims to determine if this method involves a primary dust/protein complex; either secreted by the phytoplankton or contained on the cell membrane. Biomarker studies were conducted in which phytoplankton cultures were isolated from a mineral dust Fe source by a cellulose dialysis tube in iron-deficient environments. Colorimetric analyses of phytoplankton were conducted to quantify biomass in terms of the chlorophyll a concentration using the tri-chromatic method and UV-Vis spectroscopy. Growth rates were determined as a measure of colony efficacy.
Preliminary results suggest that a primary protein iron complex is not necessary for the sequestration of iron from the separated iron containing dust. Siderophore action is suspected.

CHED 791

Water adsorption on montmorillonite clays

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The study of water adsorption on clay minerals is fundamental to soil science and can be applied to the physiochemical effects of mineral dust aerosol in the earth’s atmosphere. We have studied water adsorption as a function of relative humidity (RH) on three montmorillonite clays originating from different sources, including Texas (STx-1b), Arizona (SAz-1) and Wyoming (SWy-2). The montmorillonite samples were characterized by BET surface area analysis and particle size scanning electron microscopy. Water adsorption was monitored and quantified using horizontal attenuated total reflectance Fourier transform infrared (HATR-FTIR) spectroscopy equipped with a flow cell. Water content was determined using Beer’s law and optical constants for bulk water. BET type II adsorption isotherms show that the samples all achieve monolayer (ML) coverage at less than 20% RH. Experimental results indicate that, of the three tested clays, STx-1b contains the highest percent by mass of adsorbed water (~60% water by mass at 80% RH). It was also determined that, while higher BET surface area is consistent with higher adsorbed water contents, the primary exchangeable cation also appears to be an important factor. Upon normalizing the water contents to the BET surface area, we found that the two clays with the same primary exchangeable cation (Ca$^{2+}$) had similar water contents but the clay with the more hydratable exchangeable cation (Na$^+$) had higher water contents than those with less hydratable cations at RH values greater than 50%. At these RH values, the water had already formed a complete interior layer and had access to the exchangeable cations.

CHED 792

Influence of a metal oxide surface on ligand exchange reactions between strong chelating agents

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Chelating agents are employed by microorganisms and plants and in various human industries to bind metal ions and control free metal ion concentrations. The presence of chelating agents in the environment influences the distribution of metal species. One process affected is the exchange of the metal ion between chelating agents by a ligand exchange reaction. Our research examines how a surface, such as rutile titanium
dioxide (TiO\textsubscript{2}), influences the exchange of nickel between CDTA and EDTA, two common chelating agents. By examining these exchange reactions using capillary electrophoresis (CE) we hope to understand the role of surfaces in the exchange mechanism. As a first step to understanding the mechanism we have measured the extents of adsorption of Ni, CDTA, EDTA, NiCDTA and NiEDTA in rutile suspensions at varying pH using CE and Atomic Absorption Spectroscopy.

CHED 793

Influence of pH on ligand exchange rate with phosphonate-containing chelating agents

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The geochemical speciation of transition metals and chelating agents ultimately determines bioavailability, solubility, and the transport of nutrient or cytotoxic metals. There is wide use of phosphonate-containing chelating agents as herbicides, corrosion inhibitors, and detergent builders. Their presence in the environment necessitates a geochemical understanding of their behavior. Our research focuses on determining the reaction kinetics of ligand exchange reactions involving phosphonate-containing chelating agents and nickel. Capillary electrophoresis with ultraviolet spectrophotometric detection was used to monitor nickel(II) cyclohexaneethylenediaminetetraacetate (NiCDTA) production following the addition of CDTA to N,N-bis(phosphonomethyl)glycinenickel(II) (NiBPMG) solution. Initial rates were determined over a pH range and at varying chelating agent concentrations. A pathway for the ligand exchange reaction is proposed.

CHED 794

Sediment and water analysis of a glacially formed lake

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Mud Lake is a kettle lake, a remnant of the last glaciation, sitting on the top of a hill at approximately 1800 ft elevation in the Robert V. Riddell State Park near Davenport, NY. The lake is surrounded by a bog and no fish live in the lake. The only known water input to the lake is meteoric water and the only outlet is of anthropogenic origin. The bedrock is mainly sandstone and siltstone with some interbedded shale providing low acid buffering capacity. The goals of this study are to determine the inorganic geochemical properties of the lake water and surrounding sediment. Water samples were collected along a North-South cross-section of the lake at three depths and five locations.
Temperature, dissolved oxygen, pH and total dissolved solids were measured on site using a handheld multi-probe. Cation and anion concentrations were determined using inductively coupled plasma optical emission spectrometry and ion chromatography, respectively. Sediment core samples were collected using a split core sampler when the lake was still frozen. Sediment samples were analyzed for particle size distribution, mineralogical make up using XRD, and extractable anion and cation concentrations using UV-vis spectrometry and atomic absorption spectrometry, respectively. Water temperature decreases to 10 °C by 2.5 m depth and remains constant to maximum depth. Dissolved oxygen concentrations decrease rapidly, reaching nearly zero mg/L by 1.5 m depth. The pH values are between 4.2 and 5.3. Low values of the total dissolved solids, 12-18 mg/L, are consistent with the low cation and anion concentrations found in the lake water. Nitrate and sulfate are the dominant anions reaching 1.2 and 2.8 mg/L concentrations at the surface and decrease to 0.6 and 1.6 mg/L at the bottom of the lake, respectively. Chloride is below 1 mg/L in all samples, but it increases with depth. Calcium, sodium and magnesium are present below 1 mg/L concentrations and other metals are below 0.2 mg/L for all samples. The low amount of dissolved species support that the lake’s only water input comes from meteoric water and weathering processes of the surrounding bedrock and sediment only add small quantities of cations and anions to the water. Further investigation of the sediment can shed light on chemical processes between the lake water and the sediment, and provide additional information about sources of the chemical components of the lake water.

CHED 795

Southeastern Massachusetts student network for biodiesel research and education

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The small scale production of biodiesel fuel from waste vegetable oil (WVO) has been a popular activity for sustainability education in colleges and high schools. However, the full educational impact has not been realized due to inherent safety issues and inefficiency of the overall process. An interdisciplinary group of Bridgewater State University (BSU) students has designed, constructed and tested a bench top processor to support student research on improving the efficiency of WVO conversion into biodiesel. The optimum system design is cost effective, constructed from available materials, has integrated safety features, and is adaptable to testing a variety of experimental parameters. The project team has applied sustainability and green chemistry principles to identify priority problems leading to poor efficiency for converting WVO into biodiesel, developed specific research questions to address these problems, and proposed solutions that are laboratory testable. We are currently developing a Biodiesel Research and Education Network with community college and high school students. Students in the Network will submit research proposals to use the biodiesel
processor, thereby introducing a research-based learning component into the curriculum focused on applying sustainability and green chemistry principles.

CHED 796

Series of meso-tetrasubstituted porphyrins synthesized using mechanochemistry

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Porphyrins are useful molecules, not only as model compounds for biological systems, but also for their demonstrated catalytic, optical, and magnetic properties. Currently, the protocols for synthesizing and purifying porphyrins require a large amount of solvents which are toxic to the environment, and still yield only a small amount of product. However, it is possible to eliminate the solvent used for the cyclization step of porphyrin synthesis via mechanochemistry. Using the method of ball-mill grinding an equimolar amount of pyrrole and an aldehyde in the presence of an acid catalyst followed by oxidation of the intermediate yields an amount of tetraphenylporphyrin similar to amounts obtained through traditional synthesis. UV-Vis spectroscopy and $^1$H Nuclear Magnetic Resonance spectroscopy have been used to confirm the yields and purity of synthesized porphyrins. Through the use of mechanochemical synthetic protocol, it was possible to isolate yields and characterize a series of tetra-aryl and tetra-alkyl-substituted porphyrins, including some that are usually difficult to obtain from in-solvent synthesis. This study shows that applying mechanochemistry can provide access to porphyrins in yields as good as or better than those obtained in solution without need for solvent in the cyclization step.

CHED 797

Entrainment sublimation for purification of mechanochemically-synthesized porphyrins

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Mechanochemistry, or chemistry by grinding of reagents, is becoming increasingly prevalent in organic chemistry synthesis. Mechanochemistry can allow the solvent-free production and purification of compounds with fewer waste products and less cost than traditional solvent chemistry. This makes mechanochemistry an ideal approach for new synthetic protocols for porphyrins. As a model reaction, benzaldehyde and pyrrole are ball-milled in the presence of an acid catalyst for ten minutes. This produces a cyclized precursor to a porphyrin, which is then oxidized to produce tetraphenylporphyrin (TPP) along with a number of byproducts. Porphyrins are usually isolated from solution-synthesis mixtures by column chromatography. This research focuses on purifying TPP by separating it from the mechanochemical reaction mixture via entrainment sublimation. During this processes, a nitrogen carrier gas passes over the sample in a
Pyrex processing tube while being heated by a tube furnace. TPP is sublimed away from the impurities and subsequently deposited in a cooler area of the tube. Since TPP sublimes at around 400 °C, this process has been carried out at various temperatures near this point with various nitrogen gas flow rates. Also, different aldehydes have been tested and used to form porphyrins with different R-groups attached to the methine bridges. The highest pure, isolated yield we have obtained is 6.4%, using 2-chlorobenzaldehyde as a starting material. The conditions will continue to be optimized for various aldehydes in an attempt to raise yields to levels that match or surpass traditional solvent-chromatography yields of about 30%.

CHED 798

Effects of halide salt hydrates on isomerization of glucose to fructose

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With rapidly growing attention on lignocellulosic biomass utilization, various technologies for converting carbohydrates in the biomass into valuable products have been investigated. Among biomass sourced carbohydrates, glucose exists abundantly in nature in both cellulose and starch, highlighting it as an important renewable resource. Fructose is an isomer of glucose. It is widely used as a sweetener in food and beverage industries. In addition, fructose is an important intermediate in the glucose conversion to furan-based chemicals, which can be further converted to fine chemicals, pharmaceuticals, biofuels, and biopolymers. Therefore, it has drawn growing interests of many researchers how to efficiently isomerize glucose to fructose. This study is to develop a process to isomerize glucose to fructose in molten salt hydrates. The effects of different halide salts and reaction conditions (salt concentration, temperature, reaction time, and pH) on isomerization of glucose to fructose in the molten halide salt hydrates were investigated. Reaction kinetics and mechanism were also studied. Other possible glucose isomers such as mannose were monitored as well to observe the side-reactions during the process.

CHED 799

Plasticizing sulfur with limonene: A functional material synthesized entirely from industrial waste

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Polymers are ubiquitous in everyday life yet most common polymers—plastics, rubber, adhesives, and coatings—are derived from non-renewable feedstocks. To ensure a sustainable polymer future, alternative monomer feedstocks need to be investigated. Here we report the reaction between two industrial waste products: limonene and sulfur.
Limonene—found in citrus zest—is currently produced on the order of 70,000 tons annually as a byproduct of the citrus industry. Sulfur is a by-product of the petroleum industry and is produced on the order of 60 million tons. In this presentation, we report the use of limonene and sulfur as co-monomers in the synthesis of a novel polysulfide that can be processed into coatings and various molds (Figure 1). The synthesis requires no exogenous regents or solvents and is therefore highly atom economical. Prospects in water remediation and removal of toxic metals through binding to the polysulfide will also be presented.

![Industrial waste to useful polymer](image1)

**Figure 1**

**CHED 800**

**Malonic acid as a green alternative to formaldehyde in cell fixation**

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Formaldehyde is the main method for fixing cells prior to their usage in immunocytochemistry. In order to create the cross linkages through proteins, formaldehyde undergoes a mannich reaction in which the formaldehyde forms a methylene bridge between the amine group of two amino acids within the cell. The crosslinking of the proteins causes the cell to hold up stronger to preservation, allowing for the proper binding of fluorochrome conjugated antibodies for fluorescent imaging. Formaldehyde is also a known carcinogen as classified by the National Cancer Institute. Malonic acid, a green, plant based water soluble and relatively inexpensive polycarboxylic acid, has been shown to undergo the mannich reaction as well in the cross-linking of proteins. Using this greener compound, we hope to cross-link proteins inside the cell and compare the fluorescent images of paraformaldehyde fixed cells versus malonic acid fixed cells to see malonic acid is a greener alternative.

**CHED 801**
Oxidation of anthracene catalyzed by a recyclable vanadium(IV) oxide complex using hydrogen peroxide in an aqueous biphasic medium

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Anthraquinone is an important and widely used chemical. It is used as a raw material for the production of vat dyes, as a seed dressing, pesticide and an additive in the chemical alkaline pulp processes in the pulp and paper industry. One of the methods used for the production of anthraquinone is the oxidation of anthracene. This process involves extreme reaction conditions and use of hazardous reagents such as concentrated HNO₃ or chromic acid (a hexavalent chromium compound that is carcinogenic). Development of a greener oxidation of anthracene to anthraquinone is therefore of great interest. The simple VO(acac)₂ complex has been studied as catalyst for the oxidation of anthracene to anthraquinone in acetyl acetate using the green oxidant, hydrogen peroxide. The resultant catalytic mixture is biphasic. This aqueous biphasic medium provides the possibility to easily recover and reuse the catalyst, an aspect of great importance to green chemistry. Therefore, in this study, we have attempted to determine which layer, aqueous or organic, retains the catalyst and how efficient the catalyst can be recovered and recycled. In addition to results on the robustness of the catalyst, we will present data on the nature of the catalytically active species and the effect of pH on the catalysis.

CHED 802
Vacuum distillation via solar irradiation

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Traditionally, vacuum distillation required electricity for heating the distilling flask and running the vacuum pump. We have done vacuum distillation using PV panels to run the vacuum pump and a parabolic reflector to heat the distillation flask via solar irradiation. Several liquids have been vacuumed distilled completely off grid. The procedure and results will be discussed.

CHED 803
Further progress with Claisen condensations via solar irradiation

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Traditionally, the Claisen condensation is used to make beta-keto esters by reacting an ester with another ester using a strong base as catalyst. The reaction is usually heated
by using gas or electricity as the heat source. We will report our efforts to run Claisen condensations using solar irradiation as the thermal heat source.

CHED 804

Further progress with Fisher esterification via solar irradiation

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Traditionally, Fisher esterification involves reacting an acid with an alcohol to give an ester and water. This is often done with an acid catalyst and with electric or gas heat as the source of thermal energy. Our current work continues to exploit the sun as a source of thermal energy. Various esters have been prepared and the reactions and yields will be discussed.

CHED 805

Preparation of tetraphenylporphyrins via solar irradiation

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Several tetraphenylporphyrins have been synthesized via solar irradiation. The thermal heat source is a parabolic reflector previously published by our laboratory. Comparison of yields to conventional methods and solar irradiation yields will be discussed.

CHED 806

Research to develop a more efficient reflux process for methanol capture in biodiesel synthesis by applying green chemistry principles

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“Reflux” is an experimental technique in organic chemistry where a water-cooled condenser is used to cool, condense and recover solvent vapor from heated reactions. This process requires a constant source of cold water that ends up going down the drain, and is not efficient or sustainable. Our research on improving the efficiency of biodiesel synthesis requires heating vegetable oil with methanol for two hours at temperatures of 60-70 °C. The boiling point of methanol is 64 °C, resulting in wasteful loss due to evaporation. We compensate for this loss by using an excess amount of this flammable solvent, or use a constant flow of cold water for at least two hours. The goal of this research project is to apply Green Chemistry principles to improve reflux efficiency, reduce the amount of methanol to stoichiometric amounts, and reduce or eliminate the need for a constant flow of cold water. To accomplish this goal we
explored the use of static liquid reflux condensers to make the process more efficient, less costly, and more sustainable. We have explored a series of alternative "static" coolants that are sealed into different reflux condensers. Our choice of static liquids was made based on their heat capacities: water, ethylene glycol, and glycerol, with "air" serving as our coolant control. We also investigated different types of reflux condensers (Liebig, Allihn, Graham and air condenser), and will report our results in making the methanol reflux process less wasteful and more sustainable for the large-scale synthesis of biodiesel.

CHED 807

Development of green chemistry metrics to assess improvements to the efficiency in the synthesis of biodiesel from waste vegetable oil

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Green chemistry is a relatively new concept, but has gained significant attention in recent years. The main goal of green chemistry is to reduce or eliminate waste and improve overall safety and efficiency of chemical processes. A significant challenge is how we define the "greenness" and how to directly compare processes based on that definition. This research was focused on developing a system for analyzing green chemistry metrics. The proposed metrics will grade a chemical process based on: yield, atom economy, scale of reaction, environmental impact factor, time, cost, reaction mass efficiency, hazardousness, analysis of product, and renewability of reagents. The process will be graded on every aspect mentioned and can be directly compared to alternatives based on scores given. If a process fails on any point, it will fail the assessment entirely. This green chemistry metrics analysis system is being designed for use in a biodiesel project for the EPA P3 competition, but will be applicable to a wide variety of chemical processes.

CHED 808

Applying green chemistry principles in the synthesis of oxindole-3-acetic acid: The initial intermediate in the bromination of indole-3-acetic acid to 3-bromoxindole-3-acetic acid

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The goals of green chemistry are to eliminate the production of hazardous materials during chemical synthesis and to improve the overall efficiency of chemical reactions. We are studying the bromination of indole-3-acetic acid (IAA) to 3-bromoxindole-3-acetic acid (BOAA), a reaction that suffers from poor atom economy and low percent yield. NMR analysis has revealed that IAA bromination is a two-step process. Poor regioselectivity in addition of the first equivalent of electrophilic bromine is the critical
step, producing a mixture of oxindole products responsible for the poor overall reaction efficiency. We have found that oxindole-3-acetic acid (OAA) is the initial intermediate formed in the bromination of IAA, and this research was focused at optimizing the synthesis and isolation of OAA. Synthesis of OAA was accomplished using one equivalent of N-bromosuccinimide, and the products characterized using NMR spectrometry. We will report on how changing different reaction parameters effects the yield, atom economy and E-factor for OAA synthesis, including temperature, reaction time, stoichiometry, solvent, and the use of amides and amidines as Lewis base catalysts.

CHED 809

Synthesis of glucosamine-based single chain nonionic and cationic surfactants

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Glucosamine, a carbohydrate derived from chitin, shows promise as a natural resource for the synthesis of glycolipid surfactants. Glucosamine has not been thoroughly explored as the hydrophilic basis of glycolipid surfactants but its structure makes it particularly interesting for use as a quaternary ammonium cationic surfactant. The synthesis of surfactants based on glucosamine requires i) protection of the sugar hydroxyl and amino groups, ii) attachment of a lipid chain (which can also be derived from renewable resources) at the anomeric carbon through O-glycosylation, and iii) deprotection of the hydroxyl groups. Conditions for the synthesis of these surfactants were chosen to minimize environmental impact (i.e., greener solvents, reactions at ambient temperature, etc.) Protection of the hydroxyl and amino groups of glucosamine has been completed and the glycosylation step of the protected sugar has been optimized. This nonionic amino glucoside is then converted into a quaternary ammonium cationic surfactant through methylation. The critical micelle concentration and average aggregate size for both the nonionic and cationic surfactants were determined through surface tensionmetry and dynamic light scattering, respectively. This work aims to establish a framework for a more sustainable, cost-effective and environmentally friendly synthetic method for these single-chain glycolipid surfactants, thereby, producing products with the potential to compete with surfactants derived from petroleum based sources.

CHED 810

Endo/exo thermal isomerization of a green Diels-Alder adduct

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Green chemistry topics are important additions to subjects normally offered at any level of chemistry education. As part of a continuing effort to further green the organic chemistry laboratory curriculum, aqueous and solventless Diels-Alder reactions between 2-furfuryl alcohol and maleimide were developed. This resulted in good yields of endo and exo 3a,4,7,7a-tetrahydro-4-(hydroxymethyl)-4,7-epoxy-1H-isooindole-1,3(2H)-dione at room temperature and atmospheric pressure in the hands of students during a single four-hour laboratory period. Attempts to increase the reaction rates by heating above room temperature increased the exo:endo ratios significantly. It was then discovered that heating pure endo isomer yields a mixture of both endo and exo isomers, where the isomerization yields predominately the exo isomer.

CHED 811

Design of experiments approach to optimize the yield of 1-(4-vinylbenzyl) thymine

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The optimization of the synthesis of 1-(4-vinylbenzyl) thymine (VBT) was studied using a design of experiments (DOE) approach. VBT, a bio-inspired molecule, shows promise in a variety of applications, including as a component of a polymer that can be used as a greener photoresist. When copolymerized with charged monomers, the resulting water soluble VBT copolymers can become insoluble upon UV irradiation. The average reported yield of VBT is less than 50%, resulting in wasted reagents, materials, and energy. A DOE approach is an economical, green way to analyze the effect of many factors on the yield using the minimum number of experiments possible. A fractional factorial screening experiment was performed, investigating the significance of the length of the reaction, the temperature of the reaction, the ratio of reagents, the cation of thyminate salt, the addition of water, and the amount of solvent used for the VBT synthesis. For each run, a Microwave Accelerated Reaction System was used to synthesize VBT. Automated flash column chromatography was used to purify the product, and the yield was determined using UV-Vis analysis. Through the fractional factorial design, the time, temperature, ratio, and amount of solvent were found to be significant. The subsequent full-factorial design further investigated factors and the interactions of factors and suggested that the interaction between time and temperature was significant. The optimized time and temperature given these conditions for the synthesis of VBT will be determined through a central composite design.

CHED 812

Interactions of partially green double reduced gold nanoparticles with lead

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The use of plant extracts as reducing agents to prepare nanomaterials widens the opportunities to explore nature as a resource for nanotechnology novelties. The synthesis of gold nanoparticles has been carried out using plant extracts from leaflets of *Leucaena leucocephala* (Lam.) de Witt. together with sodium citrate as reducing agents. The prepared nanoparticles were characterized using UV spectroscopy for determine the optical properties and Dynamic Light Scattering, DLS to estimate the size. The UV-Vis results show the characteristic gold plasmon signal at 531 nm, and an additional shoulder at 624nm. The diameters obtained, according to DLS were estimated between 60-80 nm. Additionally, the optical properties of the obtained gold nanoparticles were employed as a sensing platform to detect different concentrations of lead in aqueous solutions. The UV-Vis spectroscopy results, showed a particular shoulder displacement from 624 nm to 650 nm indicating an aggregation tendency of the gold nanoparticles because of the electrostatic repulsive interaction with the Pb$^{2+}$ ions in the solution. A linear correlation of the wavelength displacement Vs Pb$^{2+}$ concentration was obtained. These results indicate the potential use of partial green nanoparticles to identify heavy metal in aqueous solutions.

**CHED 813**

Green synthesis of silver nanoparticles using extracts from *Leucaena leucocephala* (Lam.) de Witt. leaflets

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Green synthesis of nanomaterials is strategic to enhance the use of nanoparticles in environmental related processes. The chemistry profile of *Leucaena leucocephala*, a worldwide distributed mimosoid legume in tropical and subtropical regions of the world, corresponds to the allelopathic responses of this plant in nature. The leaflets plant collected in the southern region of PR were used to prepare an extract which posteriorly was employed as a reducing agent to synthesize silver nanoparticles. Additionally, a comparative analysis of single reduction using *Leucaena leucocephala* with and without ethylene glycol (EG) was performed. The obtained nanoparticles were characterized with UV spectroscopy and a Dynamic Light Scattering to determine their sizes. The UV-Vis spectrum presented the characteristic plasmon signal for silver at 415 nm, and the average diameter for green nanoparticles was estimated at 65.4 nm for the nanoparticles obtained used only the plant extract and 86.4 nm for those nanoparticles obtained using ethylene glycol. Additionally, stability studies were carried out by monitoring periodically the size of the nanoparticles for both types of synthesis, plant extract and ethylene glycol. This study confirmed that the silver nanoparticles obtained using the leaflets extracts alone remained stable for more than one month rather those
obtained using EG. These results indicate the potential of allelopathic substances such as mimosine to produce highly stabilized green nanoparticles.

CHED 814

Cross-linking and surface functionalization of polycarbonate films using thiol-ene click chemistry

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As fossil fuel sources diminish, it becomes more pertinent to seek out renewable and sustainable methodologies in both industrial and research environments – particularly in high-demand fields such as biomaterials. Combining green epoxide - CO₂ coupling reactions with highly efficient techniques such as thiol-ene click reactions, it is feasible that biodegradable and functional materials can be made through green chemistry methods. Propylene oxide, allyl glycidyl ether, and carbon dioxide were polymerized and then cross-linked to various densities using thiol-ene chemistry. Fourier Transform Raman spectroscopy confirmed the cross-linkage of polymers. Further, this research sought to functionalize the remaining olefin groups by thiol-ene reactions with various thiols in order to provide functional pendant groups for multiple potential uses. Due to unforeseen technical issues, the success of functionalization remains undetermined; therefore, further tests on this step must be conducted. If successful, this route may become a potential green method for films that could be used as biomaterials for drug delivery systems by attachment of biologically active molecules to functional pendant groups.

CHED 815

Chloride retention in biomass with the addition of lime and dolomite
This research investigated potential solutions to issues plaguing biomass gasification, including the formation of corrosive hydrochloric acid and slag deposits. Previous work has shown that chloride content is directly related to hydrochloric acid production and slag accumulation. This project studied the effectiveness of two additives to the biomass fuel - dolomite and lime - and their ability to retain chloride that would otherwise be freed to form hydrochloric acid. In an analysis that tested chloride content of corn and wood biomass before and after ashing, it was found that corn stover naturally retains about three fourths of its relatively high initial chloride content in the ash. When added at 4% by mass, both dolomite and lime were able to retain 100% of the chloride within standard error for the corn stover. Wood samples were found to naturally retain a third of the very low amount of chloride present in the ground sample, and that dolomite and lime were again able to retain 100% of chloride within standard error. The results and conclusions for wood were weakened by the low number of samples and low initial chloride content. This research provides evidence for a potential method for the drastic reduction of hydrochloric acid production during gasification and demands further exploration of dolomite and lime additives to biomass fuels.

CHED 816

Investigation of thiosemicarbazone ligands in “green” palladium catalyzed Suzuki cross-coupling reactions

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Thiosemicarbazones are versatile ligand species and their associated metal complexes have been shown to effectively catalyze a variety of reactions. This research reports the synthesis of a library of novel tridentate [O, N, S] thiosemicarbazone ligands and their associated palladium(II) complexes which were characterized by X-ray crystallography and NMR spectroscopy. These metal complexes were investigated as catalysts in the Suzuki cross-coupling reactions of aryl boronic acids with aryl halides to form biaryl products under “green” reaction conditions (aqueous solvents at room temperature). An examination into the effect of varying ligand structure on the palladium catalyst during cross-coupling reactions will be discussed.
CHED 817

Discovery of a new copper bismuth oxide material for the conversion of sunlight into a solar fuel

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The development of novel combinations of mixed metal oxides to produce a storable chemical fuel from sunlight in photoelectrochemical cells (PECs) is reported. A combinatorial approach is used for the preparation of a wide range of materials by spray pyrolysis to discover compositions able to generate a photocurrent. A copper bismuth oxide based photocatalyst was discovered and the composition, thickness, and deposition order of the metal solutions were optimized. The films were characterized using I-V curves, photoaction spectra, and absorbance spectra in order to provide information about the film’s electrochemical properties and absorption capabilities. The films were also analyzed by SEM, XRD, and an electron microprobe to confirm the crystal structure, and to identify the specific elemental composition and thickness of the film.

CHED 818

Mechanochemical synthesis of biologically relevant porphyrin targets

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Solvent-free syntheses of organic compounds are of increasing prevalence due to their “greener” aspect when compared to solvent-based synthesis. The success of solvent-free synthesis has been shown in the past with the production of tetraphenylporphyrin (TPP) and other meso-substituted porphyrins with the use of mechanochemistry, resulting in significant yields. This work presents our progress towards solvent-free synthesis of three porphyrin targets; porphine, bis-pocket porphyrin and octaethyl porphyrin (OEP) applying mechanochemical techniques. Each of our targets is relevant as a model compound for biological studies and is synthesized in-solvent giving very low yields (Porphine <10%; bis-pocket porphyrin 1%) or in very high-dilution conditions.
to give moderate yields (300L benzene for 10g OEP – 52% yield). We are investigating
mechanochemical synthesis of these three porphyrin targets. Isolated yields and green
chemistry metrics for the mechanochemical synthesis will be reported. These targets
are characterized using UV-Vis Spectroscopy and ¹H Nuclear Magnetic Resonance
Spectroscopy to verify the presence and yield, of the porphyrin molecule.

CHED 819

Conversion of ethanol to gasoline over zeolite H-ZSM-5 catalyst

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The research examined the process of converting ethanol to gasoline using a zeolite H-
ZSM-5 catalyst under different conditions. The variables tested were temperature,
catalyst composition, and weight hourly space velocity (WHSV). Findings suggested
that lower SiO2/Al2O3 ratios in the catalyst produced more paraffins whereas higher
ratios produce more olefins. The effect of temperature was dependent on WHSV and
catalyst composition. Similarly, the effect of WHSV depended on both temperature and
catalyst composition. Micro-GC and GC-MS analyses of the products indicated the
presence of hydrocarbons in the C2-C9 range. Since commercial gasoline consists of
hydrocarbons such as paraffins, olefins, and cycloalkanes in the C4-C10 range, the
results of the study are promising.

CHED 820

Hydrolysis of fungal chitin utilizing ionic liquids as a solvent and catalyst

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The depletion of petroleum has created a need for a renewable source of feedstock
chemicals for advanced materials and energy. Biopolymers have been shown to be a
potential source for these feedstock chemicals. Chitin is the second most abundant
biopolymer in the world and represents a promising source of renewable energy. A
derivative of glucose, chitin is a polymer with repeating N-acetylglucosamine units and
is a main component in the exoskeleton of crustaceans and the cell wall of fungi.
Mushrooms are a great source for chitin because they grow quickly and are abundant.
Chitin can be isolated from the cell walls of mushrooms by a series of chemical
treatments. The resulting chitin is of a lower crystallinity than that obtained from
crustaceans, making for easier processing with ionic liquids. It has been shown in the
past that ionic liquids possess the ability to dissolve a variety of polymers and
biopolymers, including chitin, and can be modified to contain an acid functionality. The
dissolution of chitin opens up the polymer matrix making it susceptible to hydrolysis
from acid catalysts such as a Bronsted acid functionalized ionic liquid. This research will focus on the use of acid functionalized ionic liquids for the hydrolysis of chitin isolated from various mushrooms such as *Trametes cubensis* and *Ganoderma lucidum*. This study will look at the effects of temperature and catalyst structure on the products obtained from the hydrolysis reaction. It will also compare the hydrolysis products from chitin sources: crustacean and fungi.

**CHED 821**

**Investigation of transesterification of canola oil using basic ion exchange resin**

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A transesterification reaction of canola oil and ethanol solvent was conducted using an anionic resin catalyst yielding ethyl ester based biodiesel. A catalyst column was prepared by packing a bed of anion-exchange resin in a chromatography column. A wash of ethoxide was prepared and percolated through the bed of resin to activate the resin with catalytic hydroxide groups. Upon washing away excess ethoxide, a continuous flow of oil and ethanol was run through the resin’s active sites yielding a conversion of oil to biodiesel without the need for extra filtration or washing. Upon reaction completion, a regeneration method can be used to prepare the resin for further transesterification reactions.

[Diagram of transesterification reaction]

**CHED 822**

**Mechanochemical reactions for green chemical synthesis**

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Polytetrafluoroethylene (PTFE) is known to charge negatively via contact electrification. This process appears to result from the formation of mechanoradicals and material transfer between PTFE and other materials. These materials tend to be solids, but we have shown previously that liquids—including many common solvents—also develop
electrostatic charge when flown through tubing made of PTFE. It is thus possible that chemical reactions may take place between PTFE and the liquid. This poster describes the chemical reaction of liquids that flow through PTFE tubing. We applied a measured amount of stress to the tubing to induce the formation of mechanoradicals in the PTFE. Based on quantum mechanical calculations, we have determined likely radicals that form from various liquid solvents. To these solvents, we added compounds known to react with these radicals and detected reaction products via GC-MS and NMR spectroscopy. Further work will conclude whether the stressed tubing promotes chemical reactions. This method may consume less energy and produce less chemical waste than thermochemical synthesis, and thus may lead to new green chemical synthetic techniques.

CHED 823

**New metric to evaluate sustainability in the undergraduate organic laboratory course**

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The Chemistry and Biochemistry Department at Carroll University will move into a new science facility in 2016. This gives the program an opportunity to evaluate and redesign the current curriculum. The project described here focused on the sustainability of the first course in the organic sequence. A metric was designed to score each lab on a series of factors: solvent use, chemical disposal, safety, and cost. Labs that did not comply with EPA standards of green chemistry were redesigned, or substituted, to make them “greener” while preserving the education objectives. The process that we designed for organic labs will be considered for other chemistry courses.

CHED 824

**Effects of cation structure on the acidity of Brønsted acid ionic liquids: A computational study**

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Ionic liquids stimulate interest in a variety of areas, from new solvents for reactions to new catalysts. One distinctive property of ionic liquids is their ability to attach different functional groups to the cation or anion in order to tailor the properties of the resulting ionic liquid. The idea of attaching various acid functional groups to one of the ions to create an acid functionalized ionic liquid has become prominent among researchers. The resulting ionic liquid is a non-volatile acid catalyst whose acidity can be controlled by structural changes to the cation group, i.e. changing from an imidazolium-based cation to a pyrrolidinium-based cation. Brønsted acid functionality is of particular interest
in the literature, especially the addition of a sulfonic acid group. These catalysts possess a unique acidity, which is very different from their molecular counterparts. To gain a better understanding of the effects structural changes have on the acid properties of the ionic liquid, a computational study using ab initio calculations was initiated. The effects of structural changes in imidazolium and pyrrolidinium cations were modeled and the changes in the acidity of the sulfonic acid group were observed. This study also investigated the phosphinic acid and boronic acid groups. The computational result will be further support by a rates of reaction study for a simple acid catalyzed organic reaction utilizing the catalysts will be performed.

CHED 825

Developing and applying new thin film combinatorial techniques for the discovery of new metal oxide semiconductors for the efficient photoelectrolysis of water

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One of the most promising sources of renewable energy is solar powered water photoelectrolysis in which energy from sunlight is stored within the chemical bonds of hydrogen (H2) and oxygen (O2). Recently, we have developed a new combinatorial metal oxide semiconductor thin film synthesis technique to aid in the discovery of new photoelectrolysis materials. The technique reproducibly generates high quality continuous gradient semiconductor films through the use of a screen-printing technique. This screen-printing technique is a cost and time-efficient method of creating a ternary phase diagrams that contain every possible three constituent alloy combination of the metal oxide. The metal oxide thin films are screened for potential photo-activity using the Solar Hydrogen Research Activity Kit (SHArK). The screen-printing technique and recently discovered photoelectrolysis semiconductors will be discussed.

CHED 826

Development of carbohydrate-based heterogeneous solid acid catalyst for biodiesel production

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A production of biodiesel utilizes a catalyst to efficiently generate product from an esterification reaction of a fatty acid. To study this esterification reaction, the reaction of oleic acid and methanol is used as a model due to being the primary fatty acid in a number of oilseed crops. This study investigates a starch-based catalyst due to its economic and environmental advantages, including being recyclable, reusable and relatively low cost.
The focus of this study is on the development of preparation procedures for high surface-area mesoporous cornstarch and the effects this material has on the model reaction. The preparation of mesoporous cornstarch is a four step process that is performed prior to sulfonating the material into a catalyst. Mesoporous materials have higher surface areas and pore volumes which allow for a higher acid density and easy access of reactants on the catalyst. Hypothetically, the higher acid density and minimum transport issues will lead to a more active catalyst and more efficient biodiesel production. BET analysis was used to verify that the cornstarch achieved mesoporous structure and an acid-base titration was performed to determine the acid density of the catalysts.

The reaction system employed consisted of the catalyst, oleic acid (10 mmol) and methanol (50-200 mmol) or ethanol (100 mmol) being inserted in a vial that was placed in an ultrasonic bath at 80°C for three hours. The findings of this study determined that a faster rate of reaction was achieved for the mesoporous catalyst as compared to a traditionally prepared catalyst. These findings were reinforced by quantitative acid density results to verify the increase in observed rate of reaction.

CHED 827

Aminebis(phenolate) complexes of palladium as catalysts for the Suzuki-Miyaura coupling reaction

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A series of new Pd complexes featuring aminebis(phenolate) ligands is reported. These complexes are evaluated for catalytic competency in the Suzuki-Miyaura coupling of aryl halides and aryl boronic acids.

CHED 828

Alternative to detection: Europium(III)-tetracycline species association with biological molecules

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The fundamental of nature is structure determines function; as such it is natural for biological molecules (biomolecules) with active functions to be dependent on structural characteristics such as chirality and anisotropy. Therefore, one field of research is to develop robust, sensitive, specific techniques capable of determining biomolecules’ proper structural characteristics and to a greater extent to be able to detect distinct molecules. A complete study of organic ligand Tetracycline (TC) chelated with luminescent
Europium(III) (Eu) associated with biological molecules in relation to pH and concentration was conducted using steady-state luminescence, time-resolved luminescence, and $^5\text{D}_0\rightarrow^7\text{F}_0$ europium excitation spectroscopy. Furthermore, we utilized circularly polarized luminescence (CPL) to monitor the change in chirality in relation to the TC-Eu complexes association with biological molecules. The resulted spectra exhibited explicit peaks of each TC-Eu species associated with biological molecules at various pH and concentration in time-resolved and steady-state luminescence that can be used as a “fingerprint” to (1) be used to identify unknown molecules similar to the usage of molecules’ distinct vibration modes in IR and NMR techniques to determine the unknown molecules’ structures. Also, CPL spectra of the TC-Eu probe associated with targeted molecules can be used to (2) give a more extensive view on chirality of targeted molecules.

CHED 829

**Triflimide activation of azaferrocene-boranes for hydroboration of simple alkenes**

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The ability to control regioselectivity in synthetic pathways is highly desirable in nanotechnology and pharmaceutical research. Asymmetric hydroboration of all alkene types has proven difficult to master. 1,1-disubstituted alkenes remain the most difficult alkene class over which to exert stereoselective control. Azaferrocene Lewis bases (L) are known to stabilize simple borenium cations such as [L-BH$_2$]$^+$. Previous work has shown azaferrocene-borenium cations are very active in the cyclic hydroboration of cyclooctadiene, suggesting they may prove successful in asymmetric hydroboration reactions.

Two azaferrocene-boranes, 1',2',3',4',5'-pentamethylazaferrocene-borane (PMAF-BH$_3$) and 1',2',3',4',5',1-hexamethylazaferrocene-borane (6MAF-BH$_3$), were converted to their respective borenium cations via hydride abstraction with triphenylmethylium (trityl cation) or trifluoromethanesulfonimide (triflimide) and mixed with two equivalents of either cyclooctene or alpha-methyl styrene in a stepwise fashion. Hydroboration products were characterized via proton ($^1$H), boron ($^{11}$B), and fluorine ($^{19}$F) nuclear magnetic resonance spectroscopy (NMR). Conversion of the hydroboration products to alcohols was achieved by overnight reaction with hydrogen peroxide. $^1$H NMR spectra of the isolated alcohol products revealed successful synthesis, but included significant quantities of impurities. Purification of these mixtures by column chromatography proved only partially successful. The chosen azaferrocene-borenium cations were successful in hydroboration, but further work must be carried out to further investigate their selectivity.

CHED 830

**Liquid sorption studies of Co$^{II}$-4,4'-bipyridine 1D chains and 2D square grid MOFs**
Metal organic frameworks (MOFs) are crystalline structures comprised of metal atoms connected by organic linkers, forming structures with connectivity ranging from 1D chains to 2D and 3D frameworks. The sorption properties of these porous materials are of interest because they have great potential for separating mixtures of small molecules and other MOF properties, e.g. magnetism, can be altered by sorbing guest molecules into the pores. Sorption studies were conducted on a 1D chain MOF and a 2D square grid MOF prepared from Co(NO$_3$)$_2$ and 4,4′-bipyridine (bpy) building blocks. The selectivity and rate of sorption of liquid guest molecules into the MOF pores was investigated.

CHED 831

Synthesis and characterization of 1-D ladder crystals grown in methanol

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A wide variety of metal organic frameworks (MOFs), such as the 2D bilayer, 1D ladder, and 3D brick wall, have been prepared from cobalt (II) nitrate and 4,4′-bipyridine using different solvent mixtures to grow crystals. Small changes in the nature of the solvent can have a substantial effect on the MOF structure. A 2D bilayer structure forms in ethanol, but while methanol has been used as a component of a solvent mixture that gives crystals, there have been no reports of crystals produced using only methanol as solvent. In this study we have synthesized and characterized 1D ladder MOFs from cobalt (II) nitrate and 4,4′-bipyridine using only methanol as the solvent.

CHED 832

Reaction of copper(II) chloride dihydrate with formamide

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The goal of this research is to identify the unknown products of a known reaction between transition metal copper(II) and formamide, which has been shown to produce 1,3,5-triazine and purine in prior studies. By dissolving copper (II) chloride dihydrate into acetonitrile it should be possible to vary the concentrations to make analysis of these unknown products possible. By identifying the additional products formed, further knowledge of the reaction’s mechanism and peptide bonding can be gathered for the previously identified polymers and newly identified products.
Synthesis and investigation of novel thiosemicarbazone ligands and their metal complexes

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Cisplatin is a metal containing compound that has been widely used as an anti-cancer agent since its discovery in 1960. Despite its success, some cancer cells have developed a resistance to the drug. The synthesis of novel metal containing complexes with similar biological activity is an active area of research. Thiosemicarbazones are a class of ligands whose metal complexes have been shown to have biological activity including anti-fungal, anti-bacterial, and anti-tumor properties. Recent research has reported the synthesis, cellular testing and DNA binding assays of thiosemicarbazone complexes with palladium and platinum. While these complexes have been shown to have anti-cancer activities similar to cisplatin, detailed mechanistic studies or structure-activity relationships have not been fully investigated. Here we report the modular synthesis and characterization of a series of novel thiosemicarbazone ligands and their palladium and platinum complexes. The palladium and platinum complexes exhibit a similar puckered square planar geometry but have different spectra by UV-vis spectroscopy.
Synthesis and characterization of a larger neutral macrocycle for transition and lanthanide(III) metal complexes

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o-Aminobenzaldehyde (oab) is known to self-condense under a variety of reaction conditions, including in the presence of metal ions. Different polymeric Schiff-base condensates are produced depending on the coordination preferences of a given metal ion, including the tetrameric ligand known as TAAB (tetrabenzo[b,f,j,n][l,5,9,13]tetraazacyclohexadecine). The objective of this research is to design an extended analogue of oab to give a larger self-condensate ligand to accommodate larger metal ions. Increasing the size of the macrocyclic ligand can potentially allow lanthanide(III) ion complexes to form. Lanthanides are highly paramagnetic, making macrocycle lanthanide complexes good candidates for contrast agents for magnetic resonance imaging (MRI).

The ligand precursor is formed in a six-step synthesis starting with the generation of the 8-nitroquinaldine from 1-nitroaniline and crotonaldehyde with phosphotungstic acid as a catalyst. The 8-nitroquinaldine is brominated at the aromatic methyl. Tribromonitroquinaldine is hydrolyzed with sulfuric acid to form the carboxylic acid. The final steps involve the reduction of the nitro group using hydrazine hydrate with zinc phthalocyanine as a catalyst, forming the amino acid, followed by reduction of the acid to an alcohol with lithium aluminum hydride and finally oxidation of the alcohol with manganese(IV) oxide to give 8-amino-2-quinolinaldehyde. The ligand is synthesized by Schiff-base self-condensation with three equivalents of 8-amino-2-quinolinealdehyde using a metal ion as a template. Progress toward the synthesis and characterization of the ligand precursor and the formation of a lanthanide complex will be presented.

CHED 835

Synthesis, characterization, and electrochemical properties of tris(3-isopropylpyrazolyl)borate nickel complexes

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An isopropyl substituted trispyrazolylborate ligand (Tp^iPr) was synthesized from sodium borohydride and 3-isopropylpyrazole using the melt method in a 65% yield. This Tp^iPr ligand was reacted in a 1:1 ratio with nickel nitrate or nickel chloride hexahydrate in methanol to generate Tp^iPrNiNO3 and Tp^iPrNiCl respectively in a good yield. These complexes were exposed to 5 eq. of NaX (X = Br⁻, I⁻, NCS⁻, and NO₂⁻) in methanol to generate, in good yields, the corresponding Tp^iPrNiX complex giving a series of complexes with varying metal environments. These complexes were characterized using ¹H-NMR spectroscopy, infrared spectroscopy, UV-visible spectroscopy and small
Results of NMR spectroscopy indicated paramagnetic behavior with peaks ranging from -15 to 85 ppm with the pyrazolyl hydrogen atoms being shifted the most downfield. The infrared spectra display a characteristic B-H stretch near 2500 cm\(^{-1}\), which is a higher energy than that of the free ligand. UV-visible spectroscopy indicated both \(d\) to \(d\) and charge transfer absorbances which varied greatly between the complexes. Small molecule X-ray analysis of Tp\(^{iPr}\)NiNCS revealed a bridging thiocyanate dimer in the solid state. Subsequent FTIR analysis, focusing on the thiocyanate ligand, suggested both monomer and dimer when dissolved in methylene chloride. Existence of a dimer supports the intermediate steric bulk of the isopropyl substituents on the ligand when compared to similar complexes with bulky \(t\)-butyl substituents that do not form dimers. The electrochemical properties of each complex were analyzed using cyclic voltammetry and the complexes exhibited similar voltammograms across the series in methylene chloride, which is surprising considering the difference in donor properties of the different \(X\) ligands. When the electrochemistry was performed in tetrahydrofuran, a coordinating solvent, the redox properties were more consistent with the donor properties of the \(X\) ligand.

CHED 836

Synthesis, characterization, and electrochemical properties of tris(3-\(t\)-butylpyrazolyl)borate copper complexes

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A \(t\)-butyl substituted trispyrazolylborate (Tp\(^{ibu}\)) was synthesized from sodium borohydride and 3-\(t\)-butylpyrazole using a melt method with a 59% yield. This Tp\(^{ibu}\) ligand was reacted with copper nitrate hemihydrate and copper chloride dihydrate to form Tp\(^{ibu}\)Cu(NO\(_3\)) (1) and Tp\(^{ibu}\)CuCl (2) complexes, respectively, in good yields. Addition of 5 eq. of NaX to complex 1 or 2 in methanol (\(X = \text{Br}^-\) and NO\(_2^-\)) resulted in the formation of the respective Tp\(^{ibu}\)CuX complex in yields ranging from 70 to 97% depending on the complex. The compounds were characterized using \(^1\)H-NMR, IR, and UV-vis spectroscopy. The NMR spectroscopy displayed paramagnetic behavior with resonances located in the range of -5 to 50 ppm with the pyrazole protons being the most shifted downfield. The IR spectra of the copper complexes exhibited B-H stretching frequencies at 2500 cm\(^{-1}\), which is higher energy than the corresponding stretch in the free ligand. The UV-vis spectra of the complexes contained a combination of \(d\)-\(d\) transitions and charge transfer bands depending on the complex. Attempts to grow X-ray diffraction quality crystals, by solvent evaporation, resulted in the decomposition of the complexes resulting from B-N bond cleavage in the ligand. The electrochemical properties of the complexes were determined using cyclic voltammetry. Each complex contained a Cu\(^{2+}/Cu^{1+}\) reduction wave with varying reversibility. The reduction potential trend was consistent with the donor properties of the unique \(X\) ligand in each complex. However, the differences in potential across the series are
larger than a similar series of nickel complexes. This suggests that the redox properties of the copper center are more sensitive to changes in ligand coordination in Tp systems.

CHED 837

Synthesis, characterization, and ion-binding studies of Ru(bpy)_3^{2+} macrocycle host complexes

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A series of ruthenium macrocycle polyamine complexes were synthesized and characterized by ^1H NMR spectroscopy and mass spectrometry. The macrocycle ligands were prepared by reacting 4,4’-diformyl-2,2'-bipyridine with the appropriate polyamine. The resulting ligands were coordinated to a ruthenium center using Ru(bpy)_2Cl_2 to yield the target tris-bipyridine host framework. These complexes were investigated as host molecules for alkaline earth cationic guests such as alkali, alkaline earth, and transition metals. Fluorescence spectroscopy titration experiments were used to investigate the binding affinities of the host complexes for the cations, as well as to investigate the effects that pH play in a host-guest system.

CHED 838

Complexation reactions of cerium (III) and cerium (IV) salts with amides

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The goal of this research is to determine the structure of products and the nature of the mechanism of the reactions of cerium (III) and cerium (IV) salts with amides (particularly formamide, acetamide, and benzamide). The cerium salts used for cerium (III) and cerium (IV) are respectively cerium (III) chloride and ceric ammonium nitrate. The following reactions have been performed with each cerium salt: 1) metal compound + sodium persulfate (oxidizer) + amide; 2) metal compound + amide; and 3) metal compound + phenylisocyanate. Additionally, hydrogen peroxide has been used as an oxidizer. The solvent in each reaction was acetonitrile. Each reaction occurred between a 24 hour to 120 hour period in order to insure precipitate formation that usually was accompanied by a color change. The reaction with phenylisocyanate was performed to give more indication as to the mechanism of the reaction since phenylisocyanate is predicted to be an intermediate. Infrared (IR) spectroscopy, GC-mass spectroscopy (GC-MS), high performance liquid chromatography, and Raman spectroscopy were all used to analyze the products. A goal of this research was to provide further understanding of the nature and behavior of lesser studied metal compounds such as
cerium. Future considerations are to involve other lesser studied metals such as molybdenum, vanadium, zinc, and possibly bismuth.

CHED 839

Synthesis and characterization of copper-thiosemicarbazone complexes: Interaction with DNA and anti-oxidant behavior

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A series of four copper complexes containing thiosemicarbazones ligands derived from 6-nitropiperonal were synthesized. The complexes were characterized by elemental analyses and spectroscopic methods. The complexes were investigated for the interaction with DNA via a number of methodologies. From competition experiments with ethidium bromide the complexes presented apparent binding constants in the range \((0.82 - 1.2) \times 10^4 \text{ M}^{-1}\) indicating that they are weak intercalators. This result is supported by viscosity studies for a representative member of the group. The interaction with DNA was also examined by electronic absorption titrations, gel electrophoresis (the complexes have exhibited a weak ability to uncoil pBR322 plasmid DNA under irradiation with 365 nm UV light) and cyclic voltammetry. The interaction of the complexes with human serum albumin was also examined by fluorescence spectrophotometry. The binding constants for these interactions were on the order of \(10^3 \text{ M}^{-1}\). Initial results of the interaction between the compounds and various proteins (studied by molecular modeling) will be presented. The results of the assays for the anti-oxidant behavior towards nitric oxide and diphenylpicrylhydrazyl are being also being reported.

CHED 840

Curcuminoids as ligands in zinc and vanadium complexes: Synthesis and biophysical reactivity

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A set of structurally diverse curcuminoids (CC) were synthesized by the reaction of 2,5-pentanediol with the appropriate aldehyde in the presence of tributylborate as a drying agent and n-butylamine as catalyst. The aldehydes used include 9-anthraldehyde, thiophene-2-carbaldehyde, ferrocenecarbaldehyde and indole-3-carbaldehyde. These curcuminoids were used as ligands in the synthesis of zinc and vanadium complexes best formulated as \(\text{Zn(CC)}_2\) and \(\text{VO(CC)}_2\) though there was some structural variation amongst the complexes. The complexes have been characterized by a variety of spectroscopic techniques and initial investigations of reactions with DNA have been carried out. A number of the complexes show a weak ability to uncoil pBR322 plasmid
DNA. Spectroscopic, viscometric, fluorescence, and electrochemical experiments suggest that the complexes interact with DNA via intercalation. For the Zn(dmabCC)₂, the binding constants are on the order of 10⁴ M⁻¹ (ΔH = 32.5 kJ) and for VO(phenCC)₂ it was 10⁵ M⁻¹ (ΔH = 40.6 kJ). On the other hand, the interaction, as measured by the binding constant, with human serum albumin is strong with binding constants on the order of 10⁶ M⁻¹.

CHED 841

New ethylene cross-bridged and side-bridged tetraazamacrocycles featuring acid and amide pendant arms and their transition metal complexes for oxidation catalysis

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Ethylene cross-bridged cyclam complexes of manganese and iron are mild oxidation catalysts that can react through a diverse range of oxidation mechanisms. We have embarked on a program of modifying the parent ligand by: (1) changing ring size, (2) adding pendant arms, and (3) exploring side-bridged derivatives. In this work, we introduce a series of cross- and side-bridged derivatives with acid and amide pendant arms. Smaller cyclen-based catalysts have shown similar reactivity to the original cyclam catalysts. The pendant arms are intended to modify the electronic properties of the metal complexes, perhaps leading to new and/or different oxidation reactivity. In this case, acid and amide pendant arms can also interact through hydrogen bonds with substrate and/or oxidant molecules, perhaps stabilizing reactive intermediates. Side-bridged derivatives are likely less kinetically stable than the original cross-bridged catalysts, but appear to have modified coordination geometries that may lead to new reactivities and may be stabilized by the additional pendant arm donors. All new ligands have been complexed to manganese, iron, cobalt, nickel, copper, and zinc. The synthesis and characterization of the ligands and the synthesis, electrochemistry, and other characterization of their complexes will be presented.

CHED 842

1,7-Dimethyl-1,4,7,10-tetraazacyclododecane complexes of Mn, Fe, Co, Ni, Cu, and Zn: Synthesis and characterization

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Tetraazamacrocycles have continued to accelerate in their importance as transition metal ligands for applications as diverse as catalysis, medical imaging, and environmental remediation in part due to their ability to make stable complexes with these metal ions. One important class of tetraazamacrocycles developed over the past two decades has been the ethylene cross-bridged tetraazamacrocycles, which form particularly stable transition metal complexes because of the rigidification of the bicyclic structure produced when bound to the metal ion. Once formed, loss of the ligand from the complex requires some flexibility for a nitrogen donor to dissociate from the metal ion, which is more difficult once the macrocycle is rigidified by the short ethylene cross-bridge. However, recent publications have hinted that simple alkylation of two non-adjacent nitrogens of a tetraazamacrocycle may yield similar results in terms of geometric control and kinetic stability as cross-bridging. In order to test this idea, and to provide "control" ligands for direct comparison between cross-bridged tetraazamacrocycles and their unbridged analogues, we have prepared the known unbridged ligand 1,7-dimethyl-1,4,7,10-tetraazacyclododecane and its Mn, Fe, Co, Ni, Cu, and Zn complexes for comparison to previously published ethylene cross-bridged analogue 4,10-dimethyl-1,4,7,10-tetraazabicyclo[5.5.2]tetradecane complexes with the same metal ions. The synthesis and characterization of these complexes and comparisons to their cross-bridged analogues will be presented.

CHED 843

Electrochemical stability of ruthenium-arene complexes

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A series of ruthenium-arene complexes with the general formulas \((\text{C}_6\text{H}_6)\text{RuCl}_2\text{L}\) and \((\text{C}_6\text{H}_6)\text{RuCl}_2\text{L}^+\) (\(\text{L} = \) phosphine- and pyridine-based ligands) have been studied electrochemically in order to determine the rate at which the arene ring is displaced when the metal is oxidized from Ru(II) to Ru(III) in the presence of a coordinating solvent. The reactions were followed using cyclic voltammetry, simulation software was used to determine the rate of arene ring displacement, and \(^1\text{H} \text{NMR}\) was used to analyze displacement reaction intermediates and products. The electrochemical properties of these compounds and the identification of possible intermediates in the displacement reaction will be presented, and the factors that affect the displacement of the arene ring in these complexes will be discussed.

CHED 844

Ion selective redox chemistry of a rhenium (I) complex using cyclic voltammetry

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A series of rhenium(I) complexes have been reported that selectively bind anions in solution. Anion binding was found to cause changes in the absorbance and luminescence properties of the compounds. This study extends these results to changes in the electrochemical properties of the compounds in solution, as measured using cyclic voltammetry. The goal of the work is to quantify electrochemical changes as a function of anion binding and to fabricate ion-selective electrodes using the Re complex bound within a polymer that adheres to the electrode surface. These ion sensitive redox couples held within a polymer matrix allow for electrochemical sensing of ions without addition of the bulk quantities of the Re complex to the solution.

CHED 845

Synthesis, NMR characterization, and x-ray crystal structure of quinoline-2-carboxaldehyde tert-butyl thiosemicarbazone: The [Pd(QCA-tBTSC)Cl] complex and MIC studies

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We have synthesized the quinoline-2-carboxaldehyde tert-butyl-thiosemicarbazone (QCA-tBTSC) ligand and characterized it via $^1$H NMR and $^{13}$C NMR spectroscopy, and we have also obtained the x-ray crystal structure of this ligand. This mono-anionic tridentate QCA-tBTSC ligand has been used to form a square planar metal complex with Pd$^{2+}$, using either potassium tetrachloropalladate(II) or dichlorobis(benzonitrile)palladium(II). This work will also show the NMR characterization of the d$^8$ Pd complex. We have performed anti-proliferative MIC (minimum inhibitory concentration) studies of the QCA-tBTSC ligand and the [Pd(QCA-tBTSC)Cl] complex using seven different microbes in order to determine their anti-microbial properties. The [Pd(QCA-tBTSC)Cl] complex is highly active against gram positive bacteria.

CHED 846

Comparison of a series of 2-acetylpyridine-thiosemicarbazone Cu(II) and Pd(II) metal complexes

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The copper complex of acetylpyridine methylthiosemicarbazone [Cu(APY-MTSC)Cl] has been shown to inhibit Topoisomerase IIa enzyme. To test the hypothesis that the palladium(II) and other Cu(II) complexes of the same ligand would also inhibit the enzyme due to the same structural geometry (square planar around the metal), a series of acetylpyridine thiosemicarbazone ligands, and their Cu(II) and Pd(II) metal complexes have been synthesized using different pathways and appropriately
characterized by NMR and other techniques. The minimum inhibitory concentrations of each compound was determined with four bacteria (Bacillus subtilis, Staphylococcus aureus, Escherichia coli, and Pseudomonas aeruginosa), two yeast (Candida albicans and Saccharomyces cerevisiae), and a mold (Aspergillus niger). The results show that the Pd(II) complexes have much the same high anti-proliferative microbial activity as the Cu(II) complexes.

CHED 847

Investigating bispyrrolidine based chiral C$_2$-symmetric tetridentate ligand

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Chiral C$_2$-symmetric ligands and metal complexes were synthesized. This type of chiral ligand is being investigated for applications in chiral sulfoxidations and dearomatization chemistry because the ligand creates a chiral environment through steric hindrances and bonding to the metal in a cis-α configuration that allow for enantioselective syntheses. Aromatics make an attractive building block for complex molecules, such as pharmaceuticals, due to their abundance, low costs, and many potential reactive sites. Chiral sulfoxides have applications in pharmaceuticals and chiral auxiliaries in stereoselective syntheses. [Ru(PDP)(DMSO)Cl]PF$_6$, [(Qnbp)W(CO)(NO)]PF$_6$, and their precursors have been synthesized. Compounds were characterized by $^1$H and $^{13}$C NMR spectroscopy and x-ray crystallography.

CHED 848

Quantitative determination of silver inhibition of halide accelerated aluminum corrosion

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The versatile properties of aluminum have established its extensive commercial and industrial roles. Aluminum forms a protective oxide layer when oxygen is present. Removing this oxide layer is the rate-determining step for aluminum corrosion, and soluble chloride is known to accelerate corrosion. The Cu(II) – Al redox reaction can be used as a model for studying the kinetics of aluminum corrosion. Halide acceleration of this reaction has been studied (Wei, Lee Chen 1994, Sobel and Cohen, 2010); halides do accelerate the Cu-Al redox displacement reaction. In this study aqueous copper(II) chloride was reacted with household aluminum foil at constant temperature. Hayes et al. (1989) studied the growth of silver halide clusters prior to formation of precipitate, and showed that silver ions can sequester halide without precipitate formation. To observe
the effects of silver(I) on the reaction rate, 0.10 M copper(II) sulfate was reacted with aluminum foil in 0.001 M silver(I) nitrate with varied chloride ion concentrations. Small amounts of silver(I) reversed halide acceleration of the Cu(II)-Al reaction. In the absence of chloride ion, the reaction was completely inhibited by Ag(I). The data suggests that sulfate anion is not a neutral actor, but rather has a positive effect on the reaction.

CHED 849

Metal – organic assemblies of meso – tetrasubstituted porphyrins

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Metal – organic polyhedra (MOPs) are 3 –D structures consisting of organic ligands as the edges or faces and metal ions as the corners, able to encapsulate molecules and be hosts to a myriad of chemical reactions. Meso – tetrasubstituted porphyrins are large, aromatic macrocycles shaped like squares with substituents at the corners suggesting they would be useful for forming the faces of MOPs. The goal of this research is to synthesize four meso – tetrasubstituted porphyrins which would be used to form porphyrin – walled MOPs. Tetrakis (3 – pyridyl) porphyrin (3PP), tetrakis (2 – pyridyl) porphyrin (2PP) and tetrakis (2, 3 – dimethoxy) porphyrin (2, 3 – diOMeP) have been synthesized and purified, and synthesis of tetrakis (3, 4 – dimethoxy) porphyrin (3, 4 – diOMeP) is underway. In the case of the latter two products, the methoxy groups will be removed to yield tetrakis (2, 3 – dihydroxy) porphyrin (2, 3 – diOHP) and tetrakis (3, 4 – dihydroxy) porphyrin (3, 4 – diOHP). These tetrasubstituted porphyrins were chosen because of their ability to act as exo-dentate ligands, meaning they can bind to a metal on the four “corners” of the porphyrin exterior. Several attempts at self – assembly of 3PP with metal salts have been made with varying metals, anions, reacting and precipitating solvents and reaction conditions. One result yielding crystals suitable for X – Ray crystallography was obtained and the structure will be presented. Although not an MOP, the structure shows promise for future isolation of porphyrin – walled MOPs.

CHED 850

Iodination and MWI cyanation of closo-dodecaborate(2-) and closo-1,2-dicarbadodecaborate

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Icosahedral boron clusters such as closo-dodecaborate(2-) (B_{12}H_{12}^{2–}) and closo-1,2-dicarbadodecaborate (C_{2}B_{10}H_{12}) are molecules whose derivatives show promise in pharmaceuticals, ionic liquids, liquid crystals, and other materials. However, before these molecules can be employed for practical applications, there must be easy and reliable methods of synthesis of their derivatives. Microwave-assisted reactions,
alongside conventional ones show promise in the efficient synthesis of new derivatives. Controlled iodination followed by MWI cyanation of each cluster is shown to produce new cyanated derivatives of B$_{12}$H$_{12}$$^{2-}$ and C$_2$B$_{10}$H$_{12}$. These compounds were characterized by $^{11}$B NMR, IR, and LC-MS. Details of the synthesis and characterization of these compounds will be discussed.

CHED 851

Investigations of the halogenation, radiohalogenation, and functionalization of CB9 carborane clusters

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Derivatives of carba-closo-decaborate(1-) carborane anion (closo-CB9) have potential uses in nuclear medicine, medical imaging, and other pharmaceutical applications. The carbon in the cluster can be functionalized by a variety of groups, making this site an ideal attachment point for proteins and other biomolecules. The boron vertices in CB9 readily undergo iodination to give highly iodinated species that have potential uses as X-ray contrast agents. This strategy could likewise be used with radiiodine or astatine-211 to give useful imaging agents or therapeutic compounds. The preparation of derivatized CB9 clusters and investigations of conditions for efficient halogenation of these clusters will be discussed.

CHED 852

Synthesis of new gold-isocyanide and acyclic diaminocarbene complexes for catalysis

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Metal-coordinated isocyanides are synthetically useful intermediates for carbene ligands, because they allow for the optimization of desired catalytic properties at electrophilic metals such as palladium and gold. Reacting metal-bound isocyanides with different amines can readily create a large library of catalysts that can be tested for various metal-catalyzed organic transformations. Two chiral isocyanides, racemic $\alpha$-methylbenzyl isocyanide and chiral (R)-(-)-1-(1-naphthyl)ethylisocyanide, were successfully synthesized and attached to gold. The newly synthesized gold-naphthyl isocyanide complex was discovered to be luminescent and was used to synthesize three new acyclic diaminocarbene (ADC) complexes using diisopropylamine, (+)-bis[(R)-1-phenylethyl]amine, and (-)-bis[(S)-1-phenylethyl]amine as the amine nucleophiles. Both enantiomers of the chiral amines were found to react with the (R)-enantiomer of the gold-naphthyl isocyanide complex to give two diastereomeric gold
ADC complexes. The three chiral ADC will be studied for their potential to create enantioselectivity in various organic catalytic reactions.

CHED 853

Copper-catalyzed triazole synthesis in the presence of halides

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Sodium halides were found to inhibit the copper-catalyzed azide-alkyne cycloaddition (CuAAC) in a model system. This presentation discusses the basis for this inhibition and experimental precautions that can be taken to enable the CuAAC when halides are present. Specifically, silver salts and various ligands can be used to outcompete the inhibitive binding of halides to the copper catalyst.

CHED 854

Mercury concentration in washed and unwashed leaves of differing plant species

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Atmospheric mercury contributes to the mercury content found within plant leaves through adsorption and/or absorption. One aspect of the current research is to better understand the relationship between atmospheric mercury which is absorbed into the leaf body and that which is adsorbed onto the leaf surface through the comparison of washed and unwashed leaf samples. Fourteen plants of varying species were observed over the growing season, collecting leaf samples once each month. For each plant type, one half of the leaves collected were left as is, while the other half were washed by sonicating for 1 min in 18MΩ pure water. The plants were dried at 40°C in an oven, homogenized using a mortar and pestle, and then analyzed to determine the mercury content of each sample. Overall, the difference between washed and unwashed samples ranged from 0.73% to 3.5%, with washed samples losing an average of 2.7% of the total leaf mercury. This indicates that the majority of the mercury is absorbed into the leaf tissue and not simply being deposited on the surface. The overall mercury concentrations and rates of accumulation varied widely among species and ranged from 2.04 μg/kg (Rhus trilobeta) to 29.92 μg/kg (Malus domestica). Of the fourteen plants studied, two groups (locus and crab apple) were monitored for within-species variations. The crab apple trees ranged from approximately 7.3 μg/kg to 27.4 μg/kg over all observations, with each of the three plants showing differing rates of mercury accumulation. The two locus trees, on the other hand, increased at similar rates while containing dissimilar concentrations. Possible causes of variations within plant species and among different species in accumulating atmospheric mercury will be discussed.
Designing novel electrodes of 3D porous V2O5:PANI films by colloidal particle lithography

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Hybrid electrodes of conductive polymers and inorganic materials are of great interest for use in Li ion batteries. Vanadium pentoxide (V\textsubscript{2}O\textsubscript{5}) and polyaniline (PANI) are attractive materials for use as hybrid cathodes for Li ion batteries due to their low-cost and ease of preparation. Additionally, V\textsubscript{2}O\textsubscript{5} has a high theoretical capacity and specific energy density; and PANI is environmentally stable and is rapidly converted between its insulator and conductor forms. However, crystalline V\textsubscript{2}O\textsubscript{5} suffers from volumetric expansion, low diffusivity and low conductivity; and PANI has slow transfer of dopant ions during charging and discharging. To overcome these weaknesses, V\textsubscript{2}O\textsubscript{5} and PANI were combined in a 3-D porous structure to facilitate Li ion diffusion and minimize the damage from volumetric expansion. A self-assembled monolayer of polystyrene microspheres was used as a template to fabricate highly ordered 3-D porous V\textsubscript{2}O\textsubscript{5} structures on indium tin oxide (ITO) slides. PANI was deposited onto this V\textsubscript{2}O\textsubscript{5} porous network via electropolymerization. The morphological features of the V\textsubscript{2}O\textsubscript{5}:PANI electrodes were investigated with Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM). Chemical composition of the electrodes was confirmed using Raman spectroscopy.

Cobalt catalyzed cyclotrimerization of alkynes using a microwave reactor

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A previously prepared cobalt compound, pentafluorophenylcyclopentadienylcobalt(I)dicarbonyl {[(C\textsubscript{6}F\textsubscript{5})C\textsubscript{5}H\textsubscript{4}]Co(CO)\textsubscript{2}} (1), has been shown to catalytically produce substituted aromatics. The particular substrates investigated, as well as their resulting aromatics, as shown in table 1. The production of triphenylbenzene was quantitative and initial yields for the remaining aromatics were greater than 65 %, however optimal purification procedures have not yet been determined. Catalytic reactions were initially performed via refluxing the reaction mixture in Schlenk glassware. It was found that using a microwave reactor, the reaction times could be significantly reduced vs. the standard reflux. Catalytic production of
aromatics with 1 versus a literature prepared catalyst, \((C_6H_5)Co(CO)_2\) (2), demonstrated that the fluorinated catalyst decreased the reaction time for all substrates. All compounds were analyzed via \(^1\)HNMR.

### Table 1. Substrates and their resulting aromatic products

<table>
<thead>
<tr>
<th>Substrate</th>
<th>Substituted Aromatic</th>
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</thead>
<tbody>
<tr>
<td>Phenylacetylene</td>
<td>Triphenylbenzene, Diphenylpicolene</td>
</tr>
<tr>
<td>Trimethylsilylacetylene</td>
<td>Tri-trimethylsilobenzene</td>
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<td>1-pentyne</td>
<td>Tripropylbenzene</td>
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CHED 857

Modulating the electrochemical properties of iron-carbonyl clusters using thiolate ligands

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We are interested in the study of iron-carbonyl complexes designed to mimic the structure and function of the active site of the efficient hydrogen producing [Fe-Fe] hydrogenase enzyme. These clusters are coupled to thiolate ligands which are used to tune the electrochemical properties of the iron-center. In this study, a series of diiron-carbonyl compounds tethered to arenethiolate groups have been prepared and characterized. The structures of the compounds have been ascertained using X-ray crystallography and spectroscopy (IR, UV-visible and NMR). The ability of the compounds to electrocatalyze the reduction of acetic acid to hydrogen have been investigated and the results will be presented.

CHED 858

Adsorption studies and immobilization of metal complexes on supports: Solid-state NMR and catalysis

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Immobilized catalysts that are covalently linked to a support are extremely useful because they are as active and selective as their homogeneous analogues, yet still easily separated from the reaction mixture. However, molecules may also be only adsorbed, and we sought to better understand catalytic systems by studying the adsorption and mobility of organic and organometallic compounds on various supports. We have characterized the interactions of adsorbed species with the support surfaces using multinuclear solid-state NMR. The results enhance the basic knowledge in important areas such as the separation sciences and heterogeneous catalysis. Additionally, we have studied Ni catalysts immobilized by new tridentate ligands to allow comparisons with previously used ligands. Our results suggest that the strongly coordinating tripod stabilizes the metal complex and sterically shields it from neighbouring molecules and the reactive surface. In this way it prevents leaching of the catalyst and subsequent formation of nanoparticles.

CHED 859

Chemical pressure effects on Ga_{(2-x)}Fe_xO_3 magnetoelastic ceramic structure

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New advances in technology and computer systems are necessary to automate and sustain world-wide networks and data. This push for innovation has sparked interest in magnetoelastic compounds because they exhibit coupling of both ferroelectric and ferromagnetism orders. The harnessing of this property has the potential for creating new generation data storage applications because it combines the advantages of both magnetic random access memories (MRAMs) and ferroelectric random access memories (FeRAMs). Magnetoelastic Random Access Memories (MeRAMs) will have a non-destructive reading step, non-lethargy components, and more importantly low energy consumption.

The difficulty for the development of these new generation devices occurs from the lack of magnetoelastic materials that express the coupling above room temperature. However, a prospective material is the orthorhombic gallium ferrite Ga_{(2-x)}Fe_xO_3 that has a Neél temperature above room temperature for x>1.3. The Neel temperature within the unit cell depends on magnetic interactions which are directly affected by both the iron concentration and the volume of the cell. Modeling the magnetic interactions is therefore complicated because of their dependence on the two parameters. Keeping the Fe content constant while modifying the volume of the cell should allow improving our knowledge on the magnetic interactions. The proposed work is to complete a cell parameter study of doped GFO with aluminum and indium and the influence to the magnetic properties. By doping with these materials, the Fe concentration will be maintained, but magnetic pathways will be distorted in the structure due to expansion or contraction of the unit cell. The size and cell parameters should vary for each compound and allow for potentially better compositions that exhibit similar magnetic behavior to be...
explored for spintronic applications. The elaboration of single-phase doped GFO with aluminum and indium were analyzed with XRD and SEM to check for doped element content. The chemical pressure on the doped ceramics was analyzed with SQUID magnetization from 5-400 K and magnetic transition temperature was determined by point of inflection when magnetization reached a zero value. The cell parameters were determined by FullProf software to determine the change in structure size correlated to the doped element content. The study has shown a dependence of magnetic behavior with change in cell parameters and doped element content.

CHED 860

Synthesis and characterization of a novel hydrozone thiophene ligand

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Copper, cobalt and nickel organometallic complexes continue to be of interest to our research group as these compounds may find use as anti-cancer, anti-fungal or antibacterial compounds. Hydrozones have shown biological activity as anti-tumor, anti-viral and anti-mycobacterial agents along with other applications. One recent water-soluble hydrazone thiophene ligand synthesized by Morales-Toyo, et.al. (J. Chem. Cryst, 2013, 43, 544-549) may offer an opportunity to increase the water solubility of select metal compounds, thereby making them potentially more biologically active. The reaction of copper and cobalt with these hydrozone thiophene ligands may result in compounds of biological significance along with improved water solubility. A new ligand, (E)-Ethyl-2-[2-(thiophen-2-ylmethylene) hydrazinyl] benzoate has been synthesized and characterized by NMR and IR. Additionally, preliminary results of bacterial testing with this ligand are shown.

CHED 861

Synthesis and magnetic characterization of lanthanide 12-metallacrown-4 complexes

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Numerous metallacrown (MC) complexes with varying metal centers have demonstrated single-molecule magnet (SMM) behavior. Recently we reported the first 12-MC-4 complexes with lanthanide ions in the central cavity. For charge neutrality, an alkali metal ion (sodium or potassium) was also bound to the central cavity. The lanthanide ions were tethered to the MC ring using four bridging acetate anions. To investigate the magnetic behavior of these molecules we have varied the bridging carboxylate anion and kept the ring metal ion constant as manganese and the central
metal ions constant as dysprosium and sodium. The resultant structural and magnetic properties will be explored and modeled. Variance of the carboxylate bridges, while maintaining constant ring and cavity metals, will ensure that any structural and magnetic properties will be the result of the carboxylate anion. The magnetic coupling constants between the ring and cavity metals will be determined and matched to those of prior MC complexes that have demonstrated SMM behavior.

CHED 862

Corrosion testing of anti-corrosion coatings by Scanning Electrochemical Microscopy (SECM)

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Using SECM (Scanning Electrochemical Microscopy), two aluminum alloys with various anti-corrosion coatings were exposed to a ferrocenemethanol (FeMeOH) solution, and the current between the sample and the tip was measured to probe the metal surface. The substrate was biased to increasingly positive potentials to induce a mediator current identifying “pinholes” (current spikes) in the coating. Effects of pH of the FeMeOH solution were explored, as well as the effects of repeated potential cyclings on the state of the coatings. Two tip sizes, 10 um and 25 um, were used, and the image resolution and the precision of detecting pinholes was evaluated.

In testing the effects of prolonged exposure to electric potential, the initial results for the samples that were freshly cut showed that the observed current were much smaller than the current observed in the “used” samples. In a series of experiments varying the pH of the buffer solution, results showed pinholes were observed primarily with the pH 6.85 solution while pH 3.00 and pH 8.00 did not yield any significant pinholes.

After conducting “macroscale” scans (100 um x 150 um) of a sample at pH 6.85, the pinholes were located, and "microscale" scans (20 um x 25 um) were performed to get a closer look at the fine details of the individual pinholes. The results of these microscale scans yielded higher-resolution data of current spikes, with a greater frequency of pinholes observed on the samples. However, based on the experiments comparing the two tip sizes, the microscale scans that were conducted with the 10 um tip did not show any noticeable visual improvement compared to the scans conducted with the 25 um tip.
2024 Al pH 6.85 25 micron tip at 1.0 V

Representative SECM area scan. Potential vs. Ag/AgCl and the Pt tip / substrate separation 25 microns.

CHED 863

DNA binding studies of \([\text{Rh(tacn)}(\text{dppz})(\text{H}_2\text{O})]^{3+}\): A new metallointercalator with a modifiable coordination site

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Metal-based coordination complexes possessing flat aromatic ligands have the capability of binding DNA through intercalation and insertion. Work by J. K. Barton and others have shown that these so-called metallointercalators and metalloinserters are capable of acting as molecular probes of DNA structure and damage, as well as, inhibitors of DNA replication. Consequently, these types of metal complexes show promise as chemotherapeutics and DNA diagnostic probes. Our group is currently examining rhodium based metallointercalators supported by the cyclic triamine 1,4,7-triazacyclononane (tacn). Unlike the traditional metallointercalators which are supported by diimine type ligands, tacn possesses N-H groups that could potentially hydrogen bond with nearby base pairs. Furthermore, complexation with a bidentate intercalator
will leave a single coordination site that can be modified in order to further tune the DNA binding ability of the complex. To this end, we have synthesized the metallointercalator [Rh(tacn)(dppz)(H₂O)][CF₃SO₃]₃ (dppz = [3,2-a:2',3'-c]phenazine) in a three step process. The procedure involves reaction of RhCl₃ · xH₂O with tacn followed by treatment with silver triflate and finally addition of dppz. We have now initiated DNA binding studies of [Rh(tacn)(dppz)(H₂O)]³⁺ with calf-thymus DNA. The synthesis, spectroscopic properties, and results of the DNA binding studies of [Rh(tacn)(dppz)(H₂O)]³⁺ will be presented.

CHED 864

Speciation of europium(III)-tetracycline species

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Tetracycline (TC) is a commonly used antibiotic that prevents the growth and spread of bacterial infections. The biological action of TC is determined by its structural and complexation behavior; however, the chemical behavior of TC is not completely understood. A working concentration of 0.5mM was used to study the species formed and its conformation in relation to metal chelation, pH, and solvent was done using steady-state luminescence, time-resolved luminescence, and ⁵D₀ ← ⁷F₀ (Europium, or Eu) excitation spectroscopy. This work has shown that the change in pH of each solution favors the formation of certain TC species that act as a “fingerprint” to (1) indicate the structural changes to the chiroptical properties of each Eu(III) – TC species and (2) be used as a probe for chiral discrimination of biologically active molecules.

CHED 865

Toward the development of luminescent metal organic frameworks for use as sensors

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The most common luminescence-based sensing approach to date involves use of a luminescent, analyte-responsive compound embedded in a support matrix such as a polymeric material which is often heterogeneous in nature and usually plays an active role in sensor response. Unfortunately, there tends to be limited predictive power in the rational design of polymer-supported sensors, and the heterogeneous nature of the polymer support matrix can lead to poor sensor-to-sensor calibration reproducibility and diminished response. In the case of luminescence-based oxygen sensors, for example, non-linear Stern-Volmer calibration curves and reduced quenching sensitivity are observed as a result of poor compatibility between the sensor molecule and support. Luminescent metal-organic frameworks (LMOFs) hold great potential in the
development of sensors, and, with their relatively straightforward syntheses that produce predictable, homogeneous, extended structures, should eliminate these constraints. More importantly, subtle differences in overall LMOF structure, metal ion coordination, pore surfaces, and host-guest interactions within pores all have significant impact on observed photoluminescence and provide numerous strategies for analyte detection. Progress toward development of prototype LMOFs incorporating carboxylated ruthenium-1,10-phenanthroline or ruthenium 2, 2-bipyridine complexes as linker molecules is highlighted. Photophysical characterization of the ruthenium complexes used in the LMOFs and of the LMOFs themselves includes luminescence excitation and emission spectra and excited state lifetimes. The potential for applications of LMOFs in luminescence-based sensing is also assessed.

CHED 866

Interaction of DNA with [Cu(phen)(4-amino-pteridino(6,7-f)phenanthroline)][PF₆]₂, a potent DNA cleavage agent

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The copper(II) complex of 4-amino-pteridino(6,7-f)phenanthroline (abbreviated L-amino), prepared from the condensation of phenanthroline dione and 4,5,6-triaminopyrimidine, was investigated for its DNA binding and cleavage properties using fluorescence titrations, thermal denaturation, and gel electrophoresis. The complex exhibits a strong affinity for duplex DNA and is a potent cleavage agent even in the absence of a reducing agent. The ligand structure is potentially favorable for intercalation and is likely responsible for its binding affinity as indicated by an increase in the DNA melting temperature of about 10 °C. Gel mobility assays showed DNA cleavage occurring in a concentration dependent fashion with a very significant amount of cleavage at concentrations as low as 3 μM while requiring no incubation. Mechanistic studies indicate the involvement of singlet oxygen in inducing the cleavage of the DNA duplex.

CHED 867

Investigation of DNA binding and photocleavage properties of [Zn(4-amino-pteridino(6,7-f)phenanthroline)(triflate)]₂

**Penny Wong**, wongp@southwestern.edu, Gulnar H. Rawji. Chemistry & Biochemistry, Southwestern University, Georgetown, Texas, United States

The DNA binding properties of the zinc(II) complex of the bidentate ligand, 4-amino-pteridino(6,7-f)phenanthroline (abbreviated L-amino), and its ability to induce photocleavage of DNA were investigated using absorbance titrations and gel mobility assays. Preliminary data indicates that the triflates exchange with water to produce a more reactive form of the complex which has a strong affinity for the calf thymus DNA.
as indicated by a binding constant of \(\sim10^6\). The complex is also effective at cleaving plasmid DNA in a concentration and time dependent manner after incubation at 37 °C for \(\sim17\) hours. However, its ability to induce concentration dependent DNA cleavage is significantly enhanced upon irradiation at 360 nm for less than half an hour. The presentation will include results of studies on the mechanism of photocleavage as well as the kinetics of binding of the complex with DNA.

CHED 868

Ligand exchange of an enzyme-mimic Schiff-base copper(II) complex: A kinetic study

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The synthesis, purification and characterization of copper(II) Schiff-base complexes is presented. The \([\text{CuLN}4]\)\((\text{ClO}_4)\)_2 complex (LN4 = N,N'-bis-(1-pyridin-2-yl-ethyldene)-propane-1,3-diamine) is highly soluble in acetonitrile, and moderately soluble in water, and exhibits Beer’s Law behavior. Previous studies have shown that the complex is unreactive with sodium hydroxide and nitric acid; however, it does react with ascorbic acid and oxalic acid—both diprotic acids that commonly function as reducing and chelating agents. The reactivity of the complexes in aqueous solvent in the presence of oxalic acid and ascorbic acid is investigated. Rapid mixing of 8 mM \([\text{CuLN}4]\)\((\text{ClO}_4)\)_2 and 60 mM oxalic acid—both dissolved in NaCl solution to balance the ionic strength (~55 mM)—was monitored by UV-visible spectroscopy at constant temperature for both inert atmosphere and air-exposed conditions. Single-point (622 nm, 960 nm) and full-spectrum data suggests the presence of intermediate(s). The decay of the reactant band (622 nm) suggests a biexponential process, and the generation of multiple products in equilibrium. Potential structures of the product(s) will also be introduced.

CHED 869

Synthesis of enzyme-mimic copper(II) Schiff-base complexes

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Inspired by their enzymatic behavior, a series of Copper(II)-centered Schiff Base complexes were synthesized, purified, and characterized. Such complexes have been shown to exhibit interesting and beneficial catalytic properties. The ligands, LN4, LC2, LN4' (LN4 = N,N'-bis-(1-pyridin-2-yl-ethyldene)-propane-1,3-diamine, LC2 = Bis-(1-phenyl-yl-ethyldiene)-propane-1,3-diamine, LN4' = N,N'-bis-(1-pyridin-4-yl-ethyldiene)-propane-1,3-diamine) were synthesized via a 1-step condensation reaction in methanol. These ligands were then coupled to Copper(II) ions, obtained as perchlorate salts, and precipitated from a methanol solution. The products were purified via bulk recrystallization (vapor diffusion of diethyl ether into concentrated acetonitrile solution),
and the purified samples characterized by IR and elemental analysis. Electronic spectroscopy was performed. X-Ray diffraction was performed on suitable crystals and the structures are presented. The final products were reacted with oxidizing and reducing agents to investigate their redox behavior, and to determine potential use as catalysts.

**CHED 870**

**Synthesis and reactivity of a enzyme-mimic nickel(II) complex**

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A Schiff-base nickel(II) complex, [(NiLC2)](ClO4)2 (LC2 = Bis-(1-phenyl-yl-ethlidene)-propane-1,3-diamine) where the LC2 ligand is prepared from 1,3-diaminopropane and acetophenone has been synthesized, characterized, and purified. A second nickel(II) complex was synthesized, (NiLN4)(ClO4)2 (LN4 = N,N'-bis-(1-pyridin-2-yl-ethyldiene)-propane-1,3-diamine). The LN4 ligand is prepared by 1,3-diaminopropane reacting with 2-acetylpyridine. Both condensation reactions are performed in methanol. The complexes were purified via vapor diffusion recrystallization and analyzed through several different instrumental techniques. The [NiLC2](ClO4)2 is slightly soluble in acetone and has a greater solubility in acetonitrile and water, and the maximum solubility of these two solvents is discussed. The synthesized complex is yellow; however, the complex changes from yellow to blue when dissolved in water or when in contact with the dissolved water in acetonitrile. This is an irreversible reaction. The X-ray diffraction structure of the blue product is known to be [Ni(1,3-diaminopropane)2(H2O)2](ClO4)2, and the reaction from the yellow form to blue form is analyzed with various oxidants and reductants. Various mechanisms of the reaction are discussed.

**CHED 871**

**Development of sulphydryl-functionalized silica particles for use in diffusive gradient in thin-films passive samplers**

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Diffusive Gradient in Thin Films (DGT) is a passive sampling technique widely used to monitor for metals in aqueous environment. A DGT sampler often contains two thin layers, namely the diffusion layer and the resin layer. When DGT samplers are deployed, metals in the solution will migrate through the diffusion layer and be taken up by the resin layer. Because the migration of metals through the former layer is strictly via diffusion, it is possible to apply Fick's law to deduce the concentration of the metal in
the solution if the amount of metal accumulated on the resin layer and the deployment time of the sampler are known.

The resin layer in DGT samplers is composed of adsorbent particles that are embedded in a polyacrylamide gel. Various types of particle can be used as adsorbent (e.g., chelex-100 resin, iron oxides, titanium dioxide), depending on the targeted metal analyte. In this study, we synthesized sulfhydryl-functionalized silica particles (i.e., SH-SiO$_2$ particles), and tested their use as adsorbent particles in DGT samplers that aim to measure for chalcogenic metals, including Zn and Hg. In particular, the SH-SiO$_2$ particles were synthesized by grafting 3-mercaptopropyltrimethoxysilane on silica gel particles. The SH-SiO$_2$ particles were then embedded in polyacrylamide gels, and the particle-containing gels (i.e., the resin layer) were exposed to solutions containing a varying amount of Hg and Zn. Preliminary tests indicated that the resin layers were able to quickly remove Zn and Hg from the solution. In addition, extraction of the resin layers with aqua regia showed over 99% recovery of the accumulated Zn and Hg. These results indicated that SH-SiO$_2$-containing gels could be used as resin layers in the DGT sampler. Thus, the resins were then tested as a part of DGT sampler. This test showed that the accumulation of Zn and Hg onto the DGT sampler obeyed the Fick’s law, which should be the case in a properly-designed DGT sampler. Overall, our study showed that the home-made sulfhydryl-functionalized silica particles can be used in DGT passive sampler.

CHED 872

Capturing carbon dioxide with metal-organic frameworks

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Climate change is one of the major environmental problems plaguing Earth. Atmospheric greenhouse gas concentrations, especially of carbon dioxide, are at all-time highs. Methods need to be developed to help reduce the amounts of these gases in the atmosphere. The research done in this study looks to using metal organic frameworks as a possible solution to this problem, due to their ability to bind gases within their structures. Metal organic frameworks are a class of porous crystals in which organic molecules link metal containing clusters. The metal organic framework used in this study is synthesized from gamma-cyclodextrin, which has a symmetrical cyclic eight residue glucose structure, and potassium benzoate. Both of these starting materials are renewable and nontoxic. The metal organic framework is then used to study its potential to trap atmospheric carbon dioxide.

CHED 873

Preparation of SnO$_2$ substrate for sensitized solar cells
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TiO$_2$ and ZnO are the most commonly used wide band gap crystals in sensitized solar cells. We used SnO$_2$ in our study, because of its lower edge of conduction band energy and higher electron mobility. SnO$_2$ is a promising substrate, because it offers possible sensitization for substances that have lower conduction bands than TiO$_2$ and ZnO. We cut, polished, annealed, and etched SnO$_2$ natural crystal to make atomically flat surfaces that can be used for fundamental sensitization studies. We used AFM to obtain information about the topography of the surfaces. Mott-Schottky was used to determine the doping density of the SnO$_2$ crystals. We found that there was variability between crystals and developed a method to vacuum dope crystals that were not naturally conductive. To test our method of crystal preparation, we sensitized crystals with cyanine dyes and quantum dots and found the photocurrent spectra to match that of the sensitizer absorbance.

CHED 874

Synthesis of novel green inorganic catalysts

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The use of N-heterocyclic carbenes (NHCs) are now known to be appropriate replacements for phosphines in the synthesis of highly active metal complexes used in homogeneous catalysis. These NHCs, more than phosphines, are easier to work with, minimally toxic, and powerful electron donors. The NHCs can bind transition metals without back-donation and result in complexes that are more stable. These NHCs can also bind to any known metal, in both low and high oxidation states. This property gives much opportunity for the design and advancement of new complexes. The goal of this experiment is to test and compare the catalytic properties of the three novel NHC complexes synthesized and to determine the crystal structure of these complexes. I would expect that the complexes with NHC would be better, more efficient, catalysts than those with the PCy$_3$, and that the iridium dimer will be more efficient than the rhodium due to stability. A comparison of all three of these complexes will allow me to validate my hypotheses and help to better understand what these green catalysts may bring to the field of chemistry in years to come.

CHED 875

Studies of cytotoxicity and cellular internalization of small-molecule conjugates of metal oxide nanoparticles in tumor cells
Metal oxide nanoparticles are a new class of inorganic nanomaterials whose studies and applications in biology and medicine have rapidly expanded over the past decades. Our research lab have prepared and characterized a wide variety of metal oxide nanomaterials conjugated with small fluorescent molecules as potential biocompatible optical probes for molecular imaging. In this presentation, we will discuss cytotoxic assays of TiO$_2$ and BaTiO$_3$ nanoparticles covalently labeled with small fluorescent molecules on glioblastoma and melanoma cells. Our results reveal that some of the titanium oxide nanoconjugates are essentially non-cytotoxic over periods of up to 72 hours. We also employed confocal fluorescence microscopy to track cellular internalization of these nanoparticles. Detailed studies and fluorescence images suggesting how the fluorescent nanoconstructs may interact with these model cells will be further addressed.

CHED 876

Investigating a hybrid organosilyl class of Dawson-Wells polyoxometalates through Langmuir-Blodgett

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Dawson-Wells lacunary structures derivatized with organosilyl hydrocarbon tails previously characterized by electrochemical and spectroelectrochemical methods have been further investigated using the Langmuir-Blodgett technique. The organic/inorganic hybrid molecules displayed tunable redox behavior and electrochromic properties that would also be expected from non-modified polyoxometalates. Inherent amphiphilic properties of these novel compounds allowed for the formation and deposition of an elastic Langmuir-Blodgett monolayer without the use of organic surfactants on the air-water interphase, suggesting additional functionality not seen in ordinary polyoxometalates. In general it was found that these materials possess properties
similar to inorganic polyoxometalates, but with added functionality analogous to surfactant encapsulated polyoxometalates.

CHED 877

Synthesis of a novel green chemical catalyst

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A new novel triazole based Iridium(I) N-heterocyclic carbene complex [(cod)Ir(NHC)PCy₃]BF₄ was synthesized and characterized using multinuclear NMR and single-crystal X-ray diffraction. The complex crystallized in monoclinic cell in P2₁/n space group. The potential green chemistry catalytic property of the complex was studied in the transfer hydrogenation reduction of a ketone and imine.

CHED 878

Synthesis and catalytic properties of a novel triazole based N-heterocyclic Iridium carbene complex

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A new triazole based N-heterocyclic carbene Iridium complex Ir[(COD)(NHC)PCY₃] with butyl and benzyl wing tips was synthesized and characterized with multinuclear NMR and single crystal x-ray diffraction. The complex crystallized in a monoclinic cell in the space group P2₁/n. The catalytic properties of the complex were studied in the transfer hydrogenation reduction of acetophenone and N-benzylideneaniline.

CHED 879

Characterization of metal dithiocarbamate complexes derived from amino acids

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Metal dithiocarbamates are used for varying applications, including antibacterial and anticancer agents, because of their biological, electrochemical and synthetic properties. The goal of this research is to characterize various metal dithiocarbamate complexes derived from amino acids specifically glycine, phenylalanine, and methionine using
NMR and TGA. We will also test the solubility of the various compounds in water and organic solvents at varying pH.

CHED 880

Corrosion of aluminum by aqueous CuCl\(_2\): An SEM-EDS study

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Aluminum metal has a high resistance to corrosion because of its protective oxide film that forms on the surface. However, without this film, aluminum becomes highly susceptible to corrosion. It was previously determined that chloride accelerates aluminum corrosion, probably by interacting with the surface oxide layer to accelerate removal. The redox reaction of aqueous CuCl\(_2\) with aluminum can be used as a model for aluminum corrosion; copper deposition is a marker of corroded areas. Aluminum stubs were polished with #600 sandpaper and treated with various concentrations of aqueous CuCl\(_2\). The corrosion areas were investigated using FEI Quanta 250 SEM and EDS Aztec software. Cu and Cl distribute according to the topographic features of the aluminum surface. Chlorine filled the deeper topographic areas; copper formed on the higher ones. Copper was found only on the outer borders of the corrosion pits, while chlorine, aluminum, and oxygen were found inside. Chlorine concentration increased, then decreased according to concentration and time, consistent with our theory that chloride accelerates aluminum corrosion through accelerated removal of the surface oxide layer. We propose that corrosion can be predicted by location; the highest chlorine concentration areas with no visible corrosion nor deposition of copper go on to develop visible copper deposition, a sign of aluminum corrosion.

CHED 881

Microwave-promoted synthesis of heavily iodinated 10- and 12-vertex boron clusters

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Heavily iodinated anionic borane and carborane clusters have potential applications as X-Ray contrast agents, isotopic markers, and boron neutron capture therapy drugs. Due to their significantly higher iodine-carrying capacity (92% molecular weight iodine for 1-carba-closo-CHB\(_{11}I_{11}\)) and greater in vivo stability, they are promising alternatives to current organoiodine X-ray contrast agents. However, the preparation of highly iodinated clusters is a synthetic challenge. Microwave-promoted syntheses of 10 and 12-vertex closo-boron clusters reduce reaction times and temperatures and require cheaper electrophilic iodine sources. In this work, salts of 1-carba-closo-CHB\(_{11}I_{11}\), 1-carba-closo-CHB\(_{9}H_{6}I_{6}\), 1-carba-closo-CHB\(_{9}H_{4}I_{5}\), closo-B\(_{10}I_{10}\), and closo-B\(_{12}I_{12}\)
anions were prepared in yields of at least 80%. All compounds were characterized by NMR, IR and mass spectrometry and the crystal structure of [Et₄N][CHB₉H₄I₉] was determined by single crystal X-Ray diffraction. The synthesis and characterization of these molecules will be discussed.

CHED 882

**Novel synthesis and catalytic properties of triazole-based N-heterocyclic carbene complexes of rhodium and iridium**

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Novel triazole-based N-heterocyclic carbene (NHC) complexes of rhodium and iridium with isopropyl and butyl wing tips were synthesized and characterized fully by multinuclear NMR. The structure of the ionic iridium carbene complex, [Ir(COD)(NHC)(PPh₃)]BF₄, was determined by single crystal X-ray diffraction. The cationic iridium complex has a square planar geometry. The complex crystallized in centrosymmetric space group P2₁/n with four molecules per unit cell. The green chemistry catalytic properties of the ionic complexes of both the rhodium and iridium in the transfer hydrogenation reductions of a ketone and imine were studied.

CHED 883

**Heteroleptic salicylaldiminate magnesium amides: Solid-state and solution characterization**

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Magnesium coordination complexes offer rich structural variation and potentially useful applications in Lewis acid catalysis. Highlighted here are two series of heteroleptic magnesium complexes containing a salicylaldiminate ligand and an amide ligand. These complexes were generated from reaction of the appropriate salicylaldiminate ligand source with either magnesium bis(hexamethyldisilazide) or magnesium bis(dibenzylamide). The complexes have been characterized in the solid state using X-ray crystallography. The solution behavior of these systems was studied using ¹H-NMR spectroscopy. Magnesium complexes are known to exhibit ligand redistribution via a Schlenk-type equilibrium. Such behavior was noted for these systems. After detailed ¹H-NMR studies in a variety of deuterated solvents, a solvent dependence on ligand redistribution was noted in each system. Effects of donor and non-donor solvents on the solution stability of heteroleptic magnesium complexes for each amide class will be detailed. Comparisons of the solution structure to that found within the solid state will be noted.
Finally, the application of these complexes to ring-opening polymerization reactions will be assessed.

CHED 884

Synthesis and characterization of ground and excited state properties of a new ruthenium(II) polypyridine complex

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The complex \([\text{Ru(tpy)(bpy)(MeO-py)}]^2+\), where tpy = 2,2';6',2''-terpyridine, bpy = 2,2'-bipyridine, and MeO-py = 4-methoxypyridine, was synthesized and the effect the electron donating methoxy group has on the ground and excited state properties of the complex was investigated and compared to a previously synthesized complex, \([\text{Ru(tpy)(bpy)(py)}]^2+\), where py = pyridine. A detectable red shift is observed in the electronic absorption and emission spectra of \([\text{Ru(tpy)(bpy)(MeO-py)}]^2+\) as compared to \([\text{Ru(tpy)(bpy)(py)}]^2+\). These data show that the electron donating methoxy group located in the para position of the pyridine ring has a slight destabilizing effect on the Ru(dp) t\(_{2g}\)-type orbitals.

CHED 885

Time-based investigation of the vapochromic response of platinum(II) complexes

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Vapochromic materials respond to particular volatile organic compounds (VOCs) by undergoing a color change and do so with specific sensitivity levels and selectivity. The discovery of such materials has been serendipitous in the past, but organized approaches to synthesizing new vapochromic salts will push the vapochromic field closer to being able to predict vapochromic behavior pre-synthesis. Here, platinum(II) terpyridyl salts with an X' ligand (X' = Cl', Br', I') and YPF\(_6^\) counter anion (Y = P, As, Sb) were studied. The absorption and desorption rates of acetonitrile vapor were monitored by systematically taking pictures every 10 s with a stationary camera. A program written in MATLAB was used to monitor the color change over time for all nine salts studied. Additionally, the color difference between pure red and the color of each individual salt was calculated over time and plotted. The derivatives of these plots were used to determine the initial/final response times and the duration of vapochromic response for each salt. It was determined that the X' ligand and YPF\(_6^\) counter anion affects the selectivity and speed of response of the platinum(II) terpyridyl salts, and the use of calculating a color difference is a novel approach to quantifying color and monitoring the vapochromic response over time in the vapochromic field.
Synthesis of Co-complexes with pentadentate ligands for catalytic hydrogen evolution

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Pentadentate ligands containing polypyridyl systems can provide metal complexes with hexa coordination having a labile sixth site which is usually occupied by a solvent molecule. The polypyridyl group stabilizes the metal complex and several reports have been published with tetra and pentadendate polypyridyl complexes. Recently we have reported the synthesis and characterization of mononuclear Co complexes, [Co(DPA-Bpy)Cl]Cl (1a) and [Co(DPA-Bpy)(H2O)](PF6)3 (1b), with a pentadentate ligand (DPA-Bpy = N,N-bis(2-pyridinylmethyl)-2,2'-bipyridine-6-methanamine). The complex 1b was found to be a good catalyst for electro- and photocatalytic H2 evolution in aqueous solution (Figure 1). The overpotential for complex 1b for electrocatalytic H2 evolution was found to be 600 mV in pH 7 buffer.3 Tuning the DPA-Bpy ligand scaffolds to get more efficient catalysts with lower overpotentials, high activity is an interesting protocol. Introducing electron withdrawing groups into the ligand scaffold may reduce overpotential while maintaining the activity. In this context, we have designed a new catalyst by introducing pyridine groups with more electron-withdrawing carboxyester moiety which may result in more positive potentials and lower overpotentials in electrocatalytic hydrogen evolution from aqueous media. Hydrolysis of ester can provide carboxylic acid groups which can produce a hydrophilic environment around the cobalt center.

Exploration of coordination chemistry with arsenazo III, DTPA and metal complexes using NMR and UV-VIS

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UV-Visible (UV-VIS) spectrophotometry and NMR spectroscopy were two methods used for studying coordination compounds of the ligands arsenazo III (AIII) and diethylenetriaminepentaacetic acid (DTPA). These ligands were tested with many metals, such as some group 1, group 2, transition, and one lanthanide which had counter ions of nitrate, acetate, and chloride. AIII has a characteristic UV-VIS spectrum. We observed the wavelength at maximum absorption shift when this ligand is bound to some metals and when those metals are displaced by other ligands. A trend in the shifts was also observed with counter ions used. Shifts in the H-NMR spectrum were also
observed for the ligands when bound to metals. This method can be used in the future with other metals and ligands.

CHED 888

Coordination chemistry of divalent group 12 thiocyanate complexes containing phthalazine

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A sequence of metal-organic frameworks containing phthalazine and group 12 thiocyanates has been prepared. Analysis of the fundamental mid- and far-range FT-IR vibrational modes of SCN\(^-\) (\(v_{CN}\), \(\delta_{NCS}\), and \(v_{CS}\)), coupled with \(^{13}\)C NMR chemical shifts have elucidated the thiocyanate mode of coordination (terminal M-N, terminal M-S or binuclear bridging). Incorporation of elemental composition allows for structural supposition. Confirming X-ray crystallographic studies are underway and will be reported.

CHED 889

Coordination chemistry of divalent group 12 thiocyanate complexes containing quinazoline

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A sequence of metal-organic frameworks containing quinazoline and group 12 thiocyanates has been prepared. Analysis of the fundamental mid- and far-range FT-IR vibrational modes of SCN\(^-\) (\(v_{CN}\), \(\delta_{NCS}\), and \(v_{CS}\)), coupled with \(^{13}\)C NMR chemical shifts have elucidated the thiocyanate mode of coordination (terminal M-N, terminal M-S or binuclear bridging). Incorporation of elemental composition allows for structural supposition. Confirming X-ray crystallographic studies are underway and will be reported. A comparison of the structural topologies and packing assemblies of this investigation versus a previous study incorporating pyrimidine will be included.

CHED 890

Coordination chemistry of divalent group 12 thiocyanate complexes containing 2-amino-5-cyanopyridine
A sequence of metal-organic frameworks containing 2-amino-5-cyanopyridine and group 12 thiocyanates has been prepared. Analysis of the fundamental mid- and far-range FT-IR vibrational modes of SCN⁻ (νCN, δNCS, and νCS), coupled with ¹³C NMR chemical shifts have elucidated the thiocyanate mode of coordination (terminal M-N, terminal M-S or binuclear bridging). Incorporation of elemental composition allows for structural supposition. Confirming X-ray crystallographic studies are underway and will be reported.

CHED 891

Imidazolium salts as reaction media for preparation of metal halide cluster networks

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The molybdenum and tungsten series of halide clusters have a number of interesting photochemical and electrochemical properties. Our lab has been particularly interested in the hexanuclear molybdenum halide clusters, which are composed of six molybdenum atoms in an octahedral arrangement with eight face-bridging halide ligands and six additional terminal ligands attached to each molybdenum atom (Figure 1). Recently, we have been interested in preparing networks composed of these clusters connected by carboxylate linkers, but previous attempts using conventional solvents have been unsuccessful.

My project has investigated using ionic liquids as the reaction media for these preparations. Ionic liquids are molten salts with melting points below 100°C. Their negligible vapor pressure, low melting points, and thermal stability over a wide temperature range make them promising reaction media to avoid product decomposition. Two synthetic schemes have been investigated. The first uses salts of 1-ethyl-3-methylimidazolium [EMIM]⁺ and 2-butyl-3-methylimidazolium [BMIM]⁺ isophthalate [IPA]²⁻, terephthalate [TPA]²⁻, and trimesate [TMA]³⁻ as both the solvent and the ligand source. The second uses 1,3-dimethylimidazolium triflate [DMIM]⁺[OTf]⁻ as an inert solvent that exhibits excellent solubility for the molybdenum clusters with triflate ligands [MoCl₈(OTf)₆]²⁻.
Catalytic activation of $O_2$ for the oxidation of alcohol is both environmentally friendly and economically desirable. Metals such as nickel and copper are not usually utilized for oxidation catalysts because of the inaccessibility of higher oxidation states. However, oxygen activation can be achieved through electron-donating ligands, which reduce the oxidation potential. Baldwin and co-workers at the University of Cincinnati have previously synthesized nickel (II) complexes with ligands that contain three oxime functional groups, one being $H_3$TRISOX (tris(2-hydroxyiminopropyl)amine). Our group increased the overall steric bulk of $H_3$TRISOX by replacing the three methyl groups with phenyl groups to form the ligand $H_3$TRIPHOX.

Oxidation of a primary alcohol (methanol, propanol, or butanol) is carried out by dissolving $M-H_3$TRIPHOX-$Cl_2$ ($M=\text{Ni, Cu}$) in the alcohol, which acts as both substrate and solvent, then adding three equivalents of potassium hydroxide. (This deprotonates the three oxime O-H groups. One of the deprotonated O atoms then forms a coordinate-covalent bond to the M center on another metal complex; in turn, an O atom on the second complex acts as a bridging to the first M center. The resulting dimer is the active catalytic species.) The volatile components are distilled from the catalyst. Gas chromatography is utilized to determine the ratio of aldehyde to alcohol, and thus estimate the turnover number.

A curious observation is the Cu-$H_3$TRIPHOX-$Cl_2$ exists as two forms: a powder-blue solid and a forest-green solid. Each oxime functional group can adopt E or Z stereochemistry. Our hypothesis is that one form has the ‘E’ oximes, and the others the ‘Z’ oximes. Molecular modeling suggests the electron density on the oxime N atoms...
does vary accordingly, and might account for different sizes of $\Delta \phi$; hence, the different colors.

CHED 893

**NKU organometallic research: Examining new synthetic strategies that functionalize fullerene and coronene for organometallic supramolecular systems**

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Our group has a long-standing interest in the incorporation of extended aromatic systems (e.g., fullerene and coronene) into organometallic supramolecular systems to study their photoinduced excited state behavior. Fullerenes exhibit the desired electron-transfer interaction with attached transition metal chromophores, but its nonpolar nature has restricted the reactivity and solution chemistry of the systems. The substitution reactions that produce these complexes are relatively inefficient. This talk describes our efforts to explore similar functionalization strategies with coronene as an alternative extended aromatic system. The modular nature of these strategies allows us to explore different reaction sequences to improve the final product. Descriptions of these strategies will be presented, along with detailed NMR (1D and 2D) analysis of the obtained products.

CHED 894

**NKU Spectroscopic Research: Studies on polymers and their subunits that incorporate fullerenes and transition metal chromophores**

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A major focus of our group has been on supramolecular systems that incorporate fullerenes and transition metal chromophores that have unique photoinduced excited state behavior. While we have successfully completed spectroscopic studies on small molecule systems containing these two units, there is still much to learn on the modifications of these molecules that would allow them to be used as building blocks for polymers. This poster provides recent spectroscopic data on some of these building blocks and their ensuing polymers, including absorption, emission, and transient absorption measurements at multiple temperatures. This data will be compared to previously explored systems to better understand if these new molecules exhibit similar excited-state behavior. Preliminary interpretation suggests that these new systems show enhanced excited-state behavior when compared to our first-generation small molecule systems.
NKU Polymer Research: Synthesis of polymers and their subunits that incorporate fullerenes and transition metal chromophores

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Our group has been focused for several years on supramolecular systems that incorporate fullerenes and transition metal chromophores with specific interest in their photoinduced excited state behavior. We have completed studies on our initial small molecule systems containing these two units and continue to develop modified systems that can be used as building blocks for polymers. This poster details recent efforts to explore multiple protecting group reactions on these building blocks to allow for the controlled addition of each subunit with minimal side products. Polymer synthesis was followed with Gel Permeation Chromotography to determine final polymer size. These foundational studies will allow for the more rapid advancement of our polymer efforts.

CHED 896

NKU solar cell research: Fullerene-transition metal sensitized solar cells - construction and efficiency studies

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Our research group has been interested for several years in the synthetic design and spectroscopic examination of fullerene-transition metal supramolecular systems. The ultimate interest of these systems is to examine their photoinduced excited state behavior and apply that behavior in devices of interest. The ability for these systems to undergo electron-transfer, along with their broadened absorbance in the ultraviolet and visible light spectrum, makes them good candidates for dyes in semiconductor-based solar cells. This poster presents our recent efforts to prepare TiO$_2$-based dye-sensitized solar cells with both our molecular systems and other baseline organic and inorganic dyes. Particular attention is paid to determining the electrical capabilities of these cells (e.g., photovoltage and photocurrent obtained from the cells under varying loads), with the intention to determine their overall photoelectric efficiency. Although our numbers remain below those obtained for existing solar cell dyes, the results expand our knowledge and allow us to continue improving our dye preparation, cell fabrication and measurement capabilities.

CHED 897

NKU organometallic research: Simplified synthetic strategies for fullerene-bipyridine ligands used in organometallic complexes for solar cell dyes

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For several years our group has been interested in the creation of supramolecular systems that link substituted fullerenes and transition metal chromophores. These systems undergo unique photoinduced excited state behavior where electron transfer occurs between the two subunits. However, our research has continually been hampered by synthetic issues surrounding the fullerene substitution. While others in our group are exploring alternate extended aromatic systems (e.g., coronene) that may ultimately substitute for the fullerene, this talk summarizes our efforts to improve the synthetic methodologies involved with preparing our original fullerene-bipyridine ligand. Typically a four step sequence is used to prepare these systems in our group – each requiring purification and resulting in reduced yields. We have explored alternative reaction strategies, including an innovative Sonogashira “one pot” strategy profiled in this talk. This pathway has been explored and tweaked through numerous reaction attempts, and results suggest that this strategy will provide a more efficient method to prepare both our fullerene systems as well as other extended aromatic systems (e.g., coronene) in the near future.

CHED 898

Dye inclusion on the {101} face of KDP crystals

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Hybrid materials consisting of organic/inorganic components are candidates for industrial applications and exhibit interesting properties[1]. KH₂PO₄ (KDP) has been observed to include a variety of anionic organic molecules on the {101} face due to electrostatic interactions between the molecules and the crystal surface[2]. Sulfonated azo dyes are shown to selectively recognize the {101} growth face during crystallization from aqueous solution. When in a high temperature environment, KDP has been observed to grow around the organic dye molecules to produce an undyed or partially dyed crystal. This research project seeks to investigate the temperature range of inclusion for three sulfonated azo dyes, find a relationship between the dye structure and the temperature at which it is included, and characterize KDP dye inclusion crystals. This information will aid in growing a large KDP dye inclusion crystal and increase what is known about the dye adsorption mechanism in growing KDP crystals.


New N-heterocyclic carbene (NHC) silver fluorides facilitate dihydrogen activation to form a silver hydride cluster where sterically demanding NHC ligands increase stability and rate of hydrogen activation

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Silver hydride complexes have been studied for their interesting molecular properties and reactivity. N-heterocyclic carbene (NHC) silver complexes exhibit uniqueness in both structure and reactivity that have been found to be useful in organosilver-mediated activation of molecules which can hearken to potential applications in renewable fuel or carbon cycles. NHC-silver fluoride complexes were found to activate dihydrogen to form 3-center, 2-electron hydride clusters that are hydridically adequate to reduce activated carbon dioxide. Steric effects were found to be an important factor concerning the stability of silver hydrides where increasing bulk substantially increased the stability of the hydride and the rate of dihydrogen activation. \(^1\)H and \(^{109}\)Ag NMR spectroscopic studies disclose the formation of hydride clusters and the presence of \(^{109}\)Ag-\(^{107}\)Ag coupling. This study indicated that dihydrogen can be heterolytically activated by hard/soft-mismatched silver complexes and that expanded-ring NHCs, with their greater steric demand and stronger electron-donating capacity, offer a clear advantage over traditional five-membered NHCs, significantly enhancing the rate of hydrogen activation as well as the stability of the resulting metal-hydride cluster.

CHED 900

Synthesis and catalytic activity of tin (IV) halides functionalized with bidentate phosphine ligands

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As carbon-based fuel supplies are depleting around the world, the development of renewable biofuels is becoming more important. Biodiesel is a renewable biofuel of interest, and it can be produced using waste vegetable oil via esterification. Production of fatty acid methyl esters (FAME) is the desired product from the reaction, and this research is centered around discovering an environmentally friendly and efficient catalyst for the reaction. The tin (IV) halides can serve as Lewis Acid catalysts and with recovery, are environmentally friendly. The tin (IV) halides are known to catalyze the reaction but are soluble and difficult to recover/reuse. In order to address this, we are investigating the binding of these compounds to commercially available solid phase synthesis resins modified to present phosphine donor groups (diphenylphosphino propane). As part of this study, solution-based analogs were synthesized to provide baseline information for spectroscopy and reactivity studies. These compounds have
been synthesized and employed as catalysts in the methylation of oleic acid. This poster will present synthetic details and catalytic studies.

CHED 901

Effect of ZnO morphology on the photodegradation of malachite green oxalate

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Zinc oxide (ZnO) has received a lot of attention in recent years; it has attractive electronic properties, it is relatively inexpensive, it is easy to prepare, and it is an environmentally friendly alternative to other semiconductors. The purpose of this research was to prepare and characterize ZnO nanoparticles to determine how size, shape, and method of preparation influences its reactivity and the effects caused by exposures to ZnO nanoparticles. Zinc oxide was synthesized by a sol-gel method, using aqueous solutions of zinc acetate and various amines, and precipitated with the addition of NaOH at 65˚C and 95˚C. Zinc oxide nanomaterials were also synthesized using aqueous solutions of ZnCl₂, ZnSO₄ and Zn(NO₃)₂ without amines by the sol-gel method. The photochemical reactivity of the different materials was evaluated by using them to photochemically degrade the organic dye malachite green oxalate in aqueous solutions under UVA irradiation. In general, it was found that for a given morphology, smaller particles yielded faster decomposition rates than larger particles. Particle size was controlled by temperature of the sol-gel reaction and rate of NaOH addition. Additionally, morphologies with a high surface area-to-volume ratio, such as rod or needle shaped crystals, also appear to increase the photocatalytic effectiveness.

CHED 902

Synthesis, characterization, and reactivity of ruthenium(II) complexes involving p-cymene and hexamethylbenzene ligands

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A Ru(II)-phosphite complex of the type [Ru(p-cymene){P(OCH₂CF₃)₃}(Ph)(OTf)] (1) has been synthesized and characterized as a potential catalyst for olefin hydroarylation. Olefin hydroarylation involves the formation of a new C-C bond via addition of an aromatic C-H bond across an olefin. Complex 1 has been isolated as an analytically pure yellow solid and fully characterized by ¹H-, ³¹P-, and ¹⁹F-NMR spectroscopy. Preliminary catalysis attempts involving benzene and 1-hexene yielded a stoichiometric amount of 2-phenyl-1-hexene based on 1 by GC-MS. The complex [Ru(Ph-Me₆){P(OCH₂CF₃)₃}(Cl)₂] (2), where Ph-Me₆ = hexamethylbenzene, has been prepared. Complex 2 has been isolated and fully characterized as a precursor on the route toward [Ru(Ph-Me₆){P(OCH₂CF₃)₃}(Ph)(OTf)] in order to compare reactivity as the neutral
arene donor is varied between $p$-cymene and hexamethylbenzene. The preparation of 1 and 2 and characterization by multinuclear NMR and single-crystal X-ray diffraction will be presented as well as initial catalytic results involving complex 1.

CHED 903

Synthesis and characterization of cyclopentadienyl- and pentamethylcyclopentadienyl-Co(III) mixed sandwich compounds containing either tridentate nitrogen, sulfur, or carbon donor ligands

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A series of mixed sandwich complexes of the type [Co(9S3)(CpR)](ClO₄)₂ or [Co(9N3)(CpR)](ClO₄)₂, where 9S3 = 1,4,7-trithiacyclononane, 9N3 = 1,4,7-triazacyclononane, and CpR = cyclopentadienide (Cp) or pentamethylcyclopentadienide (Cp*), have been prepared and characterized. These complexes are readily prepared by refluxing [Co(CpR)(I)₂(CO)] with 1 equivalent of either 9S3 or 9N3 followed by methathesis with perchlorate anion. The complexes are vividly colored orange for [Co(9X3)(Cp)](ClO₄)₂ where X = S and R = Cp* or X = NH and R = Cp or Cp*, and red for X = S and R = Cp. All complexes have been characterized by $^1$H-NMR and $^{13}$C-NMR spectroscopy, and a crystal structure of [Co(9S3)(Cp)](PF₆)₂ was obtained via single-crystal X-ray diffraction. Details on the preparation and characterization of these complexes, which includes multi-nuclear NMR spectroscopy, UV-vis spectroscopy, and cyclic voltammetry, will be presented. Preliminary results of the reactivity of a tridentate N-heterocyclic carbene ligand, hydrotris(3-methyl-imidazole-2-yliden-1-yl)cobalt, with [Co(CpR)(I)₂(CO)] will also be presented.

CHED 904

Electronic properties and composition of GaAs₁₋ₓPₓ grown by close-spaced vapor transport

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Semiconductor thin films are widely utilized in the production of photovoltaic devices. GaAs is a III-V binary semiconductor with exceptional optoelectronic properties such as a direct band gap of 1.42eV and a lattice parameter of 5.6Å, making it an attractive material for the construction of high efficiency solar cells. GaAs is not ideal by itself for some applications but can be combined with GaP, another III-V semiconductor with a 2.25 eV band gap, which allows the band gap and the lattice parameter to be tuned. Combining these binary materials to make the ternary alloy GaAs₁₋ₓPₓ is useful for multi-junction cells. This study aims to produce and characterize GaAs₁₋ₓPₓ thin films grown...
via CSVT. This work was done as a part of the NSF REU Program at the University of Oregon.

CHED 905

Synthesis and characterization of transition metal clusters/polymers supported by pyridylamide ligands

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Absorption and storage of CO$_2$ by transition metal polymers have attracted considerable interest due to the high selectivity and efficiency of these materials. In our effort to discover the new generation of transition metal polymer materials, a serial of pyridylamide ligands functionalized with multiple donors were synthesized and applied in the construction of polymeric porous structures with first row transition metal ions. Various coordination polymers/clusters with different nuclearity have been prepared and characterized by X-ray crystallography, IR, UV-vis and elemental analysis. The interesting structural and spectroscopic features of these compounds will help us obtain a deeper understanding on ligand design and polymer construction, which are major factors that impact the adsorption properties of these materials.

CHED 906

Synthesis and bacterial activity studies of acetylacetonate metal complexes

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Metal acetylacetones are common compounds used in coordination chemistry. They are derived by a synthesis reaction involving the acetylacetate anion and a metal ion, usually a transition metal, to form the acetylacetate (or AcAc) metalloid-ligand complex. This research proposes the synthesis and characterization of a class of (AcAc)$_2$ and (AcAc)$_3$ complexes that are similar to Schiff base ligands that have been shown to have antitumor activity. These ligands and metal-ligand complexes will be synthesized and characterized according to previous literature methods. These metal complexes will then be tested for anti-proliferative activity against seven microbes, including four bacteria genera, two yeast genera, and one mold genus. The minimum inhibitory concentration (MIC) will be determined for the metal complexes in order to test the possible biological activities of these compounds.

CHED 907

Stabilization of catalytic tin species with phosphine ligands
Tin has been found to have catalytic effects in many processes. The compounds SnX₄ (X=Cl,Br,I) are very reactive species which hydrolyze/oxidize readily. To stabilize the catalyst, a bis-phosphine ligand can be bound to the SnX₄ species. Several free ligands (bis(diphenylphosphino)phenylenediamine and bis(diphenylphosphino)aminoethyl) and their resin bound analogues were coupled with Sn(IV) species and their ability to catalyze the esterification of oleic acid was tested. Results suggest that the phosphine couples to tin while retaining some catalytic activity.

**CHED 908**

**Towards the synthesis of a water-soluble β-brominated cobalt(II) porphyrin**

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Water-soluble cobalt complexes have shown great potential in fuel-cell technology, water purification, and on-site nerve-agent deactivation or decomposition because of their ability to reversibly bind oxygen. The addition of halogens to a porphyrin creates an electron-deficient ligand which, in turn, increases the metal ion’s potential to bind with oxygen. Halogenation of both 4-dimethylaminophenylporphyrin and the 4-dimethylamino-2,3,5,6-tetrafluorophenylporphyrin first required insertion of a metal ion (Cu(II), Co(II)) followed by the methylation of the dimethylamino groups. Additional methyl groups rendered water-solubility while protecting the aminophenyl nitrogen atoms during bromination of the porphyrin. Results indicate that the fluorination of the phenyl groups stabilized the porphyrin during bromination while the non-fluorinated derivative decomposed.

**CHED 909**

**Synthesis of a novel water soluble porphyrin-chalcone complex**

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Preliminary results have indicated the concentration dependence of a group of novel water-soluble porphyrins at the 100 μM concentration level were the most effective in the presence of light via MTT assay. These compounds were tested on several cell lines, including tumor-derived cell lines, to assess the variability of the photoxicity between cell types. In this research, the coupling of the porphyrin, 5,10,15,20-tetrakis(4-carboxyphenyl)porphyrin, H₂TPPC, and the novel 3’-amino-4-hydroxychalcone have led to the synthesis of the new porphyrin-chalcone adduct, H₂TPP-Chalc-OH (I). Preliminary
examination of the phototoxicity of (I) may demonstrate the cytotoxicity of the porphyrins and extend the ability of the chalcones to have phototoxic effects.

CHED 910

Electronic structure and electrochemical elucidation of human serum albumin–heme complex

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Human serum albumin (HSA) is the most abundant protein in human plasma and has a remarkably high ligand binding capacity, making it a good repository for small molecules. One molecule that forms a complex with this enzyme is heme b (Fe(III) protoporphyrin IX), thereby generating HSA-heme. A crystal structure of this complex indicates a phenolate ligand forming a covalent bond to Fe via Tyr161, as opposed to the proximal histidine ligand found in globins. Interestingly, the kinetics and thermodynamic parameters for binding of diatomic gaseous ligands to wild-type and engineered HSA-heme are similar to those reported for myoglobin (Mb), making HSA-heme an artificial hemoprotein and a model complex for monomeric globins. In this study, the electronic structure and electrochemical properties of the different forms of HSA-heme are investigated using UV-vis, IR and fluorescence spectroscopies, and cyclic and square-wave voltammetries. The artificial hemoprotein is also tested for potential nitrite reductase (NiR) functionality. Preliminary studies demonstrate that nitric oxide binds to the Fe(III) and Fe(II) forms of HSA-heme, but oxygen does not (bind to Fe(II)), unlike Mb. Further, the redox potential of the HSA-heme is much lower than Mb, mirroring the redox potential of catalase which also has a tyrosine as the proximal heme ligand. UV-vis data demonstrate that the reaction between HSA-heme and nitrite generate a product similar to the pure form of HSA-heme Fe(II)-NO, alluding to the possibility that this artificial hemoprotein has NiR activity under optimum conditions. Implications on functionality of this complex based on our findings are presented in this work.

CHED 911

Contrasting the biomimetic reactions of NO\textsubscript{x} with Fe (III) porphyrins and Fe (IV) corroles

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The planet's nitrogen biogeochemical cycle and human health has been dramatically impacted by anthropogenic nitrogen loadings into the environment. The nitrogen cycle is regulated by a ubiquitous set of microorganisms' employing a vast array of enzymes, many of which contain iron porphyrin systems. Many of these enzymatic pathways and
mechanisms are not thoroughly understood nor have they been fully elucidated. This research contrasted the biomimetic reactions of various nitrogen oxide species (NOx) with iron (III) porphyrins and iron (IV) corroles. This investigation employed phenyl and pentafluorophenyl Fe centered meso substituted porphyrins and corroles insitu reactions under argon with a series of NOx species; Nitrate ion (NO₃⁻), nitrite ion (NO₂⁻), nitronium ion (NO₂⁺), nitrosonium ion (NO⁺), and nitric oxide (NO). The progress of the in-situ reactions and reaction products were characterized by UV-vis, NMR, IR, and GC/MS. A series of proposed mechanisms are postulated for each of these interactions and the extent to which higher Fe (IV) oxidation state impacts stoichiometric product formation.

CHED 912

Synthesis of a nickel(II) chloride chemosensor

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Anion detection, specifically chloride detection, is useful in biological and environmental analysis. Traditionally, synthetic receptors that use arrays of hydrogen bond donors as the association site are used for anion recognition. This approach is restricted to non-aqueous media due to water acting as a competitor with the synthetic receptor. Research has shown that a transition metal-based receptor with a high bonding affinity towards the specific anion can be used effectively in water. The goal of this research is to synthesize a new transition metal chloride chemosensor. This work has involved the synthesis of a nickel(II) complex with a high affinity towards chloride, as well as investigations into its effectiveness as a chemosensor of chloride in aqueous solution. The characterization and study of this complex will be discussed.

CHED 913

Exchange between Fe(III) and Ni(II) dithiocarbamates in solution

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Iron(III) is a d⁵, paramagnetic metal center and its diethyl dithiocarbamate derivative, Fe(S₂CN(CH₂CH₃)₂)₃, [Fe(Et₂dtc)₃], is soluble in deuterochloroform and gives a ¹H NMR spectrum which was first reported about 50 years ago. It is the CH₂ protons which are of interest; because of their proximity to the paramagnetic Fe(III), their signals in the NMR are shifted more than 30 ppm and show up as a somewhat broad signal. Two other iron(III) dithiocarbamate complexes, the dibenzyl derivative, Fe(S₂CN(CH₂C₆H₅)₂)₃, [Fe(Bz₂dtc)₃], and the morpholine derivative, Fe(S₂CN(CH₂)₄O)₃, [Fe(mordtc)₃], are also paramagnetic and exhibit broadened signals in the 20-30 ppm range.
Each of these three complexes exchange their dithiocarbamate ligands rapidly and mixing two of them in solution yields four complexes in statistical concentrations, e.g., mixing the diethyl and dibenzyl derivatives yields four complexes: Fe(S$_2$CNEt$_2$)$_3$; Fe(S$_2$CNEt$_2$)($S_2$CNBz$_2$)$_2$; Fe($S_2$CNEt$_2$)($S_2$CNBz$_2$)$_2$; and Fe($S_2$CNBz$_2$)$_3$.

Nickel(II) is d$^8$ and diamagnetic. Its dibenzyldithiocarbamate derivative Ni($S_2$CN(CH$_2$C$_6$H$_5$)$_2$)$_2$, [Ni(Bz$_2$dtc)$_2$], is soluble in deuterochloroform and exhibits signals in the 0-10 ppm range. Its dithiocarbamate ligands have been studied and do not rapidly exchange in solution.

Mixing iron(III), and nickel (II) complexes, e.g., Fe(Et$_2$dtc)$_3$ and Ni(Bz$_2$dtc)$_2$ establishes a competition between the metals for these dithiocarbamates and allows the determination of their relative stability. Preliminary results indicate no significant preference in systems studied, although the exchange rate may be estimated from the results. This combination was studied during last year’s research and the results were quite promising for a significant project. Once the exchanges of Ni(II) and Fe(III) are completed, thioseleno dithiocarbamates will be studied.

This is continued research from last year, but using different compounds such as the nickel and the thioselenodithiocarbamates.

CHED 914

Novel halometallates incorporating 2, 2'-biimidazole

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Several new halometallates incorporating 2, 2'-biimidazole (biim) were prepared via solvothermal synthesis. Single-crystal X-ray diffraction analyses reveal that biim in these structures displays a diverse mode of interaction, acting as hydrogen bond donors or acceptors, as well as serving as coordinating ligands. All of the above interactions play an important role in determining their overall crystal structures. Further, it is demonstrated here that biim may be used to increase the dimensionality of halometallates, which is a desirable feature for use of these materials as semiconductors. Full details of the crystal structures, synthesis, IR, and UV-Vis diffuse reflectance spectra will be presented.

CHED 915

Synthesis and high resolution powder diffraction pattern refinement of novel rare-earth substituted pyrochlores
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Novel quaternary pyrochlores of stoichiometry $\text{Ln}_x\text{Y}_{2-x}\text{Ti}_2\text{O}_7$ (where $\text{Ln}$ is lanthanum, neodymium, samarium, or gadolinium) were synthesized via traditional inorganic solid-state techniques and characterized by high resolution synchrotron powder X-ray diffraction. The known tertiary pyrochlore phase, yttrium titanium oxide ($\text{Y}_2\text{Ti}_2\text{O}_7$), served as the parent framework. Rietveld refinement of the new pyrochlore phases revealed that once the lanthanide element content reached values of $x = 0.1$ or $0.2$ for certain compounds, substitution became less favorable on the yttrium site and known tertiary phases of $\text{Ln}_2\text{Ti}_2\text{O}_7$ and $\text{Y}_2\text{Ti}_2\text{O}_7$ formed.

CHED 916

Synthesis and characterization of di-2-pyridyl ketone oxime complexes with transition and lanthanide metals

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The ligand di-2-pyridyl ketone oxime (dpko) was reacted with several transition- and lanthanide-metals under a variety of conditions. The resulting complexes showed nitrogen binding dpko to the metal centers. We saw one, two, or three nitrogen donors binding to a metal atom, depending on the metal center and reaction conditions—such as pH, solvent, and temperature. Here we present our synthetic pathways for several novel metal-dpko complexes, along with spectroscopic evidence supporting our structures. Spectroscopic studies include infrared, UV-Vis, magnetic susceptibility, and X-ray diffraction. We present the single crystal X-ray structure of a new Zn complex, which is structurally similar to a previously reported complex. We also present preliminary X-ray data on other metal-dpko complexes. Proton NMR was used to analyze the ZnCl$_2$ complex to determine the presence of hydrogen atoms, since it is difficult to find evidence of hydrogen with crystallography. Both the ZnCl$_2$ and ZnBr$_2$ complexes showed disorder in the oxime group of dpko when they packed. This was most likely due to the steric constraints of packing, where the halogen atoms may have caused distortion and bending in the nearby oxime group. The oxime group could have also packed facing the opposite direction in half of the molecules.

CHED 917

Synthesis and spectroscopic analysis of spin-crossover cobalt complexes

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Complexes that exhibit stable and easily controlled spin crossover behavior have immense current and future economic value in polymer chemistry and as molecular switches. We sought to synthesize a library of ligands based on bis(imino)pyridine (BIP), for which there is literature precedent of controlled spin crossover ability in Fe(II), and characterize their Co(II) complexes. Additionally, bisphosphine ligands were synthesized and their Co(II) complexes characterized. Methods used for characterization include X-ray crystallography, UV-Vis, DFT, NMR spectroscopy and measurement of magnetic susceptibility.

CHED 918

N-heterocyclic carbene ligands as supports for Cp*Co(I) fragments

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Rhodium and iridium complexes have found great utility as catalysts to induce C-H bond activation via dehydrogenative reactions. The use of cobalt to induce similar types of catalysis would be desirable due to the metal’s abundance and its lack of expense when compared to precious metals.

My project has focused on generating a reactive Co(I) complex that contains easily dissociable donor ligands to investigate the ability of 16 electron Cp*Co(L) fragments to stoichiometrically activate carbon-hydrogen bonds, where L in our case is an N-heterocyclic carbene (NHC) ligand. Upon addition of the bulky IPr carbene to the toluene triple decker complex 1, the 16 electron Cp*Co(IPr) (2) complex can be isolated and characterized by X-ray crystallography and reactivity studies. The reactivity of 2 is consistent with the desired unsaturated intermediate, undergoing ligand addition and oxidative addition chemistry. Computational and reactivity studies of 2 with C-H bonds will also be presented.

CHED 919

Developing a copper-catalyzed asymmetric reduction of 2H-azirines
Although several strategies exist that allow researchers access to chiral aziridines, one method that remains largely unexplored is the stereoselective reduction of prochiral $2H$-azirines. This body of research is focused on the development and optimization of a catalytic asymmetric $2H$-azirine reduction method that employs non-racemically ligated copper hydride. The synthetic route used to generate $2H$-azirine starting materials, and the methods explored for derivatization and resolution of chiral aziridine products will be reported along with the reaction development and optimization.

CHED 920

Investigation of the mechanism of arene perfluoroalkylation by iron perfluoroalkyl reagents

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A number of pharmaceutical drugs are trifluoromethylarenes, including the anti-depressant fluoxetine and type 2 diabetes medication sitagliptin phosphate. Direct conversion of aryl C-H bonds to aryl perfluoroalkyl groups would afford a wider variety of drug candidates more quickly than the methods currently used. An iron perfluoroalkyl reagent with a Ag$^+$ initiator has been shown to convert aryl C-H bonds to perfluoroalkylarenes. The mechanism by which the reaction proceeds is unknown, however. A kinetic isotope effect study shows that C-H bond cleavage is not the rate-limiting step, and a Hammett plot suggests that electrophilic or radical intermediates may be involved. p-bound Fe(arene) compounds were studied as possible intermediates in this reaction.

CHED 921

SNC-Rh(I) pincer complexes bearing thioether and N-heterocyclic carbene donors: Catalytic activity in transfer hydrogenation

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Although a number of symmetrical pincer-type complexes based on $N$-heterocyclic carbenes (NHCs) have been studied, unsymmetrical, mixed-donor NHC pincer complexes are far less common. Our previous work with Pd(II) complexes of a pyridine-bridged mixed thioether/NHC (SNC) pincer ligand has demonstrated some unique reactivity patterns endowed by the hybrid, non-innocent ligand system. Expanding upon this work, we now wish to describe the coordination chemistry of our SNC ligand toward Rh(I) and preliminary reactivity studies of the resulting complexes. Specifically, the SNC-Rh complexes described have been found to be efficient catalysts for the transfer
hydrogenation (TH) of a variety of ketone and aldehyde substrates. Rate data, reaction optimization, and suggestions for improved ligand design will be discussed.

**CHED 922**

**Utilization of pyrazole based copper complexes in atom transfer radical addition (ATRA) and atom transfer radical cyclization (ATRC)**

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Atom transfer radical addition (ATRA) is a fundamental and versatile organic process for C-C bond formation via addition of various alkyl halides across the double bond of an alkene catalyzed by copper complexes. Atom transfer radical cyclization (ATRC) is intramolecular ATRA with the alkene and alkyl halide on the same molecule. This reaction is important for the ability to form lactones, lactams and cyclic alkenes. The utilization of catalyst regeneration has dramatically decreased the amount of catalyst from to 5-30 mol% to 0.003 mol% with the aid of reducing agents such as 2,2′-azobis(2-methylpropionitrile) (AIBN) and ascorbic acid. Using these techniques, novel copper complexes, including [Cu(DPzPA)X]X (DPzPA=3,5-dimethylpyrazolylbis(2-pyridylmethyl)amine) (X=Br,Cl) and substituted ligands similar to this have been successfully employed for the ATRA and ATRC of alkyl halides such as CBr₄ and CCl₄ across various alkenes (1-octene, acrylonitrile, methyl acrylate, methyl methacrylate) in the presence of ascorbic acid as the reducing agent and various bromoacetamides and bromoacetates will be investigated for ATRC activity.

**CHED 923**
Iminophosphorane reagents for synthesis of electrically diverse diimine and N-heterocyclic carbene ligands

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Perturbing the electron withdrawing and donating properties of ancillary ligands can dramatically alter the reactivity of the corresponding transition metal complexes produced. In our efforts to develop general procedures for synthesis of electronically diverse diimine and N-heterocyclic carbene (NHC) ligands for supports of transition metals, we have found iminophosphorane intermediates allow for successful preparation of these ligands, as traditional condensation reactions led to low yields or intractable products with less sterically encumbering anilines. Scope of the ligand synthesis, by varying steric and electronic properties of substituents, will be addressed. The effect of diketone on the diimine synthesis will also be presented. Elaboration of the diimines to the corresponding NHC ligands will also be discussed, along with metallation reactions of both ligand classes with transition metals. With these ligands and metal complexes in hand, we hope to now explore electronic effects on catalysis from diimine and NHC metal platforms.
Comparative structural studies of $A_2B\text{TeO}_6$ ($A = \text{Ca, Sr, or Ba}; B = \text{Ca or Cd}$) double perovskites

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Tellurium (VI)-containing compounds have the potential to be useful as capacitor materials for applications utilizing microwave dielectrics. However, the synthesis and crystallography of double perovskites containing Te (VI) has not been extensively discussed in the chemical literature. We prepared six $A_2B\text{TeO}_6$ double perovskites, where A is one of the heavier divalent alkaline earth metal cations (Ca, Sr, or Ba) and B is either Ca (II) or Cd (II). Their crystal structures were determined by Rietveld refinement of X-ray powder diffraction data. This poster will focus on comparing the crystal structures of the six closely related double perovskites.

CHED 925

Design, synthesis, and characterization of zinc dithiolato/dithione (donor/acceptor) and vanadium dithione complexes

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Redox-active dithiolene ligands can exhibit multiple well-defined charged states, but their coordination chemistry is primarily focused on the ligand in the reduced state. Complexes of these ligands are not only biologically relevant, but have materials science applications as conductors, non-linear optical materials, and as tools for selective noble metal reclamation. In this study, we examined the case in which both fully reduced (dithiolate) and fully oxidized (dithione) ligands are bound to a zinc metal center. N,N’-diisopropylpiperazine-2,3-dithione ($i\text{Pr}_2\text{Dt}^0$) was chosen as the primary ligand in order to represent the desired fully oxidized character while maleonitriledithiolate ($\text{mnt}^2$) was chosen to represent the fully reduced state. We also investigated complexes of the dithione ligand with the group 5 transition metal vanadium in varying oxidation states. Complexes were characterized using $^1$H and $^{13}$C NMR, FT-IR spectroscopy, UV-vis spectroscopy, cyclic voltammetry, mass spectrometry, and X-ray crystallography.

CHED 926

Bis(oxazolinylphenyl)amines complexes
The syntheses of six bis(oxazolinylphenyl) amines complexes are the target of this research project. Iron, chromium, and scandium were the metals that were complexed, and the scandium was used as a control since it was previously synthesized. The importance of these complexes is that they have shown excellent catalytic abilities with the qualities that preserve a particular stereochemistry. Some of the examples are that the scandium complex will catalyze the polymerization of isoprene, and the resulting polymer is trans 1-4 polyisoprene, which has the same structure as balata or gutta-percha rubber that is obtained from trees in the tropic. Another reaction that has been catalyzed using these ligands is the Henry reaction. This reaction produces a nitro alcohol from and nitro alkane or nitro alkenes and ketones.

CHED 927

Synthesis metal-organic frameworks containing Mn-SALEN active sites and their catalytic properties

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Metal-organic frameworks (MOFs) are ideal platforms for the development of new catalysts due to the ability to change framework structure and tune active sites. We are exploring the synthesis of MOFs contain Mn-SALEN building blocks using direct synthesis and post-synthetic exchange. In this presentation, we will discuss the synthesis of these materials and their characterization, including powder X-ray diffraction and UV-vis spectroscopy. The results of catalytic reactions using these materials will be discussed.

CHED 928

Formation of mixed monolayers on TiO\textsubscript{2} and Ti-6Al-4V using carboxylic and phosphonic acids

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TiO\textsubscript{2} and its alloys are commonly used aerospace, high performance sports equipment, medical devices, and electronic devices. Self-assembled monolayers are being used in these industries to control and alter interfacial properties of substrates. The aim of this study is to form monolayers using a mixture of two different organic acid head groups. Self-assembled monolayers of, octadecylphosphonic acid, octadecanoic acid, and a mixture of both were covalently bound to the surface of Ti and Ti-6Al-4V metal oxide.
substrates. The result of this study indicates that the phosphonic acid head groups preferably binds to metal oxide surfaces. Diffuse reflectance infrared Fourier transform spectroscopy, matrix assisted laser desorption ionization time of flight spectrometry, contact angle analysis, and atomic force microscopy were used to determine the presence, binding, wettability, and uniformity of self-assembled monolayers on the metal surfaces. Octadecylphosphonic acids formed SAMs under the least stringent conditions, followed by mixed and then octadecanoic acid on both of these metal oxide surfaces.

CHED 929

Influence of annealing conditions on electrical properties in calcium cobalt oxide misfit layered compounds

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Polycrystalline calcium cobalt oxide misfit layered compounds were synthesized by annealing stoichiometric ratios of the powders in a furnace at varying times and temperatures. The powders were then pressed into a pellet, and again annealed under systematically varied conditions. X-ray diffraction data were collected for the samples in order to explore the structural dependence on the annealing conditions. Seebeck coefficients and electrical resistivity were then measured for the different samples, and the influence of the annealing conditions on the electrical properties explored.

CHED 930

Synthesis and characterization of symmetric and asymmetric bimetallic ruthenium(II) complexes

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Symmetric and asymmetric bimetallic ruthenium (II) complexes have been synthesized and characterized. The asymmetric complexes are of the form \([(TL)_2Ru(BL)Ru(Cl)(tpy)]^{3+}\), where TL is the bidentate ligand 1,10-phenanthroline (phen) or 2,2'-bipyridine (bpy), tpy is the tridentate ligand 2,2':6',2''-terpyridine and BL is a bridging ligand 2,3-bis(2-pyridyl)pyrazine (dpp) or 2,2''bipyrimidine (bpm). The symmetric complexes are of the form \([(TL)_{2}Ru_2(BL)]^{4+}\) and \([(tpy)(Cl)Ru_2(BL)]^{2+}\). Changing the TL ligand on the complexes should affect the light absorbing properties of the complexes and thus affect the photodynamic ability of the complexes.

CHED 931

Modification of MOF-5 hydrostability for peptide adsorption studies
Metal-organic frameworks (MOFs) are an intriguing class of hybrid materials that consist of infinite crystalline lattices formed by metal ions bridged by organic linkers. Their porous interiors have highly variable properties, depending on the metal ions and linkers used. To date, MOFs have primarily been examined for uses such as gas separation and storage and catalysis, but recently researchers have described the adsorption of proteins and peptides, such as cytochrome C and a trypsin digest of bovine serum albumin, in MOF pores. The MOF pore provides a stable, ordered environment in which to isolate and characterize peptides. Our research thus far has suggested that MOF-5 readily adsorbs proteins and peptides, however most preparations of MOF-5 suffer from water sensitivity. This is problematic because water or water-based solutions are the most relevant solvent for disease-relevant peptides. We therefore have explored reported methods to improve the hydrostability of MOF-5 through several doping techniques as well as annealing processes. We then studied the adsorption behavior of MOF-5 derivatives toward a number of peptides, the results of which are presented here. Through these studies we strive to understand which differences brought about by structural changes may facilitate selective peptide adsorption.

CHED 932

Investigating aurophilic interactions: Synthesis, structural, and photoluminescent properties of lanthanide cyanometallates containing 1,10-phenanthroline

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The preparation of lanthanide cyanometallates incorporating the organic ligand 1,10-phenanthroline (phen) will be presented. Two products result with general structural formulas of $[Ln(Au(CN)\textsubscript{2})(H\textsubscript{2}O)\textsubscript{2}(phen)]$ and $[Ln(Au(CN)\textsubscript{2})(H\textsubscript{2}O)\textsubscript{3}(phen)\textsubscript{2}][Au(CN)\textsubscript{2}]\textsubscript{2}H\textsubscript{2}O$ ($Ln$=Eu, Gd, Tb), in varying ratios, as determined by single crystal X-ray diffraction. The products are distinguishable by the number and types of aurophilic interactions, which studies have shown to facilitate energy transfer to lanthanides. Temperature-dependent photoluminescence properties of each product are also examined and can be attributed to long-range aurophilic interactions bewtween moieties, as well as intramolecular energy transfer in select compounds from the cyanometallate and/or phen ligands to the lanthanides.

CHED 933

Functionalization of the rho-ZMOF framework with fluorescent probes
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Here we report the functionalization of a zeolite-like metal organic framework of rho topology with two cationic dye molecules, methylene blue (MB\textsuperscript{+}) and a ruthenium(II) tris bipyridine complex ([Ru(bpy)\textsubscript{3}]\textsuperscript{2+}). The spectroscopic properties of both molecules are influenced strongly by host-guest interactions within the cavities of the rho-ZMOF system. These strong interactions can be seen by shifts in the absorption and emission spectra of the functionalized ZMOF with respect to the dyes in solution. The absorption and emission spectrum of MB-ZMOF are red shifted with respect to MB\textsuperscript{+} in aqueous solution, while the emission of [Ru(bpy)\textsubscript{3}]-ZMOF is blue shifted with respect to [Ru(bpy)\textsubscript{3}]\textsuperscript{2+} in aqueous solution. In the MB-[Ru(bpy)\textsubscript{3}]-ZMOF, the presence of MB\textsuperscript{+} quenches the emission of [Ru(bpy)\textsubscript{3}]\textsuperscript{2+} through an efficient energy transfer mechanism. Analyzing the lifetime of the [Ru(bpy)\textsubscript{3}]-ZMOF reveals that there are four unique environments within the system and a strong quenching of [Ru(bpy)\textsubscript{3}]\textsuperscript{2+} by rho-ZMOF network.

CHED 934

Synthesis and reactions of a tris-(tributylamine)triborate cation

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Tetrabutylammonium borohydride was heated at 130 °C under vacuum. Sublimation of the products at 100 °C leads to a viscous oil on the cold finger. The \textsuperscript{11}B and \textsuperscript{1}H NMR spectra indicate the formation of the B\textsubscript{3}H\textsubscript{5}·3N(C\textsubscript{4}H\textsubscript{9})\textsubscript{3}\textsuperscript{2+} cation. Reactions of this triborate derivative and further characterization data will be reported.

CHED 935

Reaction of 1-{2-[diphenylboryl]benzyl}-2,2,6,6-tetramethylpiperidine with hydrogen

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Frustrated Lewis Pairs (FLPs) have been shown to be able to activate small molecules such as H\textsubscript{2}. Building on last year’s reported synthesis of the new intramolecular FLP 1-
Mononuclear ruthenium complexes containing a tetradequate bipyridine dicarboxylic acid equatorial ligand and two N-heterocyclic carbene axial ligands were studied in order to determine their potential as catalysts for the oxidation of water and to determine how the structure of the complex was affected by varying the NHC ligand. In order to synthesize these complexes, [Ru^{II}(dmsos)_4Cl_2] was first prepared from RuCl_3 and dimethyl sulfoxide. Once this complex was prepared, the tetradequate bipyridine dicarboxylic acid equatorial ligand was added by reacting the [Ru^{II}(dmsos)_4Cl_2] complex with 2,2'-bipyridine-6,6'-dicarboxylic acid and dichloromethane. The ability of 5 different NHC ligands to subsequently form complexes was then studied. Characterization of these complexes via NMR and X-ray diffraction are contained herein.

Characterizing novel Mg alkoxide compounds as potential precursor electrolytes for next-generation batteries

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Novel magnesium-ion battery electrochemistries have received considerable attention from both academia and industry because such batteries have a high theoretical volumetric energy density when using a metallic Mg anode. One of the biggest hurdles facing the field is finding novel electrolytes that facilitate the reversible deposition of magnesium metal. Current state of the art magnesium electrolytes are based on Grignard-derived Lewis bases paired with Lewis acids of the type R_xAlCl_{3-x}. Our research is focused on investigating various synthetic pathways to produce halide-free Mg electrolytes, because chloride ions in these solutions corrode stainless steel battery casings via pitting. In pursuit of a halide-free electrolyte, we are focused on removing halide species from the magnesium starting material. In our research on magnesium alkoxides, we have found that the concentration of Lewis acid species has an appreciable effect on important characteristics of magnesium electrolytes, including the electrochemical window, deposition efficiency, conductivity, and peak oxidative stripping current. Characterizing and comparing alkoxide and other novel solutions under such
parameters is important in optimizing electrolyte systems. This investigation can hopefully enable future electrolyte systems to be halide-free when paired with an appropriate Lewis acid.

CHED 938

Fe₈-based MRI contrast agents targeted to breast and ovarian cancer cells

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Fe₈-based MRI contrast agents (CA) are currently being studied for potential use in breast and ovarian cancer screening. Conjugation of Fe₈ with tyramine-modified hyaluronic acid has high potential to get a new targeted MRI CA specific to CD-44 receptors. We have synthesized [Fe₈O₄(4-Ph-pz)₁₂Cl₄] and further reacted it with 4-NO₂-PhOH, which led to a model compound - molecular 4-substituted complex [Fe₈O₄(4-Ph-pz)₁₂(4-NO₂-PhO)₄]. It was characterized by IR, ¹H NMR, UV-vis, and single crystal XRD, which gives fingerprints for identification of more complicated conjugates. We have attempted conjugation of Fe₈ with tyr-HA, and final conclusions require more characterization by mass and Mossbauer spectroscopies, ¹H NMR.

CHED 939

Analysis of selective oligonucleotide release from photothermally active hollow gold nanospheres using surface enhanced Raman scattering

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Gene therapy is a rapidly developing DNA-based therapy that promises to provide treatment for oncological and inflammatory diseases. The creation of an effective DNA delivery vector is necessary for effective implementation of gene therapy. The photothermal release of single stranded DNA (ssDNA) from the surface of gold nanoparticles of different shapes and sizes is a promising mode of delivering DNA for gene-therapy applications. Here, we demonstrate the first targeted photothermal release of ssDNA from hollow gold nanospheres (HGNs). The HGNs used demonstrate a tunable localized surface plasmon resonance (LSPR) while maintaining size consistency. It was shown that HGN 760 and HGN 670 release significant amounts of ssDNA when excited via 785 nm and 640 nm lasers respectively. When excited with a wavelength far from the LSPR of the particles, the ssDNA release is negligible. This study also presents the first use of surface enhanced Raman scattering (SERS) to analyze the amount of ssDNA released from the surface of gold nanoparticles. As opposed to traditional fluorescence measurements, this SERS based approach provides quantitatively robust data for analysis of ssDNA release and lays a strong
foundation for future studies exploiting plasmonically induced ssDNA release. Furthermore, the HGN-based ssDNA system has potential to enable multi-step gene therapy treatments by utilizing different LSPR frequencies that deliver different ssDNA payloads. The DNA system demonstrated here can be applied to in-vitro studies and is expected to successfully release therapeutic DNA for treatment of disease.

CHED 940

Examining bridged oligothiophenes as small-molecule semiconductors in organic photovoltaic devices

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Organic photovoltaic devices (OPVs) have been an important focus of solar power research due to their low-cost fabrication and minimal environmental impact. Recent advancements in synthetic chemistry have enabled the tuning of organic semiconductor functionality at the molecular level, thereby enhancing device specificity and increasing OPV efficiency to levels near those required for commercial success. Specifically, oligothiophenes have been widely studied and demonstrate viability as charge transport materials in OPVs. In previous work, a series of highly redox-active fused tetrathiafulvalene-oligothiophene compounds were synthesized and exhibited complex electrochemical behavior ideal for organic electronic materials. The present study reports the synthesis of a novel family of bridged oligothiophenes with terthiophene, quinquithiophene, and septithiophene backbones (1, 2, 3) for application in OPV devices. The structures were studied with UV-Vis spectroscopy, cyclic voltammetry, and tested for OPV performance. Compound 3 exhibited the most red-shifted absorbance (461 nm) and the lowest electrochemical HOMO-LUMO gap (2.13 eV), and OPVs fabricated with this analog demonstrated successful photocurrent generation. Meanwhile, devices fabricated with 1 achieved PCEs of nearly 10 times those made with 3, even with less-desirable absorbance properties and redox behavior. Variations in the optical and electrochemical HOMO-LUMO energy levels among the three structures can be attributed to differences in the length of their conjugated backbones. While the properties of 3 were promising, its poor solubility was an obstacle for device processing and fabrication. This likely resulted in unfavorable film morphology, which impeded charge transport and limited photocurrent generation. Future efforts are needed to optimize the morphology and processing of films in order to best exploit the characteristics of bridged oligothiophenes and other organic semiconductors for energy applications.
Series of bridged oligothiophenes for OPV applications.

CHED 941

Synthesis and characterization of CdSe quantum dots via low temperature thermolysis of a single organometallic precursor

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The preparation of CdSe nanocrystals based on a low temperature thermolysis of a single organometallic precursor in different experimental conditions and their characterization are reported. This method is of interest because the single precursor synthetic route can be beneficial for facilitating the nucleation of quantum dots. However, the single precursor method poses challenges as the presence of selenium in the organometallic precursor drastically affects the solubility and stability of the organometallic precursor. The formation and growth of CdSe nanocrystals have been studied upon changing the experimental preparation conditions (solvent and stabilizer). The nanocrystals were characterized in terms of optical properties (absorption and emission spectra) and morphological properties (AFM measurements). In the synthesis involving thioglycerol as both a solvent and stabilizer, the nanocrystals grew to an average diameter of 5.4 ± 2.5 nm. The synthesis involving 3-MPA, as both a solvent and stabilizer, the nanocrystals grew to an average diameter of 5.2 ±1.1 nm. The results indicate that nanoparticles of similar size are obtained for both conditions, but when thioglycerol is used as stabilizer the dispersion in dimensions is wider.

CHED 942
Stabilization of light-harvesting complexes from *Rhodopseudomonas acidophila* in dipeptide gels

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Photosynthetic organisms have utilized light harvesting complexes as a method of harnessing energy from the sun for millions of years. Humans have mimicked this ability with the use of photovoltaic materials of various synthetic sorts, but the great environmental and fiscal benefits of more conventional biochemical systems of light harvesting make them a topic well worth pursuing. Unfortunately, light harvesting complexes can be very unstable in aqueous media. The goal of this study was to establish the stabilizing or destabilizing properties of dipeptide gel matrices when light harvesting complexes from *Rhodopseudomonas acidophila* were embedded within them. By monitoring protein stability with absorbance and fluorescence spectrophotometry, gel viscosity through rheometry, and directly observing the behaviour of the complexes in situ, it was established by this study that FmocYL and FmocYN dipeptide matrices had a stabilizing effect on both Light Harvesting complex 1 and Light Harvesting complex 2.

CHED 943

**S2O3** treated cuprous oxide electrochemical reactivity with carbon dioxide

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This poster is a study into the effects of the electrochemical properties when a polished copper disk treated with cuprous thiosulphate film is reacted with carbon dioxide. The film shows higher selectivity towards products containing two carbon atoms than other reported copper based cathodes. Our results lead us to believe that the film is stable, lasting over an hour and produces significant amounts of ethylene and ethanol. These percentages can reach over 30% for ethylene production and 20% for ethanol production. This area of research needs more investigation; however, this is a good introduction into showing the potential of the cuprous thiosulphate.

CHED 944

**Synthesis and characterization of divalent ligands with photoswitching capabilities**
The use of azobenzenes as photoswitchable catalysts has inspired the development of numerous light-controlled ligands for transition metals. The purpose of this study was to develop an efficient multi-step synthesis of novel divalent azobenzene ligands that—upon metal coordination—can be used to control reactions with light. Two different salophen azobenzene ligands (Figure 1) were proposed, and their photoswitching abilities were investigated using UV spectroscopy. This study has resulted in the successful synthesis of both ligands 1 and 2, which exhibit satisfactory photoswitching abilities between the cis and trans isomers, upon irradiation by different wavelengths of light.

**Figure 1.** Proposed and synthesized azobenzene ligands

**CHED 945**

Optimization of ferroelectric behavior in lead-strontium-titanate (PST) ceramic thin films

**Griffin Ruehl**

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Ferroelectric ceramic thin films have arisen as promising candidates for applications as capacitors, FeRAMs, energy harvesters, and sensors. A recent solution synthesis and photolithography preparation method has presented a desirable means of film preparation, but is troubled by final samples with low ferroelectric behavior. This study sought to enhance the ferroelectric behavior by optimizing the synthesis parameters of sintering temperature and film thickness.

**CHED 946**

**Synthesis and characterization of light-responsive hybrid polymer thin films**

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Stimuli-responsive polymers have a multitude of applications in the biomedical and materials science fields. Surface coatings of hybrid polymers are of particular interest because of their tunability and adherent properties. While some hybrid polymer surfaces have been designed to respond to environmental stimuli such as temperature, pH, and light, there still remains a need for shorter, less toxic synthetic routes for responsive polymers. The aim of this study was to create a light responsive thin film based off of the PMSSQ-PStCHO hybrid polymer. Functionalization was to be performed through three post-polymerization modification steps, based on the Kabachnik-Fields reaction. This pathway allowed for a diverse panel of hybrid polymer coatings ready for chromophore addition to be synthesized. Produced surfaces were analyzed with FTIR spectroscopy and contact angle measurements to determine hydrophobicity. The feasibility of the synthetic route and surface characteristics of the precursors to light-response was ultimately established.

**CHED 947**

**Synthesis and exploration of spiropyran-containing poly-(3-hexylthiophene) oligomers**

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A route was explored to synthesize a new iodine-functionalized spiropyran to later incorporate into poly-(3-hexylthiophene) (P3HT) polymers via a Stille cross-coupling reaction. P3HT oligomers of approximately 9 monomers were synthesized using GRIM polymerization and procedures known in literature, as it is a popular polymer used for studying conjugated polymeric systems and developing organic semiconductors. By synthesizing and functionalizing spiropyrans with P3HT polymers of varying lengths, we hope to analyze the effects spiropyran switching may have on the semiconductive properties of P3HT polymer systems of different lengths.
CHED 948

Growth of carboxylated UiO-66 metal-organic framework crystals for CO$_2$ capture

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A variety of methods – direct solvothermal synthesis, synthesis with a mixed ligand copolymer, and ligand exchange – are employed to grow UiO-66-(COOH)$_2$, a UiO-66-derived metal-organic framework that can be used for CO$_2$ capture. It is shown that all three of these methods result in products with high bulk crystallinity, and that synthesis of UiO-66-(COOH)$_2$ through ligand exchange increases CO$_2$ uptake by as much as 30% as compared to pristine UiO-66. The success of the ligand exchange method in particular is confirmed by these results and by NMR, which shows 5.4 – 13.3% incorporation of the new ligand. A combination of particle size, BET surface area, and CO$_2$ adsorption data suggests that ligand exchange may be the most favorable method of synthesis for this promising and difficult crystalline compound.

CHED 949

Development of a sustainable and efficient protocol for palladium-catalyzed Sonogashira cross-coupling reactions

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A focus of green chemistry research is the development of efficient and sustainable methodologies to be used in syntheses. The Sonogashira cross-coupling is a reaction which is heavily used in a variety of fields. This present research focused on developing a sustainable and efficient protocol for the Sonogashira cross-coupling reaction by (i) testing the efficiency of a palladium catalyst on a supported thiazole network, (ii)
researching the usability of green solvents, and (iii) designing and testing an easily recoverable supported base to minimize workup requirements. The results showed that use of a supported ionic-liquid phase (SILP) palladium catalyst was more efficient than that of unsupported catalysts. Additionally, the catalyst proved to be efficacious in a variety of Sonogashira cross-coupling reactions using a recoverable and reusable acetonitrile azeotrope. Piperazine was attached to three different resins and its efficacy as a base and the ease at which it filters was verified. The N-polystyryl-piperazine attached to the Merrifield resin had greater than 99% conversion and was easily filtered resulting in the same purity as work-up conditions. The use of a supported base also reduced palladium which leached into the final product from the SILP catalyst. In conclusion, because of our use of a catalyst with minimal leaching, a solvent which is recoverable and reusable, and a base that removes the necessity for a workup, a sustainable and efficient protocol has been established for the Sonogashira cross-coupling reaction.

CHED 950

Investigation of temperature dependent electrochemical CO₂ reduction on copper by gas chromatography including formic acid detection via derivatization

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With increasing levels of CO₂ in the atmosphere and limited fossil fuel resources, the electrochemical reduction of CO₂ is a promising technique to produce fuel and other industrial products from CO₂ emissions, but more research is necessary to understand the selectivity of the products and to optimize efficiency. The purpose of this project was to understand the effects of temperature on electrochemical reduction of CO₂ with a copper electrode at a current density of 10 mA/cm² and to develop a method that uses a headspace gas chromatographer (GC) to measure the formic acid produced. The esterification of formic acid to ethyl formate provides a means to quantifiably measure formic acid using a GC. In this study, the electrochemical reduction of CO₂ was tested at four temperatures: 5°C, 10°C, 15°C, and 22°C. The main products of the reaction in decreasing faradaic efficiencies were hydrogen, methane, carbon monoxide, and ethylene. The results of the temperature experiments agree with the trends found in literature for all products except CO, but the product distribution was very different, possibly due to the greater current density and more negative potentials. CO₂ reduction competes with H₂O reduction and increases as temperature decreases due to increased solubility of CO₂. Hydrogen evolution dominates the reaction, possibly due to the very negative potential of the experiment. Trace amounts of methanol were the only liquid products detected at all four temperatures, but the lower total faradaic efficiencies at lower temperatures suggest that more liquid products are produced as temperature decreases but were oxidized at the counter electrode. Since previous studies focused on the reduction of CO₂ with 5 mA/cm² current density, these results provide insight into the reduction of CO₂ at a greater current density.
Modification of ultrafiltration membranes for improved purification of nanoparticle dispersions

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The need to fractionate and purify solutions, particularly nanoparticle dispersions, poses a challenging task in multiple areas of research, including biochemical and medicinal. Many former techniques in this area, such as size exclusion chromatography and gel electrophoresis, are quite time-extensive and low-volume. Since a variety of nanoparticle properties depend on size and uniformity, the exploitation of ultrafiltration (UF) membranes provide a fast, efficient, and easily-scalable method for the purification of broad nanoparticle distributions. However, the fouling tendencies of such membranes yield a short life-span and hinder the purification properties of the material. Through the application of surface modification via polymer grafting, an anti-fouling layer may be added, extending the longevity of the membranes. The sieving properties of these modified membranes, coupled with pressure driven processes, provide for a precise fractionation with little to no dilution or contamination of target products.

Development in poly-thiophene and poly-benzotriazole block copolymer for use in polymer solar cell

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Polyfluorene, polythiophene, and polybenzotriazole syntheses were attempted with the goal of creating a block copolymer. Synthesis of polyfluorene was unsuccessful; it is believed that the presence of moisture in the air caused the reaction to fail. Due to this failure, polythiophene was focused on as the donor block of the block copolymer. Polybenzotriazole was used as the acceptor block of the block copolymer. Successful synthesis of each of these molecules was characterized with \textsuperscript{1}H and \textsuperscript{13}C nuclear magnetic resonance (NMR), mass spectrometry, gel permeation chromatography (GPC), and uv-visible absorption spectroscopy. UV-visible absorption analysis further confirmed polybenzotriazole and polythiophene synthesis with the observance of a shift in wavelength and higher extinction coefficient. The attachment of the donor and acceptor block polymers together to form D-A type copolymer was attempted, and will be studied further in future.
Experimental studies of shutdown procedures for water-gas shift catalysts in high temperature polymer electrolyte fuel cell systems

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While significant progress has been made thus far in developing fuel cell-based auxiliary power units with diesel and kerosene reforming, several key challenges remain in optimizing system performance. This study specifically addressed issues regarding shutdown behavior of the water-gas shift reactor, a critical component of the system designed to reduce carbon monoxide levels upstream of the fuel cell. In order to develop a protocol to maximize stable carbon monoxide conversion levels, this work investigated the performance of a commercial water-gas shift catalyst, with focus on the effect of two main parameters: inlet gas stream composition during operation and purge atmosphere during shutdown. The results revealed that the presence of higher hydrocarbons in the inlet gas decreased the selectivity of the catalyst but did not negatively influence activity and stability during operation or shutdown. Additionally, performing an air purge during shutdown consistently improved catalyst performance. These results will help guide future optimization efforts, contributing to the overall improvement of the fuel cell system.

CHED 954

Organoiridium catalyst as a functional mimic of both oxygen evolving complex and hydrogenase

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[Cp*Ir(κ²–N,N–pycxa)Cl] complex (1; κ²–N,N–pycxa = 2-picolinamide) is an effective catalyst for (i) water oxidation to molecular oxygen driven by CAN, (ii) hydrogenation of NAD⁺ to NADH, using HCOOK as hydrogen source, and (iii) dehydrogenation of NADH to NAD⁺. Performances are remarkable for all three catalytic reactions and particularly for (ii), for which catalyst 1 exhibits a TOF three times higher than that of the best iridium catalyst reported so far. Kinetics studies indicate that reaction (ii) is inhibited by the presence of a high concentration of NAD⁺, likely due to the formation of a 1-NAD⁺ adduct. Evidence of formation of the latter were obtained by ¹H NOESY NMR experiments that show NOE contacts between protons of Cp* and ortho protons of the pyridyl ring of nicotinamide. The production of H₂ from reaction (iii), directly evaluated by GC, consistently corresponds to the formation of NAD⁺, evaluated by ¹H-NMR spectroscopy, in terms of rate and quantity. Nevertheless, consumption of NADH is much faster due to the formation of a second “NAD⁺-like” species that we tentatively assigned as α-NAD⁺.
CHED 955

Threshold implementation and testing in local coupled cluster doubles theory (PNO-LCCD)

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In this work, Local Coupled Cluster Theory methodology is implemented and tested within the framework of the Molpro electronic structure software suite. Analysis is conducted on a threshold for neglecting a portion of the “disconnected” pair contributions in the Local Coupled Cluster Doubles (PNO-LCCD) method. This threshold, which is based on the magnitude of the overlap matrices, shows promising results in memory savings, while maintaining calculation accuracy. Local Coupled Cluster Theory Doubles is also tested and compared to density functional theory for two large molecular systems, the dissociation of a gold (I) aminonitrene complex and the reaction path of an enantioselective Strecker catalyst.

CHED 956

Identification and synthesis of novel cyclin-dependent kinase inhibitors

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Cyclin-dependent kinases (CDKs) are serine/threonine protein kinases that play major roles in the cell cycle regulation process. Alterations of CDK activity are associated with tumor growth, proliferative renal diseases, and neurodegenerative disorders. Inhibition of CDK activity can be achieved through a variety of approaches, including the prevention of ATP binding to CDK through the use of small molecule competitive inhibitors. Our recent work investigating indazole and phthalimide compounds as potential small molecule CDK inhibitors led us to the development of 2 novel indazoles and the identification of a phthalimide compound showing significant activity in CDK1 and CDK2. These compounds all showed sub-micromolar inhibition potency in CDK1 and CDK2 kinase inhibition assays in-vitro. The synthesis and biological activity of novel CDK inhibitors are presented.

CHED 957

Using isothermal titration calorimetry (ITC), circular dichroism (CD) and DNA unwinding studies to investigate the DNA binding properties of abietane diterpenes natural products
It now well established that several known medicinal drugs interact with DNA as a means of carrying out their actions. Some of the most notable members of the DNA binding medicinal drug class are either directly derived or inspired from natural products. Ongoing research into the therapeutic potential of natural products is therefore essential to the development of novel therapeutic drug candidates with improved efficacy and reduced side effects. Characterization of the DNA binding capabilities can provide insights into understanding why and how these potential therapeutics bind to DNA. The abietane diterpenes are a class of natural products isolated from certain plants (e.g., *Hyptis verticillata*) known in Jamaican folklore for their medicinal benefits, including anti-microbial, anti-oxidants, anti-inflammatory as well as anti-cancer activities. To date, many aspects of the mode of action of abietane diterpenes are still unclear. We have carried out preliminary studies on selected homologous abietane diterpenes using ITC, CD and a topoisomerase DNA unwinding assay, in order to determine whether these compounds bind to DNA, and if so, their preferred binding mode and relative affinity. Our ITC studies show strong interactions ($10^7$-$10^8$ M$^{-1}$) between the abietane diterpenes of this study and DNA. Binding of these compounds likely involve a non-intercalative mode, possibly via the minor groove. This was also supported by CD studies as well as topoisomerase I DNA unwinding assays. The strength of the DNA binding was substituent driven with 12-OH vs 12-OMe having different binding strengths. Substituent bulk/hydrophobicity may also be a factor. These early findings are very promising and warrant further investigations.
ITC data for the binding of a representative abietane diterpene to DNA

CHED 958

Study of antitumor effects of quercetin and amine or methoxy polysubstituted derivatives on metastatic and non-metastatic mouse cells

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The tumor-preventative effects of the biologically created quercetin chemical have historically been studied and found to be not efficient enough to be used as a chemotherapeutic drug. Amine and methoxy substituted derivatives of quercetin are being synthesized and tested in seeking a new molecule with better applications as a chemotherapeutic drug. Synthesized derivatives are also tested in conjunction with resveratrol—a second natural compound found to have anti-tumor effects—for a synergistic effect. The synthesized molecules are tested against several separate mouse lines, one that is a metastatic cell culture (T3HA), a non-metastatic cell culture (T2A), and a normal cell line (NIH SWISS).

CHED 959

Prevention and disruption of bacterial biofilms
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Millions of people are infected yearly with resistant pathogens, including MRSA (methicillin-resistant *Staphylococcus aureus*), a biofilm-forming pathogen that is often transferred to patients from contaminated surfaces. Therefore, improved methods to destroy biofilm-encapsulated pathogens or to prevent their initial formation are required. Development of a safe treatment against biofilms by integrating organic salts, or ionic liquids (ILs), into different surfaces will inhibit bacterial contamination and biofilm formation from the onset. Textiles were integrated with ILs to prevent formation of biofilms/bacterial growth, and were also treated post-exposure to determine if the biofilms could be destroyed post-contamination. Effectiveness of newly designed ILs were tested via inhibition zone studies on LB agar plates, and post-treatment samples were analyzed via scanning electron microscopy for presence of bacteria. The bacteria tested included *Pseudomonas aeruginosa*, *Staphylococcus epidermidis*, and *Escherichia coli*. These microbes are similar to MRSA in that they form biofilms comprised of extracellular proteins, DNA and polysaccharides. Bacterial colonies encapsulate themselves with biofilms to provide protection from threats, including antibacterial drugs. By integrating ionic liquids into textiles, formation of biofilms can be prevented by IL solvation and sequestering of the extracellular biofilm components. This research could have tremendous implications regarding defeating bacteria that are resistant to existing treatments due to biofilm encapsulation. Additionally, the results could lead to new antimicrobial textiles and new approaches to prevent adherence and growth resistant biofilm-encapsulated pathogens.

CHED 960

**Transition metal complex dual CXCR4/CCR5 antagonists**

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Chemokine receptors, together with their specific natural ligands, play a role in a number of disease states. We propose to systematically synthesize and evaluate potential CXCR4/CCR5 dual antagonists based on our published potent transition metal complex CXCR4 antagonists and the only known dual CXCR4/CCR5 antagonist (whose potency is not desirably high against either receptor). Upon synthesis and chemical characterization, and with the help of collaborators, we will evaluate the antagonism of both CXCR4 and CCR5 in cell lines previously developed for such studies—with the results of these screens feeding back into the iterative re-design of additional dual antagonist complexes. Synthetic routes were developed extending side- and cross-bridged ligand syntheses to include dichloropyridine moieties to impart CCR5 activity on
tetraazamacrocycles. Cu$^{2+}$, Ni$^{2+}$, Co$^{2+}$, and Zn$^{2+}$, complexes were synthesized. Electrospray mass spectra, UV-Visible spectra, cyclic voltammograms, and $^1$H and $^{13}$C NMR spectra were collected to characterize the complexes. The ligand synthesis of the dichloropyridine containing ligands is more synthetically challenging than our typical ethyl cross-bridged ligands. However, single-macrocycle and bis-macrocycle ligands have been made. Complexation with the desired metal ions proceeded as expected. Characterization of the metal complexes is ongoing. While CXCR4/CCR5 dual antagonist tetraazamacrocycles are challenging to produce, once synthesized, metal ion complexation proceeds smoothly following known procedures. The resulting complexes will inform our understanding of the requirements for producing efficient CXCR4/CCR5 dual receptor antagonists.

**CHED 961**

New thiazolecarboxaldehyde thiosemicarbazone ligands: NMR structure studies and complexation with Cu(II) to form [Cu(TZCA-ETSC)Cl] and with Pd(II) to form [Pd(TZCA-ETSC)Cl]

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Our research team has synthesized new compounds involving the reaction of thiazolecarboxaldehyde (TZCA) with several thiosemicarbazides to form new thiazolecarboxaldehyde thiosemicarbazone (TZCA-TSC) ligands. The different TZCA-TSC ligands were synthesized, recrystallized, and analyzed using $^1$H NMR, which showed evidence for the proposed structures of the ligands. These ligands were then used to form metal complexes with Cu$^{2+}$ and Pd$^{2+}$, and we present the NMR characterization of the d$^8$ palladium complexes. We have performed anti-poliferative MIC (minimum inhibitory concentration) studies using different microbes with the ligands and Pd and Cu complexes in order to determine the anti-microbial properties of each TSC compound synthesized, and have found Cu and Pd metal complexes of these ligands have significant anti-poliferative activities.

**CHED 962**

New 2-acetyl-6-bromopyridine thiosemicarbazone ligands: NMR and complexation with Cu(II) to form [Cu(ABrPy-TSC)Cl] compounds

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Our research team has synthesized new compounds involving the reaction of 2-Acetyl-6-bromopyridine (ABrPy) with several commercially available thiosemicarbazides to form a series of new 2-acetyl-6-bromopyridine thiosemicarbazone (ABrPy-TSC) ligands.
The new ABrPy-TSC ligands were synthesized in the lab, recrystallized, and analyzed via $^1$H NMR and $^{13}$C NMR spectroscopy. The NMR spectra show evidence for the proposed structure for the ligands. These ligands have been used to form metal complexes with Cu(II). We have performed MIC (minimum inhibitory concentration) studies using seven different microbes with the ligands and their Cu complexes in order to determine the anti-microbial properties of each TSC compound synthesized, and we have found that the Cu metal complex of the ligands have significant anti-proliferation activities.

CHED 963

Comparison of a series of 2-acetyl-6-methoxypyridine (AMOPY) thiosemicarbazone metal complexes

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We have synthesized several new 2-acetyl-6-methoxypyridine thiosemicarbazone (AMOPY-TSC’s) compounds, and characterized them by proton NMR spectroscopy. These new compounds have been used as ligands in reactions with Cu(II) and Pd(II) to form new metal complexes. The copper complex [Cu(AMOPY-tBTSC)Cl] has high antiproliferative activity against microbes, especially gram positive bacteria. The minimum inhibitory concentrations of each compound was determined with four bacteria (Bacillus subtilis, Staphylococcus aureus, Escherichia coli, and Pseudomonas aeruginosa), two yeast (Candida albicans and Saccharomyces cervisiae), and a mold (Aspergillus niger).

CHED 964

New terpenoids from the Caribbean gorgonian Pseudopterogorgia acerosa

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One new cembranoid and two new pseudopteranoids were found in the gorgonian coral Pseudopterogorgia acerosa collected in the Bahamas. Similar compounds from this species have been shown to have a variety of biological activities. Isolation of these compounds was performed using a combination of column chromatography and preparative high pressure liquid chromatography. The structural elucidation was performed using extensive spectroscopic analysis including mass spectrometry, 1D and 2D NMR spectroscopy. In this poster we will discuss the isolation and structural elucidation of the novel compounds.
CHED 965

Antibacterial activity of 4-alkyl and 4-arylbutenolides
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The butenolide and 5-hydroxybutenolide are common moieties found in a variety of synthetically useful compounds, several natural products, and drugs with diverse biological activities. As part of on-going project to discover new antibacterial compounds, several 4-alkyl and 4-aryl-5-hydroxybutenolides have been synthesized and tested against a variety of bacterial strains. This study has revealed key structural features in butenolide containing compounds necessary for bacterial growth inhibition.

CHED 966

Insulin-specific inhibition of insulin-degrading enzyme using a synthetic receptor

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Insulin is a hormone produced in the pancreas that regulates glucose metabolism. One way that insulin is degraded in the body is by a protein known as insulin-degrading enzyme (IDE). The synthetic receptor, cucurbit[7]uril (Q7), has been shown previously to bind with high affinity to the N-terminal phenylalanine of the B-chain of human insulin, which is also a site of specific interaction between insulin and IDE. In this project, we attempt to use Q7 to block the interaction of insulin with IDE and thereby inhibit the degradation of insulin by IDE. A time-resolved fluorescence assay using an antibody sandwich approach was used to determine the concentration of insulin at nanomolar concentrations before and after treatment with IDE and in the presence of Q7. In addition, the IDE-mediated degradation of insulin was monitored in time using HPLC.

CHED 967

Manganese-52: cyclotron production and PET/MR imaging

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Manganese is necessary for life because it is a cofactor for many enzymatic reactions, but can be toxic in large doses. Manganese also has medical imaging applications; manganese can be used for magnetic resonance imaging (MRI) while the radionuclide manganese-52 (52Mn) can be used for positron emission tomography (PET). Based on the biological roles of manganese and the fact that MR and PET complement one another in terms of sensitivity and resolution, 52Mn could be a useful radiotracer for PET/MR imaging.
$^{52}$Mn was produced by bombarding a natural chromium foil with ~13 MeV protons from the CS-15 cyclotron at Washington University School of Medicine (WUSM) and purified using a cation-exchange column. The foil was dissolved in concentrated hydrochloric acid to produce Cr$^{3+}$ and Mn$^{2+}$ ions and brought to dryness. It was then reconstituted in 1.5 M sulfuric acid and loaded onto the column. Most of the Cr$^{3+}$ went into the flow through, while the $^{52}$Mn was immobilized on the column. For some experiments, 0.5 M HCl was used to wash more Cr$^{3+}$ off the column. Next, 10 mM hydrazine sulfate was used to ensure proper manganese oxidation state. Finally, multiple experiments were conducted to elute $^{52}$Mn$^{2+}$ in various solutions, including hydrochloric acid and ammonium oxalate. Additionally, a variety of methods were used to quantify the Cr$^{3+}$ fractions eluted from the column.

Phantoms consisting of 28 15 mL tubes in a rack with a gradient of both $^{52}$MnCl$_2$ and nonradioactive Mn(II)Cl$_2$ were imaged using the mMR scanner, a PET scanner inside of an MRI machine that takes simultaneous PET and MR images. A 30 minute PET scan was conducted, as well as many MR scans with varying inversion times (TI). MR and PET signal gradients were observed for MnCl$_2$ and $^{52}$Mn concentrations, respectively. Two male C57-Black 6 mice were injected with 50 mL (41 uCi) of $^{52}$MnCl$_2$. The injection was prepared by eluting with ammonium oxalate, and then evaporating and reconstituting the product in 6 M HCl. Two PET scans, at one hour and three days post-injection, were taken before sacrificing the mice to investigate the manganese biodistribution. The PET/CT showed a large amount of activity in the kidney and salivary gland, and the biodistribution study showed that much of the injected manganese went to the pancreas and kidney. The study indicated that manganese-52 could be purified sufficiently for injection, and also provided a sensitive reading of the in vivo kinetics of manganese.

CHED 968

4-methylimidazole effect on extrinsic tooth discoloration: A computational model of the Maillard reaction

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Among the most common reasons for extrinsic tooth discoloration is the exposure of enamel and dentin to consumed pigments and coloring agents, where different foods and drinks are the main source of exposure. The focus of this study was on 4-Methylimidazole (4-Mel), the ingredient in commercial soda products that provides their caramel color. When 4-Mel was modeled using the computer programming software package, SPARTAN, using Density Functional Theory with the b3lyp/6-311++G(d,p) functional to address the electronic structure, we found that absorption occurred in the ultraviolet range. Further research indicated that the Maillard reaction is responsible for the color developed by this molecule. Using a fructose molecule (which is an ingredient in soft drinks) as a model, we explored the variation in ultra violet-visible absorption spectra throughout the Maillard reaction. The effects of the media were also taken into consideration to propose a realistic model for the discoloration.
CHED 969

Computational model for tooth discoloration with sunset yellow treated with H$_2$O$_2$

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Several everyday goods are known sources of extrinsic tooth discoloration. This research project focused on the reaction of a specific molecule, sunset yellow (C$_{16}$H$_{10}$N$_2$Na$_2$O$_7$S$_2$) with a commonly used teeth whitening agent. Sunset yellow can be found in foods such as Doritos and energy drinks. Our preliminary calculations for the ultra violet-visible absorption spectrum performed with Density Functional Theory with the EDF2 – 6-31**G functional using the Spartan software package showed values within the range of 380-520 nm, compatible with the yellow to red color of sunset yellow. Treatment of the discoloration effects involve the use of hydrogen peroxide. Three key aspects of the efficacy of hydrogen peroxide as an oxidizer used in teeth whitening are exposure time, intimacy of hydroxyapatite with the H$_2$O$_2$, and concentration. A possible reaction pathway for the interaction of H$_2$O$_2$ with sunset yellow was proposed as a model to study the effects listed above. Calculations were performed to fully account for the electronic structure of the molecules involved.

CHED 970

Synthesis of a highly fluorescent aminopyronin calcium sensor

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Fluorphores are widely used as probes in biology as an aid to visualize cellular activities. However, many of the fluorophores currently available to biologist often are metabolized rapidly, have difficulty passing through cellular membranes, are excreted from cells at a rapid rate, or have other complications. This is especially true for fluorescent probes used to detect calcium ions. Fluorinated aminopyronin fluorophores possess many characteristics that could lead to promising new calcium sensors, given that they are linked to Ca$^{2+}$ chelating moieties such as 1,2-bis(o-aminophenoxy)ethane-N,N,N',N'-tetraacetic acid (BAPTA). For example, aminopyronins rapidly diffuse through cellular membranes and covalently link to the side chains of lysine and arginine residues on proteins within the cell. In the synthesis presented, we have generated a fluorinated aminopyronin molecule with olephinic attachment points to which BAPTA or other molecules of interest could be tethered through palladium coupling or olephin metathesis. This aminopyronin was generated in 5 linear steps from commercially available material in an overall yield of approximately 50%. We are currently examining methods of appending BATPA to the synthesized aminopyrinin.
Evaluation of organogel nanoparticles as a means of drug delivery

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Many new active pharmaceutical ingredients cannot be easily administered due to their hydrophobicity. Recently, an innovative drug delivery system called gelosomes has been developed to combat this problem. This system is made of gelled nanoparticles of castor oil containing 12-hydroxystearic acid (gelator) and polyvinyl alcohol (stabilizing agent). These nanoparticles are formed by the emulsification of melted organogel with an aqueous polyvinyl alcohol solution and subsequent cooling below the gelation temperature. In this study, a hydrophobic drug molecule was dissolved in these particles, and the in vitro drug delivery rates were studied. The hydrophobic molecule, indomethacin (logP = 4.2), has a carboxylic acid functionality and a water solubility of 0.9 mg/mL at pH 7.4. It was shown that this drug molecule could effectively be solubilized at 3% by weight within an organogel made of castor oil and 15% by weight 12-hydroxystearic acid, without affecting gelation. Furthermore, the nanoparticle emulsion displayed stability for more than four weeks. Dialysis of the indomethacin gelosomes exhibited an almost identical release profile to the drug alone. On the contrary, a model molecule with a basic functionality and even greater hydrophobicity, nile red (logP = 5.0) (water solubility < 1 µg/mL), showed no release from the gelosomes, even after 30 hours of dialysis. Ultimately, the difference in solubility due to the molecules’ chemical structures affected their dialysis profiles, and should be considered as quite important when selecting drugs for gelosome delivery.

Progress toward synthesis of photomodulated SIRT1 activators
Sirtuin (silent mating type information regulation 2 homology, SIRT1) is an enzyme, which has been found to play a critical role in cellular signaling and deacylation of transcription factors. While, the specific function of SIRT1 is currently under investigation, it was originally thought to play a role in tumor growth until a recently identified its role in tumor suppression. The role of SIRT1 appears to vary in function depending upon cell type, location, and in a time dependent manner, increasing the need for tools to study its function in a time and location dependent way. Several small molecules have been reported that bind allosterically to SIRT1, inducing a conformational change and increasing its activity. Still, efforts to study this protein in a spatially and temporally controlled way have been slowed by the need for appropriate chemical tools. Fortunately, light-modulated small molecule activators of SIRT1 present an opportunity to answer some of the open questions regarding this protein. We herein describe the construction of a library of photoisomerizable small molecules to bind SIRT1, outline their screening for SIRT1 activating activity using a commercially available fluorescence assay, and discuss the practical applications of photoisomerizable allosteric activators of SIRT1. Specifically, we describe how the photoisomerizable feature will be advantageous in the study of cellular SIRT1 function by providing a minimally invasive methodology for in vivo control of protein activity levels through the use of light.

CHED 973

Cytotoxicity and cell cycle studies of trans-diiodophosphine Pt (II) complexes

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There is some precedence to the idea that non-conventional metallodrugs can overcome the unwanted clinical side-effects produced by the widely used antitumoral drug cisplatin. In particular, trans geometry with different ligands has further proved that improved antitumoral action of simple molecules is not only possible but that this geometry can in fact activate their action in some particular cases. Recent studies have shown that the leaving group, iodido versus chlorido, in platinum complexes has a considerable influence on the reactivity versus specific biological targets. The complexes described here bear phosphine ligands, which has been hypothesized to increase cellular permeability due to increased hydrophobicity. Three novel trans-diiodophosphine platinum complexes were tested against five different human cancer cell lines to determine the IC₅₀ for each complex and cisplatin. The dose that
corresponded to the IC\textsubscript{50} value was then applied to the cell lines and cell cycle analysis was performed. The latest results of these biological studies are presented.

CHED 974

Identification, synthesis, and biological activity of galloyl inhibitors of human low molecular weight protein tyrosine phosphatase

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Low Molecular Weight-Protein Tyrosine Phosphatase (LMW-PTP) isoform B (IFB) has been found to be over expressed in many forms of aggressive cancer and has become a target for inhibition. Competitive inhibition of LMW-PTP IFB by known inhibitor pyridoxal-5'-phosphate (PLP) shows a strong inhibition constant ($K_i$ = 7.6 µM at pH 5.0); however, PLP is a cofactor for many other enzymes. \textit{In silico} screening and \textit{in vitro} testing identified NSC107022 ($K_i$ = 10.8 ± 1.0) from the National Cancer Institute’s Diversity Set II as a lead compound for optimization as a LMW-PTP IFB inhibitor. Utilizing NSC107022’s galloyl group, compound libraries of aromatic alcohols and amines were connected (ester and amide linkages, respectively) and screened \textit{in silico}. Compounds yielding top docking scores (most negative) were synthesized and tested \textit{in vitro}.

CHED 975

Progress toward synthesizing transition metal complexes to mimic complex natural products

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Natural products provide an exceptional source of novel therapeutic agents to help fill our ever growing need for medicinal compounds, most notably antibiotics and chemotherapeutics. Unfortunately, large-scale use of complex natural products is often prevented by a lack of an economical synthetic method. We propose that the essential geometry of natural products can be mimicked by replacing key chiral carbons with a chelated metal. We intend to reproduce the three-dimensional shape of a metabolite of the natural product neocarzinostatin, NCSI-gb, through chelation of a metal to an easily synthesized ligand. Previous work has shown the degree to which steric strain and bite angles influence the resultant geometry of tricyclic tetradentate coordination complexes. We will outline the synthesis of different coordination structures with varying ring systems, and discuss the implications for their shape and stability.

CHED 976
Selective nitration of Hsp90 by peroxynitrite in the presence of ALS-linked mutant SOD

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A subset of the neurodegenerative disease Amyotrophic Lateral Sclerosis (ALS) is associated with mutations in the gene of superoxide dismutase (SOD). In addition, tyrosine nitration is present in the spinal cord of patients and animal models of ALS. Zn-deficient SOD catalyzes tyrosine nitration. In addition, tyrosine nitration is necessary for Zn-deficient SOD induced motor neuron death. We have also shown that the nitration of a singly tyrosine residue in the molecular chaperone heat shock protein 90 (Hsp90) is sufficient and necessary to stimulate motor neuron apoptosis. We have found that Zn-deficient and a mutant lacking the coordination sites for copper, preferentially nitrate Hsp90 in one of the critical residues that make the chaperone toxic. We are investigating the effects of several ALS-linked mutant recombinant human SODs on the nitration of spinal cord homogenates by peroxynitrite. The recombinant proteins are growth in bacteria with or without added copper. Bacteria homogenates are used as a source of SOD. The concentration of SOD in the homogenates is determined by Dot blots using antibodies against human SOD and human SOD as standard. We hypothesize that mutant SOD will selectively nitrate Hsp90. Our results represent the first hypothesis that link a change in SOD due to the mutations with the human pathology.

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CHED 977

Antimicrobial effect of improved antibiotics combined with Ni and semi-green Ag nanoparticles in Klebsiella pneumoniae

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Bacterial resistance to antimicrobial agents is a major problem worldwide. The daily increase of resistant strains can trigger a variety of infections. Nanotechnology offers possible alternative treatments, improving the antimicrobial activity of antibiotics, due to the properties of different metals. Our main objective is to develop more effective treatments against these resistant bacterial and nosocomial infections, combining metal nanoparticles with antibiotics. In this study, two different nanoparticles, Ni and Semi Green Ag, were combined with antibiotics. The antibiotics Penicillin, Amoxicillin, Levofloxacin and Vancomycin, were used at two different concentrations against
Klebsiella pneumoniae (ATCC # 13882), the causal agent of pneumonia and urinary tract infections in humans. Also, it revealed the antimicrobial effects of determined concentrations of antibiotics and nanoparticles, at equal and different proportions, against the bacteria. The results showed that some nanoparticles mixed with the antibiotics, at specific concentrations, increased the potential activity of the antibiotic against the bacteria, while in others the nanoparticles mixed with the antibiotics decreased the potential activity of the antibiotics.

CHED 978

Natural product discovery through bioassay methods on Ilex decidua

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Natural products obtained from locally harvested plants are an important source of common medicinals, and nearly half of current pharmaceuticals were initially discovered in plants. A large portion of earth’s flora, however, has not been chemically investigated. One such unexplored plant species is Ilex decidua, or deciduous holly, a small shrub native to the southeastern United States. Other species in the Ilex genus have shown cytotoxic, antioxidant, or other medicinal activity, and the leaves of various hollies, such as Ilex paraguensis are used in preparing medicinal teas, with yerba mate as a flagship example. In an effort to explore bioactivity of I. decidua, plant samples have been collected, dried and separated into seeds, stems, berries and bark. Some of the components have been extracted with a series of solvents with varying polarity. These extracts are being evaluated for interesting biological activity using a variety of assays, including brine shrimp bioassay, microbial toxicity assay, TLC, HPLC and GS-MS analysis. Series of other tests such as Folin-Cioloceau antioxidant activity assay and hematoma tumor cytotoxicity test are employed to broaden the array of assays and identify the fraction with highest beneficial activity. The samples will be then isolated for detailed study in an attempt to purify the active compound. Where possible, the structures of the molecules responsible for a new activity will be identified by NMR. Investigating the phytochemistry of unexplored plants will allow us to better understand the bioactivity of plants in the Arkansas flora and could potentially lead to the discovery of new pharmaceuticals.

CHED 979

Design and synthesis of a new mGluR$_5$ modulator

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Metabotropic glutamate receptors (mGluRs) are involved in numerous cellular mechanisms ranging from neural development to the processing of cognitive, sensory
and motor information. Several neurological and psychiatric disorders like Parkinson’s disease, Fragile-X syndrome, depression, schizophrenia and addiction have been linked to derailed signaling pathways associated with mGluRs. Due to the therapeutic benefits of targeting allosteric binding sites of these receptors, a synthetic pathway to new mGluR$_5$ NAM chemotypes is being investigated in which a new scaffold has been designed. Careful spatial arrangement of substituents and a balance of physicochemical properties required to penetrate the CNS as well as metabolic innocuousness are considered in the design.

CHED 980

Investigation of a synthetic approach to new substituted 1,2,3-triazoles

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5(4H)-Oxazolones substituted in 4-position with an exocyclic double bond can easily be obtained through the reaction of aldehydes with N-acylglycines under dehydrating conditions. This project investigates the utility of these oxazolones as dipolarophiles, substrates in 1,3-dipolar cycloadditions. Specifically, substituents on the exocyclic double bond are chosen and reaction conditions are elucidated that can lead to highly substituted 1,2,3-triazoles when the oxazolones are reacted with azides. The stability of the resulting heterocyclic systems towards hydrolytic ring opening and the stability of the hydrolysis products under physiological conditions are part of this project. Molecules with lipophilicity constant values in a suitable range for cell permeation are targeted through careful selection of substituents on the oxazolone and azide building blocks.

CHED 981

Search for an ideal selective estrogen receptor modulator (SERM)

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Selective estrogen receptor modulators (SERMs) are class of compounds heavily utilized in the treatment of breast cancer. Despite their importance, utility is limited by side effects due to unfavorable estrogenic activity in other tissues. An ideal SERM would inhibit mammary carcinogenesis while maintaining positive estrogenic activity in the brain, bone, and fatty tissues. Herein, we report the design and progress towards the synthesis of a novel SERM.
Investigating pancreatic anticancer activity of spiroxin A derivatives

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Spiroxin A, a natural product isolated from a marine fungus, has been shown to exhibit both antitumor and antibacterial activities. Our group has conducted a structure-activity relationship (SAR) study examining the structural components of spiroxin A that result in biological activity. Several compounds were synthesized and tested against pancreatic adenocarcinoma cell line PANC-1 under nutrient-deprived and nutrient-rich conditions. Pancreatic cancer is the fourth leading cause of cancer-related deaths in the United States and recent studies have demonstrated the ability of pancreatic cancer cells to survive nutrient starvation, a unique characteristic not possessed by normal human fibroblasts. Herein, we report the identification of a lead compound possessing cytotoxicity against PANC-1 cells selectively under nutrient-deprived conditions, as well as the ongoing SAR studies.

Effect of cell culture components on the preferential cytotoxicity of isoprenylated coumarin derivatives

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Pancreatic cancer is one of the most devastating forms of human cancer. The lack of effective clinical treatments for pancreatic cancer has led to one of the lowest five-year survival rates among all cancers. Recently, our laboratory has developed a novel series of isoprenylated coumarin derivatives that have exhibited anti-pancreatic cancer activity exclusively under nutrient-deprived conditions. In this study, we report the effect of the
various cell culture components on the preferential cytotoxicity of the coumarin derivatives against pancreatic adenocarcinoma cell line PANC-1. In addition, two other pancreatic cancer cell lines were examined under both nutrient-rich and nutrient-deprived conditions.

**CHED 984**

Design of tautomerically ambiguous cytosine-based nucleosides as potential anti-HIV agents

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Antiretroviral therapy for treatment of human immunodeficiency virus (HIV) has developed with great success over the last few decades. While the current therapies are successful, patients often meet with severe side effects and the mutagenic nature of the HIV virus leads to a constant need for new drug development. One such method of development involves incorporation of bases that exist in multiple tautomeric forms and thus containing ambiguous hydrogen bonding faces. We have synthesized a set of cytosine-based nucleosides with such characteristics, which, when incorporated into the viral DNA, lead to destabilization of the DNA. When combined with the high error rate of the RNA polymerase enzymes of the HIV virus, such incorporation may lead to an error catastrophe thus resulting in collapse of the virus. Presented here are the results of the synthesis and initial work on the thermal denaturation of DNA duplexes containing the ambiguous nucleosides.

**CHED 985**

Using rational drug design toward the synthesis of novel flavonoid derivatives as acetylcholinesterase inhibitors for the treatment of Alzheimer’s disease

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Research has shown that the neurotransmitter acetylcholine (Ach) is less expressed in the brain of Alzheimer’s patients when compared to normal patient’s levels. It is proposed that this decrease stems from the hydrolysis of Ach by the enzyme acetylcholinesterase. As a result, acetylcholinesterase inhibitors have been identified as a viable option for the treatment of various symptoms associated with cognitive function in patients with Alzheimer’s disease. Flavonoids, natural products that exhibit acetylcholinesterase inhibitory activity, can potentially serve as promising leads for the treatment of Alzheimer’s disease. Through the use of rational drug design, this research project will investigate the design and synthesis of novel flavonoid derivatives that incorporate nitrogen-containing fused heterocyclic rings, which were identified through
SAR as crucial structural elements, in pursuance of an effective treatment of Alzheimer’s disease.

CHED 986

Molecular modeling and docking studies of peptide macrocycles as potent inhibitors of the 20S proteasome

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The cyclic peptide metabolite TMC-95A is a potent inhibitor of the 20S proteasome. Due to TMC-95A’s synthetically challenging structure, designing simplified TMC-95A analogs without compromising inhibitory potency is of great interest. Using Molecular Operating Environment (MOE), the binding of these TMC-95A analogs in the proteasome active site was explored in order to optimize enzyme subsite and inhibitor interactions. It was found that anti-parallel beta sheet interactions form between the peptide backbone and the conserved residues Met45-Gly47-Ala49. Based on this information, side chain residues were modified to enhance binding. Asparagine and glutamine residues in the P2 and P4 positions, respectively, as well as introduction of an oxindole moiety in the peptide macrocycle establish additional H-bonding interactions. It was also determined that a C-terminal amide may facilitate coordination of the terminal threonine in the enzyme active site.

CHED 987

Design and synthesis of sphingolipid derivatives

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Sphingosine ((E)-2-aminooctadec-4-ene-1,3-diol) is an amino alcohol with an unsaturated hydrocarbon chain, and is a member of the sphingolipid family. Sphingosine also acts as the backbone for the other members of the sphingolipid family. Sphingolipids have numerous key roles in cell metabolism, signal transmission, and regulation. Their cellular importance has made them a new target for anti-cancer drug design. Breast cancer is the leading form of cancer among American women. Many women suffering from breast cancer possess breast cancer cells that are resistant to chemotherapy and endocrine therapy, the most common cancer treatments. This resistance to chemotherapy and endocrine therapy results in treatment failure. Treatment failure may result in death, which increases the urgency and importance of developing alternative treatment methods for these resistant cells. Previous research results suggest that bioactive sphingolipids play an integral role in the regulation of cancer pathogenesis and can be used as new chemotherapeutic agents. In this project, D-sphingosine moiety was conserved and coupled with benzaldehyde derivatives in
order to design and synthesize novel sphingosine derivatives. The resulting products were then analyzed and studied.

CHED 988

Design, synthesis, and evaluation of a novel hydroxamic acid series for treatment of human African trypanosomiasis

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Human African trypanosomiasis (HAT), also known as African sleeping sickness, represents a serious health threat to the people of sub-Saharan Africa. Travelers to wildlife reserves in Kenya, Tanzania, and other areas in which HAT is endemic are also at risk. HAT is fatal if left untreated, causing convulsions and serious sleep disturbance that proceed to coma and death. The disease is caused by a parasitic protozoan, *Trypanosoma brucei*, which is transmitted to humans by the bite of the tsetse fly. Rising global temperatures are expected to increase the range of the tsetse fly in the coming decades, leading to new and far-reaching outbreaks of HAT. The only available HAT medicines, all discovered prior to 1950, do not meet current standards for drug efficacy or safety: nearly 25% of advanced-stage HAT patients do not respond to these medicines, and an additional 5% of patients die from adverse reactions to them. A safe, orally administered drug that is effective against HAT is urgently needed and could set the stage for eradication of the disease. SCYX-7158 is a new drug candidate in human clinical trials for HAT. Due to its promising efficacy against HAT in infected mice, SCYX-7158 serves as a useful structural “template” from which our laboratory is designing and preparing new drug leads. Using SCYX-7158 as a starting point, we have used computational modeling to hypothesize that hydroxamic acid analogs display a similar pharmacophore, and should therefore maintain similar anti-trypanosomal activity. Our proposed analogs have never been previously prepared, and would thus represent a novel approach for HAT. The concept of exchanging a hydroxamic acid for a boronic acid has precedent with other drug targets, but has not been widely explored. Our progress toward the synthesis and evaluation of our new series of hydroxamic acids will be presented.

CHED 989

Synthesis of coumarin derivatives as potential inhibitors of human cytochrome P450 enzymes

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Cytochrome P450s are a superfamily of heme-containing monooxygenase enzymes that are mainly responsible for the metabolism and detoxification of endogenous and
xenobiotic substances. However, these versatile enzymes may also bioactivate procarcinogens into carcinogens. As a result, inhibiting family I P450 enzymes has become a target for cancer prevention and carcinogenesis studies. The project reported here focuses on the development and synthesis of selective inhibitors towards P450 family I enzymes 1A1 and 1A2. As part of a larger project, five novel coumarin derivatives were designed, synthesized, isolated, and structurally studied for use in in vitro P450 inhibition bioassays. Bioassays for P450 1A1 and 1A2 inhibition have been conducted on the synthesized coumarin derivatives. The derivatives reported here are 7,8-pyra-no-4-phenylcoumarin (78P4PC), 7,8-furano-4-methylcoumarin (78F4MC), 7,8-pyra-no-4-trifluorocoumarin (78P4TFC), 7,8-furano-4-trifluorocoumain (78F4TFC), and 7,8-dioxolo-4-phenylcoumarin (78DO4PC).

CHED 990

Design and synthesis of coumarin propargyl ethers as potential cytochrome P450 inhibitors

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Cytochrome P450 enzymes are a large superfamily of hemoproteins that are involved in the metabolism and detoxification of endogenous and exogenous compounds. Their specific interactions with, and bioactivation of, certain procarcinogens have resulted in their popularity as targets in cancer research. Developing selective and potent mechanism-based inhibitors for these enzymes is expected to be the key to understanding their mechanisms of action. Previously our group has shown that certain aryl and arylalkyl acetylenes act as inhibitors of these enzymes. Coumarin, a natural substrate of cytochrome P450, possesses fluorescent properties which make it easier to view enzymatic activity. In an attempt to increase the number of selective P450 inhibitors available for enzymatic studies, a novel group of coumarin ethers possessing an acetylene moiety have been designed and synthesized. Results of the inhibition studies of the novel compounds will also be presented.

CHED 991

Design and synthesis of flavone propargyl ethers as potential inhibitors of human cytochrome P450 1A1 and 1A2 enzymes

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Cytochrome P450 enzymes are a versatile superfamily of heme containing proteins involved in the metabolism and detoxification of endogenous and exogenous compounds including environmental chemicals. In addition, these enzymes play an important role in the bioactivation of procarcinogenic compounds into their ultimate
Carcinogenic forms. Most recently, we have discovered that some ethynyl coumarin derivatives can inactivate certain P450 enzymes involved in carcinogenesis and DNA mutation. Flavones are also known natural substrates for a number of important P450 enzymes. Cytochrome P450 activity assays point out that the addition of certain functional groups such as the ethynyl group to the flavone backbone can cause inhibition activity towards certain P450s such as P450s 1A1 and 1A2. For this project, we utilized the results of our previous structural-activity relationship studies and the geometry of the active sites of P450 enzymes 1A1 and 1A2 to design and synthesize new and promising inhibitors with potential use as cancer chemo-preventive agents. Here we report the synthesis of four flavone propargyl ethers (2’-flavonyl propargyl ether, 5-flavonyl propargyl ether, 6-flavonyl propargyl ether, and 5-hydroxy-7-flavonyl propargyl ether) as potential inhibitors of P450s 1A1 and 1A2.

CHED 992

Synthesis of beta-lactam analogs of belactosin A

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Belactosin A is a naturally occurring proteasome inhibitor with potent anti-tumor activity. Activity is conferred by enzymatic acylation of the beta-lactone. Several syntheses have been reported, however only a few analogs have been prepared. An approach to the synthesis of analogs is reported here, with the key step being the nitrocyclopropanation of an amino-acid derived enone. Efforts to improve stereoselectivity in the cyclopropanation are reported here. Reduction of the nitro group, followed by coupling to a beta-lactam affords belactosin A analog which may have improved stability over the beta-lactone. The use of alanine, phenylalanine, leucine and valine as starting materials leads to methyl, benzyl and isobutyl and isopropyl analogs of the natural product.

CHED 993

Synthesis of new toll-like receptors 2 (TLR2) ligands for pancreatic cancer imaging

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A cornerstone of pancreatic cancer treatment is the surgical resection of the primary tissues infected with cancerous cells. Without surgery, the American Cancer Society
reports a five year survival rate of 6%. However when the tumor tissue can be completely removed by surgical resection, the five year survival rate has been shown to be as high as 20 – 25%. Toll-like Receptor 2 (TLR2) is a type I transmembrane glycoprotein that plays a role in the activation and regulation of the innate immune system, and is overexpressed on pancreatic tumor cells. By taking advantage of TLR2 as a biomarker of pancreatic cancer, there is a potential to monitor the removal of pancreatic tumors in the operating suite. Additionally, structure activity relationship research has already developed hit motifs with agonistic binding activities for TLR2 (EC50 = 674 nM, Ki = 22 nM). This project was designed to elucidate a peptidomimetic ligand for TLR2 incorporating a fluorescent molecular tag meant to improve the distinction between cancerous pancreatic cells and normal cells. The first challenge was to optimize our synthetic strategy for the monoacylated PAM monomer of the ligand. This building block was a L-cysteine amino acid analog with a palmitic acid like motif. It was subsequently incorporated into the polypeptide using conventional Nα-Fmoc solid phase peptide synthesis technique. Because this peptide was being designed for pancreatic cancer imaging, a fluorescent dye (IRDye780CW) conjugate was prepared using a Suzuki coupling reaction, and then attached to the N-terminus of the TLR2 ligand using typical peptide coupling reagents. The ligand was prepared with high yield and purity levels. Future work will characterize the importance of this fluorescent ligand in imaging pancreatic cancer through cell binding assay, functional bioassay, and fluorescence imaging of murine tumors.

CHED 994

Synthesis of novel heterocyclic naphthoquinone imines and evaluation of their biological activity

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The goal is to design, synthesize, and evaluate the biological activity of novel imines derived from naphthoquinones using green chemistry techniques that limit the use of toxic chemicals and solvents and reduces the waste generated during synthesis. Reacting various primary amines in a microwave for 45 seconds with 1,2-naphthoquinone and 1,4-naphthoquinone and 3-formylchromone formed various novel imines. Depending on the heterocyclic amines used, we isolated imines or rearranged enones in this reaction. The structures are determined by various spectroscopy techniques. The compounds have been tested against two cancer cell lines and the preliminary cytotoxicity data will also be presented.

CHED 995

Ketoconazole activates CYP3A4-mediated metabolism of letrozole
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Letrozole is an aromatase enzyme inhibitor prescribed to post-menopausal women with estrogen-receptor sensitive breast cancer. It is mainly metabolized by Cytochrome P450 3A4 and 2A6. Ketoconazole is a well-known inhibitor of CYP 3A4. In this study, we investigated the interaction between ketoconazole and letrozole using steady state kinetic assays and HPLC-fluorescence to quantitate the letrozole metabolite compared to standard curves of commercially available standard, 4,4'-hydroxymethylene-dibenzonitrile. In human liver microsomes, which contain a high concentration of Cytochrome P450 enzymes, the metabolism of letrozole increased in the presence of ketoconazole. This effect was observed across multiple human liver microsome sources, and with recombinant CYP 3A4. Increasing the concentration of ketoconazole increased the degree of activation, indicating this is a concentration-dependent effect: 11.29\% and 23.28\% activation at 1.11 \(\mu\)M (\(p < 0.02\)) and 10 \(\mu\)M (\(p < 0.01\)) ketoconazole, respectively. The effect was also dependent on substrate concentration. Increasing the letrozole concentration from 0.5 \(\mu\)M to 10 \(\mu\)M reduced activation from 17.41\% to 1.51\%. These results give an in vitro example of heterotropic cooperativity in CYP 3A4. In addition, the results show that ketoconazole can lead to heterotropic activation, and does not act solely as an inhibitor.

CHED 996

Determination of inhibitor specificity for low molecular weight protein tyrosine phosphatase isoforms A and B

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Overexpression of low molecular weight protein tyrosine phosphatase (LMW-PTP) has implications in the onset and proliferation of aggressive, invasive tumors in breast, colon, bladder, and kidney cancers. Pyridoxal 5'-phosphate (PLP), the active form of Vitamin B\(_6\), is a known inhibitor of LMW-PTP, but lacks specificity due to its many other cellular roles. Non-hydrolyzable analogs of PLP have been synthesized and tested in vitro for their inhibitory activity on the two different isoforms of LMW-PTP expressed from recombinant genes in \(E.\ Coli\). Analogs that are potential anti-cancer agents show specific inhibition of Isoform B, which is oncogenic, without significantly affecting the activity of Isoform A, which is anti-oncogenic.
Potential antiviral effects of phenazine derivatives on the La Crosse virus

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The La Crosse Virus (LCV), which is transmitted by mosquitos, can cause serious problems especially when contracted by children. Some complications that can arise can range from a simple fever to encephalitis. We have data suggesting that a component of the supernatant of the genus pseudomonas may display antiviral activity against LCV. It is well known that pseudomonads produce phenazines. These phenazines show antibacterial and antifungal activity. We have an interest in investigating whether these phenazines are involved in the observed antiviral activity. Phenazines are redox-active compounds that can generate reactive oxygen species (ROS) that can have a potential toxic effect on bacteria and fungi. By synthesizing an array of phenazine compounds, we can analyze them against LCV and test their potential antiviral effects.

Quantification of longevity of aminopyronin in E. coli

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Aminopyronin compounds are a new line of fluorophores that can give us the ability to track the reproduction of various cell types. Using a library of aminopyronin compounds with substituted amine groups, the aminopyronin can cause various degrees of fluorescence that is released by the cell. Aminopyronin compounds have the ability to penetrate the cell membrane to emit fluorescence through many cell generations. Past studies have proven that through nuclear aromatic substitution the aminopyronin passes through the cell membrane to label amino acid residues. Due to the bonding nature of the aminopyronin compound it can and will advance through many generations. Treatment of E. coli with an aminopyronin compound causes the bacteria to fluoresce for up to six generations. The data suggests that treatment of mammalian cells with an
aminopyronin will allow the cell to fluoresce for days at a time. Not only does this method for studying cell lineage allow us to track cell growth over prolonged periods of time, the method is relatively uncomplicated.

CHED 999

Developing controlled-release chloroquine

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In this research, a process for creating control-release chloroquine by an oil-in-water emulsion method was developed. The aqueous phase was composed of a polyvinyl alcohol with octanol surfactant, and the organic phase consisted of base-form chloroquine with polycaprolactone in methylene chloride. Variables such as addition rate, stir time, container configuration, and amount of organic solvent were adjusted to optimize the shape and composition of the resultant microparticles. The products were filtered through stacked sieves to separate particles of consistent size. Elution profiles of chloroquine in solutions of varying pH were determined by HPLC analysis.

CHED 1000

Cyclic sulfinimidamides prospective use as non-GAT1 inhibitors

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Deficiency in the neurotranmitter GABA has been implicated in CNS disorders such as epilepsy, anxiety/depression, neuropathic pain, and cognitive impairment. Neurotransmission of GABA is terminated via transport by GABA transport proteins (GATs). Inhibition of GAT effectively increases the amount of GABAergic neurotransmission, which would be a amount likely therapy for the above listed CNS disorders. Currently there are four isoforms of GAT: GAT1, BGT-1, GAT2, and GAT3. These isoforms differ in their pharmacological role and location within the CNS. The FDA-approved compound tiagabine is a GAT1 inhibitor and is used as an antiepileptic drug (AED). Surprisingly there is limited knowledge as to what therapeutic significance inhibition of the other isoforms (non-GAT1) may offer due to the lack of potent and selective inhibitors of these non-GAT1 isoforms. Here in, we propose the synthesis of GABA mimics containing a cyclic sulfinimidamide- a carboxylic acid bioisostere- in hopes that these compounds will exhibit non-GAT1 activity.

CHED 1001

Synthesis of 2-(2-sulfonamidophenyl)benzothiazole and 2-(2-sulfonamidophenyl)benzimidazole as potential inhibitors of anthrax lethal factor and other zinc metalloenzymes
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Anthrax is a contagious and virulent disease caused by *Bacillus anthracis*, a bacterium. It has been reported that only 2500 to 55000 spores constitute the human lethal inhalation dose. Lethal factor is a metalloenzyme found in anthrax that contains a zinc ion in its active site. We have synthesized a variety of 2-(2-sulfonamidopheny)lbenzothiazole and 2-(2-sulfonamidophenyl)benzimidazole derivatives in order to evaluate their zinc binding capacity as well as their inhibitory capacity against lethal factor and other relevant metalloenzymes.

CHED 1002

Triflic acid mediated thiophenyl sulfonylation of arenes and subsequent antimicrobial activity determination of thiophenyl aryl sulfones

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The preparation and investigation into the antimicrobial activity of a wide variety of thiophenyl aryl sulfones through super acidic regioselective coupling of thiophene sulfonyl chlorides/arenes, by usage of trifluoromethanesulfonic acid is shown. The extent of the reaction was evaluated with a wide variety of aromatic substrates/aryl sulfonyl chlorides under superacidic Friedel-Crafts conditions. Literature QSAR parameters for the known antimicrobial action of diphenyl sulfones, were then comparitively optimized allowing directed synthesis of the thiophenyl aryl sulfone isosteres.

![Chemical structure](image)

Triflic Acid mediated Thiophenyl Sulfonylation of Arenes

CHED 1003

Oxadiazoles as biofilm and bacterial growth inhibitors

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Biofilms present a serious challenge in medicine and industry. These aggregate cell colonies are problematic in a wide range of scenarios ranging from cystic fibrosis patients to industrial water tanks. Compounds that can inhibit the growth of these films are needed. This paper reports heterocyclic small molecules with an oxadiazole core that are synthesized and assessed as antibacterial agents. Optimization of the synthetic route is presented, including a cyclodehydration reaction and a Suzuki cross-coupling. This optimized route allows for the synthesis of a small library of compounds. This library was tested against *Streptomyces* and *E. coli* strains for biofilm and general cell growth inhibition. Both qualitative and quantitative data are presented.

**CHED 1004**

**Synthesis of multitarget ligands for the treatment of Alzheimer’s disease**

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Alzheimer’s disease is the 6th leading cause of death in the United States and is the most fatal neurodegenerative disorder worldwide. There is no cure for Alzheimer’s and current treatments are relatively ineffective against the progression of the disease. The number of cases of Alzheimer’s continues to increase as the population lives longer. For this reason new treatments for Alzheimer’s disease are of paramount importance. The purpose of this project was to create multi-target ligands to combat Alzheimer’s disease processes. A series of substituted (1E,4E)-1,5-diphenylpenta-1,4-dien-3-ones were synthesized from various benzaldehyde derivatives and a linking molecule. The molecules were based on the structure of other ligands that have shown promise to inhibit the effects of Alzheimer’s. The molecules were tested for their capacity to inhibit amyloid-beta aggregation in vitro using a thioflavin-T fluorescence assay. Antioxidant and metal chelation ability of these molecules was determined using ORAC-FL and UV-Vis spectroscopy respectively. The characteristics of the synthesized molecules were compared to curcumin and quercetin which have demonstrated anti-amyloidogenic properties.

**CHED 1005**

**Development of autophagy-inducing agents for the treatment of human diseases**

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Autophagy is a survival mechanism that maintains cellular integrity by digesting and recycling intracellular components. Reports have suggested autophagy to be widely linked to various human diseases, such as cancer, infectious diseases, and neurodegenerative diseases. Since a limitation to cancer therapies is that many cancers have developed a resistance to autophagy, treatments targeted towards autophagic cell
death have gained considerable attraction. Although there is no conclusive evidence indicating the existence of the signaling pathways leading to autophagic cell death, regulating the level of autophagy has become a potential target for therapeutic approaches to various diseases. Here, we synthesized a library of small molecules by chemically modifying the autophagonizer, an inducer of autophagic cell death in human tumor lines, and screened this library for autophagy modulators. Selected derivatives generated through this approach demonstrated improved effectiveness in inducing autophagy. In this study, we present small molecule derivatives of the autophagonizer that may have beneficial clinical implications in the treatment of various diseases.

CHED 1006

Saccharin and its carbohydrate-conjugate shows promise for isoform selective inhibition of carbonic anhydrase IX: A lead approach to anti-cancer drug development

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Carbonic anhydrase IX (CA IX) is a zinc metalloenzyme that is highly expressed in several aggressive cancer types and its expression has been linked to a poorer prognosis in patients. Inhibition of CA IX has shown to be advantageous in terms of reducing tumor cell proliferation, growth, and inducing chemo- and radiosensitivity in solid tumors. As such, CA IX has been characterized as an ideal anti-cancer target due to its minimal expression in normal human tissue and its physiochemical properties. Despite inhibition of CA IX showing great therapeutic promise, designing selective CA IX inhibitors has been challenging due to its high homology with other ubiquitously expressed human isoforms. Here we demonstrate that saccharin, the main additive in “Sweet N’ Low”, can be used as a lead compound for structure-based drug design of CA IX selective inhibitors. Furthermore we show how the linkage of a carbohydrate fragment to saccharin enhances CA IX inhibition by >1000-fold over other isoforms and provide insights into the structure-activity relationships of such compounds. This data presents a new class of CA IX inhibitors that will potentially aide in the treatment of several cancers.

CHED 1007

Using essential oils to combat the threat of multidrug resistant bacteria

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Bacteria, particularly those common in health care settings, have been developing mechanisms making them resistant to prevailing antibiotics. Consequently, bacterial infections occurring in hospitals are becoming very difficult to treat because available antibiotics are becoming ineffective to inhibit the bacterial growth. These drug resistant pathogens, which can be both gram-positive and gram-negative, can cause infections that can risk lives of affected people. The present research focused on the bacterium, Vibrio vulnificus, which is known to cause infections in health care settings. Before the discovery of antibiotics, people relied on natural remedies such as essential oils to treat bacterial infections. In this research, several commonly used essential oils were tested against Vibrio vulnificus to determine their effectiveness to inhibit its growth. We used the Kirby-Bauer disk diffusion method and measured the diameter of the zone of inhibition for the bacterium when treated with the individual compounds. Cinnamon, wintergreen, lemongrass, and methylglyoxal (major component of Manuka Honey) showed the most antibacterial properties. In addition to investigating the antibacterial activity of these essential oils, this study included experiments to find suitable carriers for these compounds so that the combination could be used as topical applications on the patients to treat the bacterial infections. Lanolin and Aloe Vera were found to be effective carriers to produce emollients with the three essential oils and methylglyoxal. Most of the compounds tested were observed to have antibacterial activity when individually combined with Lanolin and Aloe Vera even at concentration of 12.5% (v/v). The results of these experiments and other published work on the topic suggest a cost-effective way to deal with the bacterial infections using the essential oils and methylglyoxal incorporated in lanolin and Aloe Vera.

CHED 1008

Optimization of thiadiazole small molecule inhibitor of the hippo signaling pathway to reduce pro-EMT cancerous cell growth

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The Hippo signaling pathway holds a key role in cancer metastasis through the induction of epithelial-mesenchymal transition (EMT) and thus stands as an opportunity for novel anticancer drug targets. We identified a small molecule (C19) that demonstrates inhibitory activity towards the Hippo pathway, as well as the Wnt and TGF-β pathways. C19 suppressed cancer cell migration, proliferation, and antitumor activity in a mouse tumor model through activation of the Hippo kinases Mst/Lats and the metabolic regulator AMPK. Our small molecule inhibitor contains a core 1,2,5-thiadiazole ring, which was optimized with respect to both the aromatic and the aliphatic side chain, to improve cellular introduction, cytoplasmic stability, binding pocket interactions, and IC₅₀ values. Through computational protein-ligand modeling, biological signaling analysis, and bioisostere optimization, we have synthesized and characterized...
several derivatives of C19 that also hold potential as small molecule inhibitors of these signaling pathways for novel cancer therapeutics.

CHED 1009

Targeting sphingosine kinase 2: Converting highly selective substrates into inhibitors

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Sphingosine kinase 2 (SK2) is one of two kinases responsible for the phosphorylation of the membrane lipid sphingosine to produce sphingosine 1-phosphate (S1P). S1P is a key agonist at five G protein-coupled receptors and has been shown to be a regulator for angiogenesis, neovascularization, and cellular survival and proliferation. An inhibitor of SK2, therefore, holds potential as a possible cancer therapeutic, and would be invaluable in the study of the roles of SK2 in cancer. While many excellent substrates of SK2 have been synthesized, there are few effective inhibitors. Our goal is to modify a highly active substrate of SK2 in order to generate a very selective, potent inhibitor. We have previously synthesized VPC202147, a molecule that is phosphorylated by SK2 at a level comparable to that of sphingosine. This substrate is now the scaffold for our inhibitors. Four derivatives of VPC202147 (Figure 1) are currently being synthesized that utilize steric hindrance, decreased nucleophilicity, and opposite stereochemistry near the site of phosphorylation in order to convert this substrate into an inhibitor. Once synthesized, the molecules will be evaluated for effectiveness in depressing S1P production by SK2 in vitro.

Substrate VPC202147 and four inhibitor derivatives.
CHED 1010

Novel anticancer drugs on the basis of diversely functionalized N-containing heterocycles

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Recently, the potent anticancer compound Rigidin 35(D1) was synthesized in our laboratory. The compound possess low nanomolar activity against cell lines representing cancers with dismal prognoses, tumor metastases, and multidrug resistant cells. In this work, corresponding pyrroline and pyrrole precursors of the Rigidin 35 compound were synthesized and isolated with moderate yields. The new compounds were tested against cervical adenocarcinoma HeLa cells. The compounds exhibit submicromolar antiproliferative activity. Pyrrole 35 and Rigidin 35 show similar killing effects against HeLa cells. Correspondent mixture of pyrrolines shows much stronger toxicity in high concentrations.

CHED 1011

Diastereoselectivity in an exhaustive bromination of anthracenyl-isoxazoles

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The focus of this project is to improve the efficacy of anthracenyl isoxazolyl amides (AIMs) by adding axial chirality via strategic halogenation. AIMs are a new class of antitumor agents specially synthesized to bind and interact with G-quadruplex (G4) DNA; binding G4 DNA has been shown to repress the replication of oncogenes in cancerous tumors. By using asymmetric halogenation our goal is to introduce axial chirality into the AIMs. Many biologically active molecules are chiral and the stereoisomers often display a significant difference in activity due to interactions with chiral targets, such as DNA. Methods of over halogenation of unsubstituted anthracenes, in synthetically useful yields, have been published by Cakmak. However, with the added complexity of a substituted anthracene, the addition of halogens has been a challenge. We have successfully isolated a 1,2,3,4,10-pentabromo-anthracenyl-isoxazole-ethylester. The methods that yielded the overbrominated product require consideration of the mechanism of the reactions, in which ionic and radical intermediates are expected to predominate. The current focus is the selective reductive elimination of the overbrominated compound. The future focus will shift to selective substitution that will afford an axially chiral final product. The benefit of stereospecific
activity is that a patient may be able to take less of the chemotherapeutic agent and achieve equally beneficial results with fewer side effects. Our progress will be described.

CHED 1012

Preparation and photolysis of non-glucosinolates

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Brassica vegetables are rich in glucosinolates, the chemical precursors to isothiocyanates (ITCs); several ITCs display pronounced anticancer properties. This work attempts to artificially replicate the natural production of ITCs through photolysis of a synthetic non-glucosinolatate. Initial photochemical reaction of these substances suggest partial removal of the photoactive group and additional methodological studies will be required.

CHED 1013

Activity and selectivity of PVP-capped palladium nanocatalysts immobilized on silica microspheres for the hydrogenation of phenol

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A key concern that arises with using colloidal nanoparticles as catalytic materials is their stability during the course of the reaction. To this end, we are preparing colloidal palladium nanoparticles immobilized on silica microspheres by a simple adsorption method. Alcohol reduction and seeded growth methods are being used to prepare nanoparticles of various sizes and with different molecular weights of polyvinylpyrrolidone (PVP) as the capping agent. Colloidal and immobilized nanocatalysts are being characterized by transmission electron microscopy (TEM) for particle size, with flame atomic absorption spectroscopy also being used to determine the percent mass of Pd on the microsphere surface. The hydrogenation of phenol using the synthesized catalysts is being carried out in a benchtop reactor with gas chromatography/mass spectrometry being used to follow product formation. We are performing catalytic reactions at moderate temperatures and hydrogen pressures, with the kinetic data being used to calculate turnover frequencies, reaction orders, apparent activation energies, and reaction selectivities. Taken together, this information will allow us to elucidate catalyst stability during catalytic reactions in aqueous solution.
Luminescent gold nanoparticles-based fluorescence and dynamic light scattering dual-modality sensor for copper (II) detection

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Luminescent gold nanoparticles (AuNPs) have begun to emerge as a new class of nanoprobe for chemical and biological sensing applications owing to their unique optical properties and easy-to-modified surfaces. Here, we report a highly selective and sensitive Cu$^{2+}$ ion sensor by synthesizing ~2.5 nm glutathione/cysteamine-coated luminescent AuNPs. These AuNPs can be used as dual-modality sensors for both fluorescence and dynamic light scattering assays under physiological environment.
Nanostructured metal oxides with tunable Lewis base sites for the conversion of L-α-phosphatidylcholine to biodiesel

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Lewis basic metal oxides have shown to be highly effective at breaking the phosphoester bond in many molecules such as chemical warfare agents. In this study high surface area calcium oxide and strontium oxide were synthesized by converting various commercial precursors to metal hydroxides followed by thermal conversion to oxides. The catalysts were used in a one-pot reaction to destructively adsorb L-α-phosphatidylcholine followed by transesterification to produce biodiesel. Qualitatively, all catalysts break apart L-α-phosphatidylcholine and convert it into its constituent methyl esters. Nanostructured, high surface area CaO was found to be the best pure catalyst. Mixtures of high surface area and commercial CaO, SrO, MgO, Al₂O₃ and TiO₂ were then tested to tune the base properties of the catalysts and increase the rate of conversion.

Characterizing the partitioning of hydrophobic solutes into the surfactant bilayer on gold nanorods

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In recent years the applications of gold nanoparticles in biological and medical fields such as photothermal therapy, drug delivery, and biological sensing have increased drastically. However, there is little fundamental understanding of how these nanoparticles interact with small molecules inside and outside of the body. Our work focuses on the interactions of small hydrophobic solutes with the surfactant bilayer of gold nanoparticles. The nanoparticles are synthesized via a seed mediated growth mechanism, which utilizes cetyltrimethylammonium bromide (CTAB) as the capping agent, and results in a surfactant bilayer of CTAB on the surface of the gold. The goal of this research is to determine the partitioning coefficient of hydrophobic molecules into the CTAB bilayer of both nanospheres and nanorods. The molecules, 1,5-dihydroxynaphthalene and 2,3-dihydroxynaphthalene have been used to determine the amount of molecule that partitions at a specific gold nanoparticle to molecule ratio. By determining the partitioning of the molecule at several ratios both the partitioning coefficient (K) and the number of molecules that partition into the surfactant bilayer (Cₘₐₓ) can be determined. Preliminary results suggest that the differences in size and polarity of the 1,5-dihydroxynaphthalene and 2,3-dihydroxynaphthalene cause a significant difference in the K and Cₘₐₓ values of these molecules. This gives insight
about the impacts that molecular properties have on the partitioning of molecules into the bilayer. In addition, data shows that differences in the partitioning between spheres and rods also exist. Through the use of these partitioning experiments, it will be possible to indirectly probe the structure of the CTAB bilayer.

CHED 1017

Investigating the interactions between gold nanoparticles and \textit{L. catesbeianus} and \textit{L. sylvaticus}

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Nanoparticle technology is widely utilized in today's society and shows a pattern of increasing use. In 2013, the Project on Emerging Nanotechnologies reported their updated Nanotechnology Consumer Products Inventory contained 1,628 consumer products, a 24% increase from 2010. With a rapid increase in nanoparticle technology, it is likely that more nanomaterials will enter the environment through manufacturing waste, landfills, and runoff. The effect of nanoparticles entering the environment and interacting with land, water and animal systems is still widely unknown. Bioaccumulation of nanoparticles and the potential for toxic effects at increasing levels could be a concern across the food chain. In this research, gold nanoparticles were utilized due to their relative inertness, minimal toxicity, and low environmental background. The aim of this study was to quantify the uptake of gold nanoparticles in varying sizes of tadpoles, \textit{L. catesbeianus} and \textit{L. sylvaticus}, as model organisms that would most likely encounter nanoparticles in wastewater runoff.

CHED 1018

Low temperature, size-selective fluorescence spectroscopy of PbSe quantum dots

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The electronic structure of lead selenide quantum dots (QDs) has been investigated via low temperature photoluminescence excitation (PLE) and fluorescence line narrowing (FLN) spectroscopies. PLE and FLN spectroscopies only sample QDs in a narrow spectral range (<10 meV) and can provide important information about the QDs' electronic structure that is “averaged out” of traditional room temperature absorption measurements (peak widths ~50 meV). PLE and FLN spectra were collected at 77 K for PbSe QDs with a first (room temperature) absorption peak between 1200-1500 nm (corresponding to particle diameters of 3.5-5.0 nm). The low temperature spectra exhibit distinct features compared to room temperature absorption measurements (eg,
narrowing, peak shifts, and line shape differences). These features will be analyzed and discussed in the context of fine structure splitting of the lowest PbSe exciton state.

CHED 1019

Templated gold nanorod arrays for improved plasmonic biosensing

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Localized surface plasmon resonance (LSPR), a property exhibited by noble metal nanoparticles, has proven very useful in label-free biosensing. When a protein of interest binds to the surface of a gold nanoparticle the index of refraction around the nanoparticle changes and produces a shift in the plasmon resonance frequency. Noble metal nanoparticles have their LSPR in the visible region making them amenable for use with UV-Vis absorption spectroscopy or even detection by eye. Surface enhanced Raman spectroscopy (SERS) has been shown to yield exquisite sensitivity for biosensing as well. Herein, we have fabricated gold nanorod arrays for both LSPR and SERS biosensing. Gold nanorod arrays are fabricated using electrochemical deposition through a polymer mask. Indium-tin-oxide (ITO) or thin film gold coated glass, which has undergone hole-mask colloidal lithography (HCL) to create 15 and 24 nm in diameter wells down to the ITO or gold surface, is used as the working electrode and is the base for the array. Continuous application of voltage in a range near the redox potential of gold reduces aqueous chloroauric acid into the wells to create nanorods. Nanoparticle arrays are characterized with atomic force microscopy (AFM), UV-Vis spectroscopy, and SERS.

CHED 1020

Developing a silica-coated nanovehicle for targeted cancer therapy

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Due to their small size, nanoparticles (NPs) are a suitable platform for building the next-generation targeted therapy for cancer. The high surface-to-volume ratio and well-studied surface chemistry of NPs allow for efficient loading of treatment and targeting moieties, which would maximize drug delivery and ensure high tumor specificity, all the while sparing healthy tissue. Silica-coated superparamagnetic iron oxide (SPIO) nanoparticles, a type of magnetic resonance (MR) contrast agent, combine the small size of nanomaterials with the benefits of MR imaging to provide a non-invasive method for tracking NPs inside the human body. Relaxivity studies of NPs revealed that T2
relaxivity of SPIO NPs were well above clinical-use limits. Previous efforts successfully synthesized silica-coated SPIO NPs with a diameter of approximately 50 nm and a shell thickness of 10-20 nm using a reverse micro-emulsion method. Current studies focus on attaching monoclonal antibodies (CHO31.1 or As33), which target glycoprotein A33, a tumor antigen that is over-expressed in certain pancreatic cancer cells, to silica-coated NPs. Preliminary experiments in our laboratory showed evidence of cellular particle uptake using fluorophore-labeled, As33-conjugated silica-coated NPs and pancreatic cancer cells that over-expressed A33. In order to study live cells, MR imaging phantoms are being designed and constructed to enable quantification of cellular particle uptake via MR imaging, in addition to conventional bioimaging methods.

CHED 1021

Synthesis of activated palladium nanoparticles (PdNPs) on carbon microspheres (CMs) for use as a hydrogenation catalyst

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We have developed a method to fabricate composite material consisting of palladium nanoparticles tethered directly to high surface area, porous carbon microspheres. This approach is advantageous because metal nanoparticles have been shown to be effective catalysts, however, due to their small size, unsupported metal nanoparticles can be difficult to recover and reuse. A composite material, such as ours, allows for the isolation and reuse of the nanoparticles. Other procedures for fabricating composites call for the synthesis of nanoparticles in one step, then attaching them to a support in a second step. Our approach circumvents this second step, saving time and energy. Here we present results of the fabrication and characterization of our composite materials. To demonstrate the utility of our nanoparticles as catalysts, we employed the hydrogenation of methyl trans-cinnamate as a model system. Results of the hydrogenation reactions will also be presented.

CHED 1022

Self assembly and ordering at the nanomaterial liquid crystal interface

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To enhance our understanding of fundamental interactions between nanomaterials and liquid crystals (LCs) and exploit them for specific applications this project focuses on the synthesis and investigation of two types of nanomaterials. The first type is hydrophobic carbon dots (C-dots) with small core diameters (<2 nm) featuring an excitation wavelength-dependent luminescence wavelength and intensity, which we are testing as
luminescent NP alignment layers for nematic LCs based on our recently published ink-jet printing technology. The second type of nanomaterial is functionalized gold nanorods (GNRs) for the creation of mechanic stimuli response optical metamaterials based on porous LC elastomers and GNRs. Both nanomaterials were characterized by TEM, UV-vis-NIR, TGA, FT-IR and fluorescence spectroscopy (C-dots). Preliminary data will be presented on the alignment of the GNRs in the LC elastomers and the formation of patterned homeotropic alignment of nematic LCs using the as-synthesized C-dots.

CHED 1023

Investigating the integrity of novel nanovehicles for targeting pancreatic cancer

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Our goal is to create a nanotherapeutic agent that will target pancreatic cancer cells, serve as a vehicle for radiative therapy, and enable noninvasive imaging using MRI. To optimize the particles, we are concurrently investigating the behavior of protein-conjugated gold nanoparticles in protein-rich environments, modeling conditions within the human body.

Our proposed nano-vehicle consists of an iron core for tracking with MRI and a gold shell to which we can attach various decorations: stealth-coating polymers, antibodies, and a polymer loaded with 10B for boron nuclear-capture therapy. Herein, we report results with pure gold nanoparticles (AuNPs), which serve as a simple model. Nanoparticles are coated in thiol-terminated poly(ethylene glycol) (PEG), some of which are biotin-terminated. Biotin-avidin interactions are used for the conjugation of antibodies and boron-10 rich polymers to our nanoparticle. Two antibody conjugation schemes have been successful in this study, and conjugating 10B-rich polymers is underway. With progress made in the construction of this nanovehicle, we are also testing the stability of these nanoparticles in the presence of proteins. This project evaluates the protein resistance of two types of polymer coatings: PEG and PEK. PEK is a peptidic polymer with an alternating sequence of five glutamic acid and four lysine units. To probe protein interaction, samples of AuNPs coated with PEG or PEK were synthesized and then characterized with UV-visible spectroscopy, dynamic light scattering, and Zeta-potential to monitor size, charge, and extent of aggregation. Protein resistance was evaluated by incubating each type of coated AuNPs with negatively-charged bovine serum albumin (BSA) and with positively-charged lysozyme. We found that stealth-coating the AuNPs minimizes protein adsorption and increases biocompatibility of the nano-vehicle. Further studies investigating protein adsorption to nanoparticles with directionally conjugated antibodies, BSA competition with stealth
coating, and the impact of polymer chain adjustments to adsorption resistance are underway.

CHED 1024

**UV spectrophotometric titration of graphene oxide with ascorbic acid to follow reduced graphene oxide formation**

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Graphene oxide (GO) is a promising new nano-scale material that has the potential to revolutionize electronics and applications. This material is a single layer of carbon atoms in a honeycomb lattice dotted with oxygen functional groups in the basal plane and at its edges. While graphene is a good electrical conductor, graphene oxide is an insulator with a typical band gap of approximately 2 eV. By controlling the degree of oxidation the physical and electrical properties of GO can be "tuned" or controlled. Hydrazine has been the commonly used reagent to reduce GO. Our results show that the "greener", safer, and more economical reducing agent ascorbic acid can replace hydrazine to produce reduced graphene oxide (rGO). Graphene oxide was titrated with ascorbic acid and UV spectra were collected at 30 minutes intervals over 4 hours. The formation of rGO was monitored by following the UV peak shift from 233 nm to 268 nm. These results show promise for an easy method for “tuning” the properties of rGO by controlling the level of oxidation.

CHED 1025

**Nanosized organometallic building block synthesis for the formation of a polyoxometalate-based framework**

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The ability to utilize recent developments in coordination chemistry has given way to the formation of metal-organic frameworks. One framework in this category uses polyoxometalate anions (POMs) consisting of transition metal cations surrounded by oxo anions, linked through organic ligands. These two building blocks allow for the precise formation of nano-sized compounds bridging the gap between nanotechnology and traditional synthesis. The variation in the framework’s pore size is directly a result of the organic ligands and its individual structure. The formation of a tetrahedral organic ligand is the main focus of this project and how it may be used to self-assemble into a three dimensional POM organic framework (POMOF). This framework will have the redox capabilities of the POM along with the tunable structure from the organic ligand. The synthesis of the starting tetrahedral organic ligand was accomplished through reacting tin(IV) chloride with dibromobenzene, resulting in \((p-\text{BrPh})_4\text{Sn}\). Following the synthesis of this compound the Sonagashira coupling was used to extend the arms of
the tetrahedral ligand with added rigidity through the addition of an acetylene subunit, followed by another Sonagashira addition with \( p \)-bromobenzoate. After each step the product was purified using flash chromatography and characterized using NMR spectroscopy. Future work includes an amidation between the ester and TRIS, which will allow coordination of the ligand to the POM, forming the POMOF through self-assembly.
Organic dyes improving the efficiency of dye-sensitized solar cells

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In this research dye-sensitized solar cells were constructed using an organic dyes with titanium dioxide nanocrystals. Difference formulations of Titanium Dioxide with different sized particles were used and the properties and performance of the solar cells were compared. These cells consist of titanium dioxide nanocrystals that are coated with light-absorbing dye molecules and immersed in an electrolyte solution, which is
sandwiched between two glass plate. Different dyes both commercially available and synthesized in our laboratory were tested to determine which dye produced the highest voltage when tested. Light striking the dye frees electrons and creates "holes"--the areas of positive charge that result when electrons are lost. The semiconducting titanium dioxide particles collect the electrons and transfer them to an external circuit, producing an electric current. The cells can be connected in series to produce cells with voltages as high as five volts which can be used to power a small motor.

CHED 1027

Activation and stabilization of electrodeposited p-Cu₂O with underpotentially deposited Ni

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In order to keep reactive p-Cu₂O surfaces from decomposing to Cu, deposition of Ni monolayer was carried out via underpotential deposition (UPD) of Ni from Ni acetate aqueous solution (0.6 and 0.08 M) by applying various potentials for 15 min. After the UPD of Ni, the Cu₂O films were dissolved in 1.1 wt% HNO₃, and deposited Ni was quantified by atomic absorption spectrometry via electrofurnace atomization. Although there are only a few papers on UPD of metal on oxides, we have confirmed the UPD of Ni on p-Cu₂O. The UPD at -0.2 to -0.3 V vs. SCE completed a monolayer coverage of Ni on p-Cu₂O while the Nernst potential for Ni deposition from the Ni solutions was approximately -0.5 V vs. SCE, indicating 0.2 to 0.3 V more positive UPD potentials and, thus, 38 to 58 kJ stronger attractions between Ni and Cu₂O surfaces than subsequent Ni-Ni interaction. The Cu₂O films with underpotentially deposited Ni overlayer do not undergo decomposition during four hours of illumination with a 100 W tungsten lamp, and gas evolution at p-Cu₂O and the Pt counter electrode has been observed. The x-ray photoelectron spectroscopic data will be presented to verify the oxidation states of underpotentially deposited Ni at various potentials.

CHED 1028

Synthesis of silver gallium sulfide nanoparticles

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A process that allowed the synthesis of effectively monodisperse silver gallium sulfide nanoparticles (AGS) was developed in an air free, high temperature procedure. This procedure included an injection at reaction temperature in order to nucleate crystal growth. The particles were uniform and could be grown over a range of sizes. Additionally, the ligand system has been optimized for both growth and photoluminescence. The particles were isolated at room temperature and cleaned
through centrifugation. Following cleaning, the AGS was characterized with UV-Vis spectroscopy, fluorescence analysis and TEM.

CHED 1029

Tailoring cadmium selenide nanocrystals with mixed ligand systems

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We are exploring the tethering of conjugated organic ligands onto the surface of semiconductor nanoparticles for the development of solar heterojunction chromophores. Organic ligand exchange on the outer surface of CdSe semiconductor nanocrystals was evaluated using NMR and fluorescence spectroscopy and properties correlated with ligand identity. NMR data will be presented on the coordination of 4-aminobenzoic acid, aniline, and thiophenol in single and mixed ligand systems. The NMR analyses afford quantitative study of ligand exchange and composition. Nanoparticles tethered with 4-aminobenzoic showed improved water processibility. These tailored mixed ligand systems offer new routes to realize photo-activated nanomaterials with improved water solubility and dispersity for use in thin film active layers.

CHED 1030

Surfaced enhanced infrared absorption on optimized copper nanostructures

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The goal of this research is to develop optimal copper metal nanoparticles (MNPs) for applications in surface-enhanced infrared absorption spectroscopy (SEIRA). Various optimized MNPs are formed by oblique angle deposition (OAD) through metal evaporation onto CaF$_2$ substrates at angles ranging from 75$^0$ to 80$^0$. These nanostructures are characterized with AFM, SEM, and UV/Vis-NIR spectroscopy. A monolayer of p-nitrobenzoate ion was deposited onto the copper nanostructures to determine the degree of vibrational enhancement in SEIRA. These optimized MNPs show SEIRA enhancement factors up to x50 better than MNP grown at incident. We observe SEIRA enhancement factors of ~x200 for optimized silver MNPs and enhancement factors of around x100 and x25 for optimized gold and nickel MNPs, respectively. This work will influence a range of biological, medical, catalytic, environmental, and nanotechnological applications.

CHED 1031

Noble metal-TiO$_2$ and noble metal-ZnO nanocomposites for improved photocatalysis
In this project, the photodegradation of phenol using a photocatalyst was studied. In an effort to extend the absorptive response, 2-4 nm Au and Ag nanoparticles (NP) were synthesized and attached to TiO$_2$ and ZnO nanomaterials. TEM and XRD characterization confirmed the presence of Au. Due to concern over possible oxidation of the very small Ag particles, the Ag NPs were attached to the TiO$_2$ in an inert environment under N$_2$. This preparation resulted in a dark coloration of the photocatalyst, confirming Ag attachment. The photocatalytic activity of each catalyst was tested through the decomposition of phenol under UV radiation (350 nm) for up to 60 minutes. Rates were determined and compared to unmodified TiO$_2$ and ZnO. Ag-TiO$_2$ was not as good at degrading the phenol as the unmodified TiO$_2$. For the Au-ZnO loading studies, we found that intermediate Au loading on ZnO showed faster phenol degradation than unmodified ZnO or ZnO with very small or high Au loadings. Attachment of Ag to TiO$_2$ under inert conditions provided better results compared to preparations in air. The data collected from this study will be directly applied to photocatalytic degradation of environmental pollutants including oil remediation strategies for spills such as the Deepwater Horizon disaster.

Comparative interactions of gold and silver nanoparticles and lead in the rates of germination and root elongation of radish plants

Studies of the impact of the interactions between nanoparticles and heavy metals at different ratios is an innovative way to study environmental toxicology. Gold and silver nanoparticles were prepared using a double reduction reaction. Silver and gold nanoparticles were characterized with UV Spectroscopy. The average diameters according to Dynamic Light Scattering was 50-70 nm for both nanoparticles. Seeds of radish plants were incubated in aqueous solutions of different proportions of nanoparticles and lead concentrations (1:1, 1:0.5, 1:0.3). The germination rate was determined counting germinated seeds in 24 hours. Primary roots were measure at 72 hours. Silver nanoparticles were more effective than gold nanoparticles for germination and root elongations. Comparing to lead and other controls nanoparticles may act as stimulators or inhibitors for the metabolic processes during germination and root elongation.
Functionalization of indole-3-acetic acid with gold nanoparticles synthesized through a double reduction reaction using leaflets’ extracts of *Leucaena leucocephala* (Lam.) de Witt

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The chemical profile of *Leucaena leucocephala*, a worldwide distributed mimosoid legume, is suitable to explore its role in the synthesis of nanoparticles and their functionalization with organic molecules such as plant hormones. Functionalization of plant hormones with nanoparticles is an innovative strategy to enhance the impact of nanotechnology in environmental stress situations and biotechnology. In this work gold nanoparticles were synthesized making a double reduction using leaflets' extracts of *L. leucocephala* and citrate. The obtained nanoparticles were characterized, using a UV spectroscopy and a Dynamic light scattering to estimate the nanoparticle size. Results of green gold nanoparticles functionalized with hormone Indole-3-Acetic Acid shows a red shift displacement at 545-572 nm, indicating functionalization. The nanoparticle remained stable for four weeks and the size ranged between 65-80 nm. These results indicate the effectiveness of the *Leucaena* leaflets’ extracts in the synthesis and functionalization of the gold nanoparticles.

CHED 1034

**Synthesis of small, ligand-stabilized copper nanoparticles as building blocks for electroreduction catalysts**

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Nanoparticles are being investigated as electrocatalysts for a wide variety of redox transformations. The use of preformed nanoparticles in contrast to those synthesized through electrodeposition allows for the nanoparticles to be well characterized before examining their electrocatalytic properties. Copper has shown promise as an active catalytic material for CO\(_2\) electroreduction, however, little is known about the synthesis and chemistry of preformed, small copper nanoparticles. Hexanethiol-stabilized copper nanoparticles (CuNPs) were synthesized using a modified two-phase Brust preparation method. Characterization with small angle x-ray scattering (SAXS) and transmission electron microscopy (TEM) revealed these nanoparticles to be spherical with a mean core diameter of 2 nm. X-ray photoelectron spectroscopy (XPS) of this material did not show a significant presence of oxidized copper on the surface. Preliminary studies with these CuNPs dropcast onto glassy carbon electrodes suggest their ability to electrochemically reduce bicarbonate. With the aim of linking the nanoparticles to an electrode surface, through the ligand shell of these nanoparticles, ligand exchange
reactions with 2-mercaptoethylphosphonic acid (2-MEPA) were investigated. Future work will focus on expanding the library of functional ligand shells for copper nanoparticles with the goal of covalently attaching these materials to electrode surfaces for further studies of their electrocatalytic properties.

CHED 1035

Probing nanosize-dependent oligomerization by using fluorescence dynamics of fluorescein amyloid beta 1-40 peptides

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The formation of oligomers of amyloid beta (Aβ) is regarded as a critical onset stage of Alzheimer's disease. While oligomers are produced as a heterogeneous ensemble of different types of oligomeric forms (e.g., dimer, trimer, tetramer, etc.), the presence of a nanoscale surface may selectively produce a specific oligomeric form. It has been hypothesized that the order of the oligomer is considered to increase proportionally to the size of nanoscale surface available. For example, dimer, trimer, and tetramer units are selectively produced as the gold nanoparticle increased in size from 10 nm to 100 nm. In order to establish a new methodology to probe a specific oligomeric form, we investigated the fluorescence dynamics of a fluorescein-attached Aβ₁₋₄₀ monomer (FAβ₁₋₄₀). The fluorescence decay times of FAβ₁₋₄₀ on various sizes of gold nanoparticles, ranging between 10 nm and 100 nm in diameter, were observed as the folded and unfolded conformations of the monomer formed. The folding and unfolding conformations were induced by altering the pH between 10 and 4, respectively. Faster dynamics were observed in acidic environments as well as in the presence of the larger gold colloids implying that larger oligomer units provide a higher density for nonradiative channels.

CHED 1036

Influence of pore size on cobalt loaded mesoporous materials for oxidation catalysis

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Mesoporous materials with SBA-15 and SBA-16 morphology were synthesized as a support for cobalt catalysts. Pore size was tuned to study the effect of pore size on the resulting cobalt particles. The SBA mixes were made at varying temperatures and times to tune the pore size and surface area. Pore sizes ranged from 2.54 to 4.76 nm and surface area varied from 344 to 824 m²/g. Cobalt chloride was loaded by wet
impregnation and the material was heated under air at 600°C. The percent cobalt ranged from 1 to 10 wt%. The catalysts were also characterized by XRD and electron microscopy. The cobalt catalysts were studied in oxidation reactions to evaluate the effect of pore size and cobalt loading on reactivity.

CHED 1037

Comparative study of the application of nanostructured materials to fingermarks impressions

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In the last decade, forensic investigations have increased the effectiveness to complete criminal cases due to the development of specialized equipment and technology. However, the development of fingermarks techniques remains under research. Nanotechnology offers new ways to fill the gaps by the employ of powder nanomaterials for fingermarks as an innovative alternative for detection. Our work consists in the evaluation of the effectiveness of nanopowders for the enhancement of the resolution of fingermarks’ impression. This study was performed using silver and gold nanoparticles alone and coupled to fluorescent semiconductor nanoparticles like ZnO, and CdS. Fresh and aged fingermarks on dry porous and nonporous surface materials were immersed in the nanoparticle solutions. The surfaces used for the study included: crystal, Aluminum foil, polyethylene and A4- regular paper. The sebaceous fingermarks and natural sweat fingermarks impressions were obtained from volunteer students. The impressions samples were divided in three groups of study. In the first group the fingermarks were sampled and analyzed the same day. In the groups two and three the samples were aged during four and ten days, respectively. Results showed that samples treated with ZnO nanopowder presented higher definition and details in comparison with the samples treated using aluminum powder. Additionally, samples with the natural fingers sweat last more than the samples with sebum. This proposed method offers a great sensitive forensic alternative to enhance the detection of fingermarks.

CHED 1038

Comparative study and characterization of MgO, ZnO and CuO nanoparticles using amino acids as capping agents

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Synthesis of ZnO, MgO and CuO nanoparticles was done using sonochemical methods. Colloidal and powder nanoparticles were obtained using zinc sulfate hydrate, magnesium chloride and copper sulfate as zinc, magnesium and copper sources respectively. Tetramethyl ammonium was employed as a surfactant. Polyvinyl Alcohol (PVA) and Polyetheneteylglycol (PEG) were used as stabilizers. Characterization, following synthesis, was done using optical spectroscopy (Ultraviolet Spectroscopy), Infrared Spectroscopy (FT-IR) and Diffracted Light Scattering (DLS). Kinetics studies were done to further information on nucleation and growth. These studies include changes in: reactants concentrations, sonication time and titration rate and heating time. Optical studies show the formation of the clusters and the nanostructures. DLS results showed that the mean average size was 34nm for ZnO, 68nm for MgO and 14nm for CuO. The absorption bands for the nanostructures formation were centered in 358 nm for ZnO nanoparticles, 600 nm for CuO nanoparticles and 335 nm for MgO nanoparticles. Additionally stabilization experiments using amino acids were performed. The ZnO nanoparticles and MgO nanoparticles were stabilized using cysteine and methionine amino acids and CuO with lysine. These results show the potential impact of nanoparticles on bioapplications like drug delivery or nanoprobes for disease detection at the cellular level.

CHED 1039

Functionalization and characterization of bimetallic silver-gold nanoparticles with antibiotics

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New methods for drugs detections are necessary to improve the time and sensitivity for drug testing. Our work is focused in the development of a strategy to produce bimetallic silver-gold core-shell nanoparticles for the study of drugs interactions. Formation of the nanoparticles was achieved by the reduction of the AgNO$_3$ with NaBH$_4$ and HAuCl$_4$ with sodium citrate and polyethylene glycol. A conventional microwave was applied to complete the synthesis. This technology offers minimization of reaction times and stabilization of nanoparticles. In this research, we explore the interactions with Penicillin, Ciprofloxacin, Vancomycin and Clindamycin with the silver-gold core shell nanoparticles. Characterization of the nanoparticles was performed using UV-Vis absorption spectroscopy with a band absorption center at 523 nm, Diffracted Light Scattering (DLS) study shows a mean diameter of 75 nm. Interaction with antibiotics results in a red shift between 15-70 nm. Also a change in color is produced with the addition of the antibiotics to the bimetallic nanoparticles.

CHED 1040

Preparation of metalloporphyrin nanoparticles
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A study was done to determine the best method to prepare metalloporphyrin containing nanoparticles. Two methods of preparation were examined to determine which yields higher quality nanoparticles. Previous synthetic procedures were first studied to determine the optimal method. Cetyltrimethylammonium bromide (CTAB), was used to catalyze the self-assembly process of the nanoparticles, as well as graphene oxide nanosheets (GO nanosheets). Each method was tested with zinc-5,10,15,20-tetra(4-pyridyl)-21H,23H-porphine (ZnTPyP). The research was then expanded by using the method that had higher success with zinc-5,10,15,20-tetra(4-phenyl)-21H,23H-porphine (ZnTPP), 5,10,15,20-tetraphenyl-21H,23H-porphine nickel(II) (NiTPP), and 5,10,15,20-tetraphenyl-21H,23H-porphine copper(II) (CuTPP). The effect of aging time on the size of the nanoparticles was also studied.

CHED 1041

Synthetic methods of CTS and CZTS nanocrystals

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The synthesis of various morphologies of copper zinc tin sulfide (Cu₂ZnSnS₄) and copper tin sulfide (Cu₂SnS₃) nanocrystals were explored to find a more energy efficient synthesis. Reactions were all carried out at 220°C under either inert atmospheres or normal conditions. Variations in synthetic methods included reaction time and solvents used. Products were analyzed with powder X-Ray diffraction and compared to simulated powder patterns of zincblende and wurtzite nanocrystals. The synthesis of CTS nanocrystals required the reaction to be heated to 220°C overnight under an inert atmosphere. The reaction used for the synthesis of CZTS nanocrystals required less energy and only required the reaction to be heated to 220°C for four hours. The effects of solvents were found to be that 1-octadecene (ODE) yielded predominantly a zincblende morphology, oleylamine (OAm) yielded predominantly a wurtzite morphology, and the use of 1-dodecanethiol (DTD) as the only solvent yielded a mixture of zincblende and wurtzite nanocrystals. The various nanocrystals produced assisted in achieving our overall goal by narrowing down an energy efficient and effective synthesis of CZTS and CTS nanocrystals using earth-abundant and low cost reagents.

CHED 1042

Thin films of gold nanoparticles: Temporal stability and mechanisms of degradation
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Thin films of gold nanoparticles (AuNPs) are of interest because of their unique, physiochemical properties. These thin films have potential applications in electrical devices, chemical sensing, and biosensing. Retaining the integrity of the thin film is important for such applications. The purpose of this project is to assess the temporal stability and determine the mechanisms of degradation of thin films of AuNPs on glass substrates. Thin films were fabricated through a layer-by-layer deposition process. Clean glass substrates were sequentially immersed in solutions of 3-aminopropyltrimethoxysilane, synthesized AuNPs, and 1-dodecanethiol (DT). The wettability of each layer was characterized with contact angle goniometry. Upon the completion of thin film fabrication, slides were immersed in ultrapure water and changes in wettability were observed over a 7-day period. Although thin films of gold had more hydrophobic surfaces than DT-containing controls lacking AuNPs, there was still a significant decrease in contact angle once the films were immersed in high purity water. Preliminary results from inductively coupled plasma–atomic emission spectroscopy indicate that the degradation of the thin film does not result from the loss of AuNPs from the slide. Another potential source of degradation is the desorption of DT via oxidation of the thiolate headgroup. Thin films with an additional immersion in an antioxidant were investigated. Results from these studies will be described.

CHED 1043

Synthesizing dendrimer-ligand conjugates for peptide mediated cellular delivery systems

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In recent years nanomaterials have been studied in efforts to design a potential platform for cancer treatment as drug delivery agents. Polyamidoamine (PAMAM) dendrimers are a class of nanomaterials that are star-branched macromolecules containing internal tertiary amines, amide bonds, and terminal primary amines. Conjugation of small molecules to the dendrimer results in nanomaterials that are suitable for treating cancer with greater selectivity and efficacy. Dendrimers conjugated to targeting agents, such as peptides, dyes, and anti-cancer drugs have been used to track and selectively deliver chemotherapeutic agents to cancerous tumor cells. However, due to the high number of conjugation sites, the conjugated dendrimer product results in a distribution of populations varying in the ratio of small molecules per dendrimer including a non-functionalized population. Conjugating first a polar ligand with unique chemistry to the dendrimer would allow for easy separation of the populations with precisely defined numbers of ligands. In this work, generation 5 (G5) PAMAM dendrimers were conjugated with 3-(4-(2-azidoethoxy)phenyl)propanoic acid and 3-(4-(prop-2-ynyloxy)phenyl)propanoic acid as “click chemistry” ligands. The individual populations
are able to be separated by rp-HPLC in order to produce nanomaterials with precisely defined numbers of ligands. Subsequently, biomolecules, such as a peptide, could then be conjugated stochastically resulting in a material with a defined number of peptides per dendrimer. Once conjugated, the G5-ligand products were characterized by HPLC, Proton NMR, and Matrix Assisted Laser Desorption Ionization-TOF.

CHED 1044

Diazonium-derived nitrobenzene layers on nanoporous gold

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The electrochemical reduction of diazonium-based salts is a promising reaction for the functionalization of gold surfaces because it creates a stable carbon-gold bond to the surface. We have investigated the binding of diazonium-based aryl molecules to nanoporous gold electrodes, a novel form of gold with high surface area and conductivity that is well suited for sensing applications. Infrared spectroscopy and cyclic voltammetry were used to characterize the density and stability of the resulting molecular layers. This work examines the viability of electrochemical diazonium functionalization as a scaffold for adding functionality to the nanoporous gold surface.

CHED 1045

Stability of alkane-thiol monolayers on nanoporous gold surfaces

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Nanoporous gold has a high surface area and high conductivity, making it an attractive platform for surface chemistry. However, the nanoporous gold surface lacks the functionality necessary for many applications. Self-assembled thiol-based monolayers are a popular method for adding functionality to gold surfaces, however, many aspects of their performance including density and stability remain unexplored on the nanoporous gold surface. We have investigated the stability and packing of alkane-thiol monolayers on nanoporous gold surfaces using infrared spectroscopy and cyclic voltammetry. This work demonstrates that the resulting molecular layers are dense and well ordered and alkane-thiol monolayers are a promising method for adding functionality to nanoporous gold.

CHED 1046

Zinc oxide and zinc sulfide nanoparticles for DNA detection: Synthesis, functionalization, characterization, and applications
The study of nanoparticles has been a large area of focus in recent years as their applications are widespread and interdisciplinary. Zinc sulfide (ZnS) and zinc oxide (ZnO) nanoparticles have been synthesized using previously-published protocols and functionalized with the lanthanides terbium and europium. The nanoparticles were characterized using UV-vis and fluorescence spectroscopy. The interaction of these lanthanide-functionalized nanoparticles with DNA has been investigated using frequency-domain lifetime and fluorescence experiments with the goal of developing probes that can distinguish between different forms of DNA (duplex, quadruplex).

CHED 1047

Nano size, pH, and temperature dependence of interfacial self-assembly of α-synuclein peptide

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The formation of α-synuclein peptide (α-syn) oligomers on neural cells is regarded as a pathological hallmark of the onset of Parkinson’s disease. This research focuses on a folding or unfolding process of α-syn under an interfacial environment. We use an approach to provide surface potential required for folding through nanogold colloidal particles. The folded or unfolded conformation of α-syn can be prepared by externally changing the pH to pH 10 or pH 4, respectively. Corresponding the folded or unfolded conformation of the α-syn pre-adsorbed over the gold particles create either dispersed or aggregated condition of gold particles, resulting in a no-shift or red-shift SPR (Surface Plasmon Resonance) band for various sizes of gold colloids. Under 25 °C conditions, the reversible self-assembly mechanism was most enhanced over the gold colloidal size of 60 nm, and least over the 10 nm gold colloidal size. When temperature was raised to 55 °C, the reversible self-assembly was enhanced for 10 nm of gold colloidal size. Dissimilarly, the enhancement of the self-assembly was observed for the gold colloidal size of 60 nm as temperature was decreased to 5 °C. Our observations regarding nanosize-, pH-, and temperature- dependence confirmed that a plausible oligomeric unit of α-syn constructed over nanogold colloid must be dimer and trimer over 10 nm and 60 nm gold colloidal surfaces, respectively.

CHED 1048

Solvent interactions in vegetable oil solutions of C₆₀ fullerene

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Solutions of C\textsubscript{60} fullerene dissolved in vegetable oils and a variety of alkane solvents were prepared by using sonication, stirring, and simple dissolution. The effects of these different techniques was compared by studying the UV-VIS spectra of the solutions. Small changes in the nature of the alkane solvent occasionally gave significant changes in the spectra. The formations of suspensions involving clusters of C\textsubscript{60} molecules is common in C\textsubscript{60} solutions and evidence of cluster formation was observed. The effect of varying the temperature from 25° C to 200° C on the spectra was studied. At the higher temperatures decomposition and chemical reactions were indicated for some of the solvents. This research is being conducted because olive oil and other natural oils are used as solvents in the study of fullerenes in biological systems and in commercial products such as cosmetics.

**CHED 1049**

**Ambient and UHV STM studies of metal surface restructuring by amino acids**

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Surface studies of amino acids are beneficial to a variety of scientific fields and questions ranging from the origin of homochirality to the fundamental study of noncovalent supramolecular interactions. The requirement for pristine molecular resolution of these systems requires the use of ultra-high vacuum scanning tunneling microscopy (UHV STM) in the initial characterization of the systems. Importantly, it is also possible to study the assembly of these molecules with liquid or in situ STM in an attempt to bridge the temperature and pressure gap of ultra-high vacuum studies. In this way, these amino acid systems can be studied at more relevant conditions, and solvent choices can be made to mimic biological environments. Through the examination of the self-assembly behavior of five amino acid molecules on a Cu(111) single crystal in UHV, an unexpected phenomenon was discovered. All of the amino acids assisted in the immobilization of copper atoms on the surface. The extension of this extreme and unique interaction will also be studied with ambient STM experiments on Au(111), also a coinage metal. While the UHV studies are critical for the preliminary examination, it is important to determine if the islands are also formed under more biologically relevant conditions, like room temperature and in liquid. It is known that amino acids form complexes with metal ions, like Cu, in the body and that these interactions are critical to the development of neurodegenerative diseases like Alzheimer's. The study of these fundamental interactions on a 2D scale under appropriate conditions could provide useful knowledge to multiple fields from medicine to nanotechnology.

**CHED 1050**

**Probing the interactions of polyethylene glycol-coated magnetic nanoparticles with human hemoglobin**
The interactions between polyethylene glycol (PEG)-coated magnetic nanoparticles (MNPs) and human hemoglobin (Hb) were investigated using various spectroscopic techniques. UV-Vis spectrophotometry and dynamic light scattering (DLS) indicated strong binding between Hb and MNPs. Fluorescence quenching experiments were used to determine the binding constant ($K_a$), enthalpy changes ($\Delta H^\theta$), entropy changes ($\Delta S^\theta$), and free energy changes ($\Delta G^\theta$). Results indicated that PEG-coated nanoparticles quenched hemoglobin fluorescence mainly by a static quenching mechanism. The binding constants ($K_a$) were determined as $1.12 \pm 0.18 \times 10^7$ M$^{-1}$, $0.95 \pm 0.12 \times 10^7$ M$^{-1}$, and $0.78 \pm 0.16 \times 10^7$ M$^{-1}$ at 297, 302, and 307 K, respectively. The changes of secondary structure of hemoglobin due to binding with nanoparticles were also investigated using circular dichroism (CD) spectroscopy.

CHED 1051

Solution-processed templated organic semiconductor nanowires

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One of the most promising fields of alternative energy research is photovoltaics. Organic solar cells offer a potentially cheap, flexible, easily processable alternative to inorganic solar cells. To improve organic solar cell performance, we propose to integrate organic semiconductor nanowires. In this study, we use a template method to create organic semiconductor nanowires of controlled size within the pores of anodic aluminum membranes. We determined that surface functionalization with hexamethyldisilazane (HMDS) leads to improved pore filling. This new process was shown to be effective for producing nanowires made from poly(3-hexylthiophene-2,5-diyl) (P3HT) and 6,6-Phenyl C61 butyric acid methyl ester (PCBM), two common components in organic solar cells. So far, we have been able to produce nanowires with diameters as small as 55nm. These findings could potentially be used to develop efficient organic nanowire-based photovoltaic cells.

CHED 1052

Toxic heavy metal removal via a recyclable gold nanoparticle complex

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Chelating agents in combination with gold nanoparticles (AuNP) can be used to remove heavy metal contamination from a variety of media. Current methods involving AuNP-
Chelate complexes utilize only the complex’s heavy metal detection, rather than removal, abilities. This study was conducted to develop an AuNP-chelate complex that can be removed from the media via centrifugation and then recycled for further heavy metal removal. By attaching thiolated EDTA to AuNP, this remove-then-recycle effect can be achieved. After optimizing the attachment of thiolated EDTA to the gold nanoparticle, the effectiveness of the recyclable gold nanoparticle complex to remove Pb$^{2+}$ from aqueous media will be investigated.

CHED 1053

Nanostructured polymer lithography for photovoltaic applications

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The self-assembly of diblock copolymers into ordered domains holds great potential to furthering the efficiency of photovoltaic devices. Solutions containing polystyrene-block-poly(ethylene oxide) (PS-b-PEO) and poly(methyl methacrylate) (PMMA) were applied to silicon wafers from toluene solutions. Hexagonally ordered domains, with pore sizes ranging from 10-30 nm, were obtained by annealing films in solvent vapor, with the best results produced from a humidified benzene environment. Exposing the films to UV light cross-linked the polystyrene matrix and degraded the PMMA. Removal of the PMMA and PEO produced an ordered polystyrene template, which can be used for nanolithography for the deposition of quantum dots onto the wafers. Details of the film preparation, annealing times and conditions, and characterization will be presented.

![Figure 1. Atomic force microscope image of PS-b-PEO polymer film on Si wafer. Polymer was annealed in humidified benzene environment at low temperature.](image-url)
Impact of poly(ethylene glycol) molecular weight and degree of conjugation on the thermodynamics of DNA complexation and colloidal stability of polyethylenimine-graft-poly(ethylene glycol) copolymers

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Although polyethylenimine (PEI) is a widely used gene delivery agent, poor blood circulation times of the DNA complexes and cytotoxicity lead to inefficient delivery in vivo. Poly(ethylene glycol) (PEG) conjugation to PEI is one solution to these issues, however the extent to which the modification affects DNA binding remains to be quantified. Here, a library of nine cationic copolymers was synthesized by grafting three molecular weights (750, 2000, 5000 Da) of PEG to PEI at three conjugation ratios. The thermodynamics of the copolymer-DNA associations have been quantified by isothermal titration calorimetry and results compared to common assays such as ethidium bromide exclusion and electrophoretic mobility shift. Low conjugation ratios of 750 Da PEG to PEI resulted in little decrease in DNA affinity, but a significant decrease - up to two orders of magnitude - was found for the other copolymers. Dynamic light scattering of the DNA complexes at physiological ionic strength showed that only PEI modifications that reduced DNA affinity conferred significant colloidal stability, a finding that was supported by thermodynamic aggregation data. These results indicate there is an optimum PEG chain length and conjugation ratio in the design of gene delivery agents that will be most effective in vivo.

Deposition of gold nanoparticles on silicon via a galvanic displacement using a block copolymer technique

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A nanoparticle patterning method, the block copolymer technique, has been implemented to control the pitch and diameter of gold nanoparticles, which will be further used as the metal catalyst for silicon nanowire growth. A block copolymer, two polymer chains covalently linked together at one end that self-assemble into nanoscale structures, has been synthesized using the monomers styrene and 2-vinylpyridine and the initiator, n-butyl lithium. This polymer, polystyrene-b-poly-(2-vinylpyridine), was then deposited on silicon wafers via spin coating. These polymers formed spherical domains, with size depending on concentration of polymer, and ratio between monomer concentrations during synthesis. These spherical domains can be used to deposit gold nanoparticles on silicon wafers via a galvanic displacement.
Double shell CdSe/ZnSe/ZnS nanoparticle spectral shifts before and after a manganese dopant is introduced

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Double shell nano-particles, or better known as quantum dots have a very unique and uniform ability to fluoresce under UV light. This project studied the fluorescent properties of CdSe/ZnSe/ZnS quantum dots, and how those properties changed when an Mn dopant was introduced. The dots were grown and synthesized at temperatures above 190°C. Quantum dots have the ability to change wavelengths depending on how long they are grown at those high temperatures. Three different types of quantum dots were observed. The first set was the undoped CdSe/ZnSe/ZnS dots, second was with a doped ZnSe subshell and the final stage was the doped outer ZnS shell. For each quantum dot, the UV-Vis spectrometer and the fluorimeter were used to observe spectral shifts. Double shell quantum dots are more stable, and have a smaller chance of oxidizing under UV light. Manganese is used as a parallel to test whether or not other molecules can attach onto different shells of the quantum dot.

Structural and electronic properties of endohedral and exohedral derivatives of C_{20} and C_{24} fullerenes; TM@C_{20}, TM-C_{20}, TM@C_{24}, and TM-C_{24} (TM = Group 11 & 12 metals): Density-functional theory investigations

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Density functional theory (DFT) is employed to investigate small fullerenes composed of transition metals (TM) that are either encapsulated inside the structure or attached to the outer surface of a small nanocage. Exohedral and endohedral derivatives of the smallest fullerenes, with general formulas of TM@C_{20}, TM-C_{20}, TM@C_{24}, and TM-C_{24} (TM = Group 11 & 12 metals), are systematically investigated in order to evaluate their respective energetic stabilities along with an assessment of the electronic and structural properties of the molecular species. The cation form for each transition metal is incorporated into the fullerene systems and subsequently assessed on the resulting binding energy, HOMO-LUMO gap, and Gibbs' reaction energy. Preliminary calculations on the Cu@C_{20}^{1+} endohedral fullerene indicate that the derivative is energetically comparable to that of the C_{20} nanocage; however, the C_{20}Cu^{1+} exohedral is predicted to increase the HOMO-LUMO gap, relative to the C_{20} cage, by 14% and possess negative binding energy and thereby increasing the energetic stability of the system. The remaining Group 11 and 12 transition metals will be subjected to identical calculations in both the endo- and exohedral C_{20} and C_{24} derivatives. Analysis of the results will then
be conducted in order to evaluate the potential feasibility of synthesizing this class of fullerenes in the laboratory.

Endohedral derivative Cu@C_{20}

Exohedral derivative Cu-C_{20}

CHED 1058

Synthesis of graphene and its derivatives by chemical reduction, mechanochemical ball-milling, and electrochemical exfoliation

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Graphene, a two-dimensional carbon layer, has recently attracted significant research attention because of its impressive thermal, elastic, optical, electrical, and mechanical properties. Current methods of producing high-quality graphene are expensive, toxic, and complex. Developing an alternative path for the production of scalable graphene-related materials while improving upon commonly used methods are the goals of this study. Because pure graphene can be difficult to make, our study focuses on producing more cost-effective graphene derivatives, including few-layer graphene mixtures and reduced graphene oxide (rGO). This report introduces several methods to produce graphene-related materials, including chemical reduction by organic solvents, mechanochemical ball-milling, and electrochemical exfoliation of raw graphite. Samples were characterized using Thermogravimetric Analysis (TGA) for thermal stability studies, Fourier Transform Infrared Spectroscopy (FTIR) for the determination of
functional groups, Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM) for visualization of surface diagram and atomic structure, and Raman Spectroscopy for graphene identification. The results conclude that each method successfully produced graphene mixtures with improved qualities and exfoliated structures.

CHED 1059

Inkjet-printed multisensor arrays on flexible substrates

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This presentation describes the design, fabrication and analytical applications of flexible multi-sensor arrays. The sensor arrays were fabricated on flexible substrates using simple inkjet-printing technology. To achieve this, two types of nanoformulations were prepared: one formulation composed of conducting nanoparticle ink and the other composed of polymeric semiconducting nanoparticle ink. The polymeric and conducting inks were synthesized via chemical methods. Characterization of these inks was performed by cyclic voltammetry, Fourier-transformation infrared spectroscopy, UV-visible spectroscopy, Raman spectroscopy, and scanning electron microscopy. The sensor arrays were designed and printed such that the semi-conducting polymeric layer bridged the electrodes fabricated from the conducting nanoparticle ink. The polymer bridge layers acted as the sensing elements while the conducting ink layer acted as the electrodes as well as the interconnects for the circuits. The sensor arrays will be employed for the detection of various analytes. The goal is to achieve reproducible, cost efficient, and flexible sensor array fabrication with the potential for mass production.

CHED 1060

Direct growth of alpha-Fe$_2$O$_3$ by vapor deposition on stainless steel as anode for Li-ion battery

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$^{3d}$ transition metal oxides have been studied widely as an anode component for lithium ion batteries due to their high reversible capacities, chemical stability, and low cost. Fe is one of the more abundant metals among the various transition metals and its oxide form, Fe$_2$O$_3$, possesses fairly high capacity of 960 mAh g$^{-1}$. Direct growth of nanomaterials on current collectors leads to efficient charge transport, and no need of polymer binder and conductive carbon. Because of the preceding facts, Fe$_2$O$_3$ nanoparticles have been deposited directly on stainless steel by chemical vapor deposition (CVD) method using a volatile precursor material, Fe(acac)$_3$. 
(acac=acetylacetonate). As prepared materials were characterized by powder x-ray diffraction and field emission scanning electron microscope techniques. Cyclic voltammetry and galvanostatic charge-discharge experiments were carried out versus Li metal and the details will be presented.

CHED 1061

Chemical vapor deposition of cubic NiO nanoplates on stainless steel substrates as anode for lithium-ion battery

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2D-dimensional nickel oxide (NiO) nanoplates were prepared using a low pressure chemical vapor deposition (LPCVD) producing metallic Ni directly on stainless steel current collectors followed by annealing under ambient oxygen atmosphere. The structural identities of the as-deposited nanomaterials were examined by X-ray diffraction, which revealed the formation of NiO (111 preferred orientation) after annealing. The morphology was examined by field emission scanning microscopy, which displayed the uniform arrangement of NiO nanoplates. The electrochemical properties of the as-deposited NiO nanoplates were investigated galvanostatic discharge-charge experiments in the range of 4.0 to 0.1 V versus Li/Li⁺ at a constant current of 100 mA for the first 10 cycles. A capacity of 1377 mAh g⁻¹ was observed during the first discharge process. The rate was increased to 200 mA which displayed a capacity 1291 mAh g⁻¹. After 70 cycles at 100 mA a capacity of 1542 mAh g⁻¹ was calculated. A capacity of 1723 mAh g⁻¹ was shown at a constant current reading of 500 mA after 110 cycles. The as-deposited NiO nanoplates stabilize around 1650 mAh g⁻¹ after 140 cycles at 500 mA. The NiO nanoplates exhibited better reversibility and higher
capacity than previously synthesized NiO anodes. It is interesting that the NiO
nanoplates held the extra capacity even after 150 cycles. The origin of the extra
capacity in the NiO nanoplates will be discussed.

Plan view image of NiO nanoplates (15-30 nm)

CHED 1062

Cyclic voltammetry study on the origin of excess capacity on ruthenium oxide

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Synthesis and understanding of nanomaterials with improved properties are critical in
the development of high capacity electrochemical cells for application in lithium ion
batteries. Nanostructured materials have been shown to have exceptional storage
capabilities. In this project, we have prepared nanostructured columnar self-assembled
ruthenium oxide (RuO₂) directly on stainless steel current collectors using low pressure
chemical vapor deposition. The as-prepared materials were examined by powder X-ray
diffraction. 3D pyramidal structure ranging from 50 to 80 nm was self-assembled.
Galvanostatic charge-discharge experiments versus Li/Li⁺ in the range of 4 to 0.1 V
have demonstrated that these nanostructures are reversible at extremely high capacity
(~1150 mAh g⁻¹, 5.70Li per mol of RuO₂). The capacity retention was approximately
100% from the first to second cycle and 87% after 60 cycles. The origin of the excess
capacity was probed using cyclic voltammetry (CV), which was performed at various
different voltage ranges. The CV results will be discussed.
Transition metal oxides are a class of anode materials for lithium ion batteries. They possess higher theoretical capacities than that of graphite and store charges through conversion reactions with lithium, within which electrochemical reduction leads to the transfer of at least two Li ions. Carbon coating is required for transition metal oxides in battery application. However, utilization of low cost and abundant metals such as Mn provides a variety of scalable electrode alternatives. Direct growth of nanomaterials on current collectors has several benefits such as sufficient empty space to accommodate the volume change, electrical contacts to the current collector, efficient charge transport, and no need of polymer binder and conductive carbon. We have deposited MnO nanoparticles directly on stainless steel by chemical vapor deposition (CVD) method using a volatile precursor material, Mn(acac)$_2$ (acac = acetylacetonate). As prepared, the material was characterized by powder x-ray diffraction and scanning electron microscope techniques. It possesses cubic MnO structure with a film thickness of 1 μm. Electrochemical charge-discharge experiments were carried out versus Li metal. High experimental capacity of ~975 mAh/g was achieved during the first cycle with high cyclability and an increase in capacity for subsequent cycles.
Galvanostatic charge-discharge capacity of as-deposited MnO nanoparticles shows an increase in capacity for the first 275 cycles. Measured at constant current 100 mA in a mixture of 1 M LiPF₆ in EC-DEC-DMC in a 1:1:1 volume ratio.

CHED 1064

Vapor phase synthesis of cubic CoO nanocrystals as anode in lithium ion battery

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The synthesis cobalt oxide has great importance but is quite challenging due to the complexity of its chemical formation. A one step synthesis for the growth of CoO nanoparticles and their performance as anode for rechargeable lithium ion batteries are described. Low-pressure chemical vapor deposition was used to deposit CoO directly on stainless steel current collector from cobalt acetylacetonate precursor. CoO nanoparticles were synthesized at a temperature around 400° C and 3 torr. The crystal structure was characterized by X-ray diffraction and the morphology was studied by field-emission scanning electron microscopy. Electrochemical measurements were performed and the nanoparticles electrode exhibited high discharge capacity and good cycling performance with >95% Coulombic efficiency. The nanoparticle shows excellent cyclability. The enhancement of the electrochemical performance is attributed to the high specific surface are excellent contact between the nanoparticles and the current collector. This work is promising in that it provides a reproducible method for the synthesis of cobalt oxide.

CHED 1065

Energetic effects of metal nanoparticle fuel additives on the combustion of ethanol

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The purpose of this project was to study the effects of metal nanoparticle fuel additives (magnesium, aluminum, scandium, and indium) on the combustion of ethanol. Metal nanoparticles were synthesized using electrolytic reduction of the appropriate metal acetate in tetrahydrofuran. The compositions, sizes, and shapes of the nanoparticles were characterized using X-ray powder diffraction and atomic force microscopy. The heats of combustion for ethanol-nanoparticle mixtures (containing up to 10% of the metal nanoparticles by volume) were measured and compared to the heat of combustion of pure ethanol.

CHED 1066

Fluorescence quenching in organic and inorganic solutions using gold nanoparticles

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Due to the unique properties of gold nanoparticles, applications across many fields can be found, ranging from drug delivery to ceramic coloring. One such application utilizes the strong and unique fluorescence quenching ability of gold nanoparticles, which arises due to the plasmonic nature of the particles. This research examines the quenching effects of gold nanoparticles when in solution with fluorescent organic and inorganic compounds such as naphthalene and cerium salts.

CHED 1067

Cheap and cost effective synthesis of metal (gold, silver)/reduced graphene oxide nanocomposites for antibacterial applications: A comparative study

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Noble metals such as silver and gold have been recognized since antiquity for their antimicrobial properties, but with the advent of antibiotics, their use in this regard was discontinued. The advancement in nanomaterials science in the past decade has resulted in a growing interest in their use as an adjunct to microbial control, particularly because of the rise in antibiotic resistant bacteria. Indeed, silver nanoparticles (Ag NPs) and gold nanoparticles (Au NPs) are currently being used as broad spectrum antimicrobials in a wide range of commercial products such as toys, cosmetics, fabrics, water filters and detergents. However, the widespread use of these metals poses another set of problems, such as toxicity to mammalian cells, pollution to the environment and cost effectiveness.

It has been shown that the antibacterial activity of these nanoparticles is dependent on particle size and distribution. Indeed, because of its unique properties in terms of
mechanical strength, electrical conductivity and non-toxicity to mammalian cells, rGO is an ideal substrate for the tethering of metal nanoparticles. In this work, in order to assess the relative effectiveness of different noble metal/ rGO nanocomposites, we have prepared AgNPs and AuNPs/rGO nanocomposites using cheap and cost effective route and are currently measuring their antibacterial activity in terms of colony inhibition and bacterial DNA damage. We have shown that by bonding AgNPs and AuNPs to sheets of reduced graphene oxide (rGO), we are able to achieve similar levels of bacterial inhibition using far lower levels of metal ions compared to pure preparations of Ag NPs and Au NPs alone.

CHED 1068

Enhanced visible light driven photocatalytic degradation of organic dyes and antibacterial properties of iron oxide/RGO nanocomposites

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Environmental problems such as organic pollutants and toxic water pollutants produced by some industries are harmful to human health. Semiconductor-assisted photocatalytic degradation of organic pollutants has attracted considerable attention because it shows promise for solving environmental pollution problems. In addition, the emergence and increase of microbial organisms which can cause severe infections and have developed unmatched resistance to drugs, result in a number of deaths caused by multi drug resistant (MDR) bacteria in developed economies every year. Therefore, new strategies are needed to design antibacterial agents. Among various oxide semiconductor photocatalysts, α-Fe2O3 has been recognized as excellent material for visible light photocatalysis and antibacterial agent due to high photosensitivity, nontoxic nature and low cost. Graphene surface has been of significant interest as a means of tuning the properties of the nanosheets for enhanced performance in various applications. In this work, α-Fe2O3/ RGO nanocomposites with tunable size and shape were prepared by microwave irradiation based solution method. The as-grown nanostructures were characterized using X-ray diffraction (XRD), field emission scanning electron microscopy (FE-SEM), energy-dispersive X-ray (EDX) spectroscopy, transmission electron microscopy (TEM), Raman and ultra violet- visible (UV-Vis) measurements. XRD showed that the nanostructures were highly pure and well crystallized. FESEM and TEM images confirmed the nanometer size range of nanostructures. The photodegradation of methyl orange (MO) using α-Fe2O3/RGO nanocomposites was measured under visible light irradiation and observed that α-Fe2O3 showed higher activity than commercial α-Fe2O3. Antibacterial activity of α-Fe2O3/RGO nanocomposites as a function of concentration against gram-negative bacterium Escherichia coli (E. coli) was carried out in solid growth media. Nanocomposites showed better antibacterial activity than that of other antibacterial agents.

CHED 1069
Synthesis, characterization, and antibacterial activity of reduced holey graphene

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With increasing antibacterial resistance, the effectiveness of antibiotics will decrease. Which means, future antibiotics will be weak and not be able to fight life-threatening diseases. Graphene surface has been of significant interest as a means of tuning the properties of the nanosheets for enhanced performance in various applications. Herein, we will present synthesis and characterization of Holey Reduced Graphene Oxide (HRGO) nanosheets via microwave irradiation and its antimicrobial activity will be presented. The as-prepared HRGO are expected to present effective antibacterial activity towards E. coli. The ultimate quest of this work is to use the HRGO in the filtration system for killing microorganisms which may cause biofouling in downstream filters.

CHED 1070

Facile synthesis of reduced graphene oxide layer supported cobalt nanoparticles and their antibacterial activity against E. coli

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Graphene has unique physical properties, and a variety of proof-of-concept devices based on graphene have been demonstrated. A prerequisite for the application of graphene is its production in a controlled manner because the number of graphene layers and the defects in these layers significantly influence transport properties. In this work, well dispersed Co nanoparticles (NPs) supported on the reduced graphene oxide (rGO) were synthesized by simple solution method. The synthesized nanocomposites were characterized using UV/Vis absorption spectroscopy and transmission electron microscopy (TEM) measurements. UV/Vis study revealed the formation of cobalt/ rGO nanocomposites with characteristics surface plasmon absorption maxima. From TEM analysis, it is observed that the nanocomposites have uniform size distribution. Antibacterial activity of Cobalt and rGO nanocomposites as a function of particle concentration against gram-negative bacterium Escherichia coli (E. coli) was carried out in solid growth media. The nanocomposites show good antibacterial activity against E. coli.

CHED 1071

Tuning the forces between conjugated nanoparticles
Organic photovoltaic (OPV) devices have garnered considerable attention as a renewable energy source, due in large part to their low production costs, mechanical flexibility, and their potential to revolutionize the energy landscape by providing sustainable, clean power. We aim to develop a next-generation OPV device morphology that uses organic nanoparticles. The production of any photovoltaic device consists of efficiently assembling donor and acceptor materials in a 3-D structure such that continuous conduction paths exist between electrodes. The so-called bulk heterojunction morphology thus far has achieved the most success, but the formation of this morphology requires material specific process conditions and is quite Edisonian. Self-assembly of semiconducting polymer nanoparticles provides a route to desired morphologies with control at multiple length scales.

We propose a method of controlling packing between donor and acceptor nanoparticles by tuning the van der Waals force between them. For neutral particles dispersed in a solution we have shown that the dominant force of interaction at the scale of nanoparticle packing is the van der Waals force. The magnitude of the force between two nanoparticles is inversely proportional to the distance between them. Using mathematical techniques in QED, one can find that, magnitude the proportionality constant depends upon the dielectric constant and the refractive index of the dispersant. Using this theory, we show that, for reasonable ranges of refractive indices and dielectric constants, the force between two nanoparticles at the 1 nm distance can range over a full order magnitude. Additionally, we have shown that changing the solvent from water to an organic solvent like decalin or benzene can change in the magnitude of the force by hundreds of pico-Newton. We show that with organic nanoparticles used in OPV’s, the van der Waals force is strongly dependent upon changes in the refractive index of the dispersant. Based upon these calculations, dispersing solvents can be specifically selected to tune the van der Waals forces between particles which can significantly affect the geometry of the packing of nanoparticles. This study provides new insight into the possible methods of controlling OPV morphology by tuning the van der Waals forces of semi-conducting polymer nanoparticles by taking advantage of the myriad solvents available.

CHED 1072

Investigation of the ability of dibenzyl sulfoxide and triphenylphosphine oxide to form cocrystals with carboxylic acids and phenols

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A binary cocrystal is a crystalline structure composed of two different compounds in a definite ratio. Our cocrystal design consists of one compound containing two hydrogen-bond donors in combination with a compound containing a single hydrogen-bond acceptor. The ten didonor compounds we have tested in this research consist of an aromatic core appended with a carboxylic acid and a phenol. We have investigated the ability of these compounds to form cocrystals with two different acceptor compounds: dibenzyl sulfoxide and triphenylphosphine oxide. A total of over 150 cocrystallization experiments were carried out and analyzed by infrared spectroscopy to identify the formation of cocrystals. HNMR was then used to determine the stoichiometry of any cocrystals that formed. In this poster the cocrystal design strategy, the experimental methods, and the analyses will be discussed along with applications in future work.

Possible Cocrystal

CHED 1073

Complete synthesis of analogs of a tuberculosis medication, ethambutol, with known intermediates, diethyl ethylmalonate and diethyl phenylmalonate

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Ethambutol is a medication given when diagnosed with tuberculosis and this research presents two pathways that will facilitate a total synthesis of four analogues of this drug. Both pathways use well known malonate intermediates in a five and seven step synthetic route. The pivotal portion of the synthesis is using a lipase in order to generate an alcohol with stereochemistry around a chiral carbon. The first pathway will take the malonate compound and reduce it into a diol. An acylation with acetic anhydride will take place with the diol and then lipases will react to
hydrolyze the compound into an alcohol with a chiral carbon. Once the hydrolysis is completed, the material will be subjected to SN$_2$ conditions in order to replace the hydroxide functional group with an azide. The last step in the first synthetic pathway will be to perform a reduction and the final product will be a β-amino alcohol.

The second pathway is the same as the first until the compound is hydrolyzed. After the hydrolysis a protection of the hydroxide will be performed and then the protected compound will undergo a reduction to yield a terminal alcohol. From there the product will replace the hydroxide group with an azide group through a SN$_2$ reaction. The final step will be to reduce the azide into a terminal amine.
Investigation of the ability of sulfisomidine to form cocrystals with carboxylic acids
Cocrystals, defined as multicomponent neutral molecular complexes that form crystalline solids, have important applications in the pharmaceutical industry due to their ability to change the physical properties of drugs. This research builds upon past research on sulfisomidine and sulfamethazine, two nearly identical antibacterial drugs both of which contain an amidine group known to hydrogen bond to carboxylic acids. Prior work has shown that sulfamethazine forms cocrystals readily with carboxylic acids and has several cocrystal structures in the Cambridge Structural Database. Sulfisomidine, in contrast, does not and has no cocrystal structures in the database. Previous work with sulfamethazine has shown that conditions that favor cocrystallization can be produced by either using an ideal solvent to decrease the solubility differences between the drug and acid or by increasing the initial amount of the more soluble component. In this research, these conditions were applied to sulfisomidine/carboxylic acid solutions in attempt to enhance cocrystallization conditions. Solids formed from slow evaporation of sulfisomidine/carboxylic acid solutions were analyzed by infrared spectroscopy for shifts in the absorbance of hydrogen bonding functional groups, and by proton nuclear magnetic resonance spectroscopy to determine the ratios of components by comparing the integrations.

CHED 1075

Synthesis of novel bactericidal aminoglycosides

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With the proliferation of multi-drug resistant bacteria, the synthesis of novel antibiotics is of the utmost importance. As such, we propose to functionalize simplified analogues of common antibacterial agents—specifically certain well studied, but underexploited, aminoglycosides—to produce a library of new, potentially bactericidal molecules. Toward this end, we chemically modified the neamine-like substructure of the aminoglycosides butirosin B, neomycin, and paromomycin with azide and alkyne moieties, as depicted in Figure 1. In the future, via the high-yield azide-alkyne click reaction, each of these molecules will be 'clicked' with an array of alkyne- and azide-modified small molecules to produce a library of novel semi-synthetic aminoglycosides, as described in Figure 2. These semi-synthetic aminoglycosides will then be tested for antibacterial activity via antibiogram and, depending on the results obtained, further chemical modifications will be considered.
Palladium-catalyzed coupling of O-benzylbenzimidoyl iodides and boronic acids

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The synthesis of O-benzylbenzimidoyl iodides [Ar¹C(I)=N-O(CH₂)Ar²] has been developed. These compounds are made by converting the corresponding O-benzylated hydroxamic acid into the O-benzylbenzimidoyl tosylate followed by reaction with iodide ion to produce the O-benzylbenzimidoyl iodides. These iodo compounds were subjected to a palladium-catalyzed coupling reaction with arylboronic acids to form single geometric isomers of O-benzylxime ethers of substituted benzophenones [Ar¹C(Ar³)=N-O(CH₂)Ar²]. Various approaches to install the N-benzyloxy group are outlined. Characterization data for the E and Z isomers are compared.

Palladium-catalyzed Songashira coupling reaction between diaryl telluride and alkynes

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The Sonogashira reaction is a cross-coupling reaction used in organic synthesis to form carbon–carbon bonds. It employs a palladium catalyst to form a carbon–carbon bond between an aryl or vinyl halide and a terminal alkyne. Due to its usefulness in the formation of carbon–carbon bonds, the Sonogashira cross-coupling reaction has been employed in a wide variety of areas such as pharmaceuticals, natural products, organic materials, and nanomaterials. Organochalcogen compounds have been used extensively in carbon–carbon bond forming reactions. In our research, a highly efficient new protocol for C–Te bond formation leading to symmetrical diaryl tellurides has been developed.

The synthesis of symmetrical diaryl tellurides employed aryl iodides and elemental tellurium as starting materials in the presence of KOH. It is a one-pot reaction without using any catalyst. Utilizing this new protocol, a variety of aryl and heteroaryl iodides are reacted with elemental tellurium to afford the corresponding diaryl tellurides in good to excellent yields.

In this work, diaryl tellurides were used as coupling partners in Pd-catalyzed Sonogashira reactions under exceptionally mild conditions. Several palladium catalysts and bases were attempted but the coupling product alkynyl arene was formed in a favorable yield at room temperature only when Pd(dppf)Cl$_2$ was used as the palladium source and K$_2$CO$_3$ as the base in the presence of Cul. Under the optimized conditions, the coupling between various diaryl tellurides with alkynes was studied.

The new method for Sonogashira reactions will lead to a more benign alternative to the various fields in the synthesis of alkynyl arene-containing molecules.

CHED 1078

Investigation of the non-covalent binding between benzo-crown ethers and bis(trifluoromethyl)dibenzylammonium ion

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We are exploring the non-covalent interaction between bis(trifluoromethyl)dibenzylammonium hexafluorophosphate ion (1) and a series of variously-sized benzo- and dibenzo-crown ethers. The guest and host combine in 1:1 stoichiometry to form a [2]pseudorotaxane as evidenced by isothermal titration calorimetry and $^1$H NMR spectroscopy. These methods also permit the association constants to be measured, which are on the order of 1,876 M$^{-1}$ in 1:1 chloroform / acetonitrile. In addition to the expected host-guest threading interaction in the slow exchange regime, we also observed an unusual concentration-dependent fast exchange process by NMR. The signals corresponding to the aromatic protons of 1 exist as a pair of doublets in the presence of sub-stoichiometric amounts of benzo-24-
crown-8, but coalesce into one singlet in the presence of equimolar (or higher) amounts of crown ether. Equally puzzling, the apparent multiplicity of these protons also varies with concentration, even when the host:guest ratio is maintained at a 1:1 stoichiometry. We are examining the hypothesis that pi-pi stacking plays a role in this unexpected phenomenon. Further investigation by UV-Vis spectroscopy and attempts to grow X-ray quality crystals are underway.

CHED 1079

Tethered quionolide ligands for stereoselective lactide polymerization

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Lactide can be polymerized via a ring polymerization mechanism, producing polylactic acid (PLA). PLA is a carbon-neutral, biodegradable plastic; a plastic that is an alternative to petroleum based plastics whose lifetimes far exceed their use. Recently, we explored the efficacy of a series of chiral aluminum-based catalysts, each with uniquely substituted 8-hydroxy quinolide ligands, to facilitate the ring opening polymerization of lactide with iso-stereoselectivity. The success of these catalysts invites the study of a new series of tri- and tetra-dentate ligands based on the quinolide core, designed to form chiral aluminum catalysts with greater thermal stability than its predecessors.

The synthesis and characterization of several such ligands, and their subsequent incorporation into active catalysts, will be discussed. Most of the ligands described are made with a pair of quinolide ligands tethered together via carbon bridges constructed using well-developed synthetic approaches such as olefin metathesis, palladium catalyzed cross-coupling reactions, or thiol-ene reactions. Subsequent lactide polymerizations will be described, including polymerization rates, thermal properties and polymer tacticities for polymers formed from each catalyst will be measured.

CHED 1080
Diversifying covalent organic framework designs through nonreversible linkages and non-planar aromatic monomers

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Covalent organic frameworks (COFs) are an emerging class of two- and three-dimensional polymers linked entirely by the covalent bonds of light elements such as carbon, nitrogen, boron, and oxygen. These materials can be predictably designed to form highly organized, crystalline networks with high-surface area and porosity, and are suitable candidates for a variety of applications such as gas storage, charge storage, and photovoltaic cells. COFs are often constructed from planar aromatic monomers, providing two-dimensional polymer sheets that stack into a layered crystal. Although the mechanism of COF formation is not fully understood, the reversible bond formation during the polymerization process is thought to be necessary for the formation of crystalline networks.

Dynamic bond formation provides a mechanism for the network to correct defects as it crystallizes. Tailoring COF design to this requirement constrains the types of linkages, and expected properties of these materials. As a result, COFs that can achieve crystallinity under non-reversible reaction conditions based on the rigidity of their monomers, or have limited aromatic surface areas available for stacking, will diversify the potential designs and applications of future COFs. Two such approaches for COF formation will be discussed.

(1) A non-reversible, nucleophilic aromatic substitution is a potential candidate for the formation of a crystalline COF from a non-reversible reaction. Computational modeling has shown this linkage to be rigid and planar, which suggests that the polymer network would be forced into the typical, planar COF sheet.

(2) The formation of a COF as a single-layer 2D polymer might be promoted by reducing the high surface-area contacts between adjacent sheets. Triptycene is a three-fold symmetric monomer whose aromatic groups are arranged in a 3-dimensional fan, rather than in a flat plane, and has been incorporated into COFs previously. Condensation reactions of triptycene-based monomers orient the π orbitals into the pore of the COF, which limits interlayer interactions and might facilitate the isolation of single-layer structures.

Progress toward the syntheses of these two COF networks will be presented, including the optimized solvents, temperatures, and catalytic conditions.

CHED 1081

Studies on Suzuki and Hiyama coupling of halopyridines with bromoacetates
In the context of synthetic studies toward phantasmidine analogs, we sought a method which would allow efficient access to dihalohomonicotinic acid synthons. A promising route would be the direct coupling of 3-pyridyl anions to haloacetates. However the acidity of the haloacetate precludes direct reaction with highly basic organolithium derived from directed ortho metalation using LDA. Transmetalation to the organozinc using ZnCl₂-TMEDA also failed to give product, as did attempted coupling of the Reformatski zinc enolate with the iodo halopyridine. We next investigated cross-couplings based on boron (Suzuki-Miyaura) or silicon (Hiyama) derivatives of halopyridines. Thus 2,6-dichloropyridine and 2-chloro-6-fluoropyridine were lithiated and quenched with TMSCl and B(OMe)₃ to give the corresponding silyl and boroxine derivatives, while attempts to obtain silicate derivatives using Si(OEt)₄ failed. Results of our efforts at cross-coupling under Pd-catalysis to date will be discussed.

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**CHED 1082**

**Design and synthesis of multifunctional peptoid-NSAID conjugates**

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To date, there is no cure for Alzheimer's disease (AD), a debilitating neurodegenerative disorder affecting an estimated 5.1 million Americans, because there is a lack of potent medications with suitable blood-brain barrier (BBB) penetrability. Recent research has linked cyclooxygenase-1 (COX-1) to amyloid-beta (Aβ)-induced neuroinflammation, and metals, such as iron and copper, may also play a role in Aβ-associated oxidative damage. Clearly, a multifunctional approach is necessary to treat such a complex disease. As such, COX-1 inhibitors and metal chelators have been explored as potential treatments for AD. In this work, peptoids, or N-substituted glycine polymers, containing polyphenolic arms are linked to anti-inflammatory drugs in order to generate dual-acting AD agents with enhanced BBB penetrability. The synthesis, characterization, and membrane permeability of these novel molecules will be presented.

**CHED 1083**
Desilylation and deuterium enrichment of ethynyl substituted pyridines

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Cross-coupling followed by desilylation of terminal alkynes is a common method for building complexity in organic synthesis. In the course of other studies, our work required deuterium enriched ethynylpyridines. Replacement of the trimethylsilyl group with a deuterium atom can be difficult to complete with many current desilylation techniques. We will discuss the first reported one-pot microwave assisted desilylation and deuterium incorporation of ethynyl pyridines. Using tetrabutylammonium fluoride and deuterium oxide, we observe rapid reactions with high deuterium incorporation for various ethynyl substituted pyridines.

CHED 1084

Synthesis of 3,4-bis(2-acetoxybenzoyl)-1,2,5-oxadiazole-2-oxide

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Acetylsalicylic acid (aspirin) can cause ulceration of the mucosal lining of the stomach. Nitric oxide is an endogenous compound that inhibits ulcer development. Therefore, taking aspirin in unison with a drug capable of releasing nitric oxide would help alleviate the side effects associated with aspirin. 1,2,5-Oxadiazole-2-oxides, also known as furoxans, have been shown to release nitric oxide in the presence of thiol cofactors. Furoxan derivatives have also been seen to serve therapeutically as nitric oxide generators in vivo. In this presentation, the results from the synthesis of bis-acetylated dibenzoylfuroxans will be discussed.

CHED 1085

Investigating the stereochemistry of 2-pyridinecarboxaldehyde in aldol reactions

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In basic solution, 2-pyridinecarboxaldehyde rapidly undergoes tandem aldol condensation - Michael addition with acetophenone at room temperature. In the presence of two equivalents of acetophenone, only the Michael adduct is recovered and it is not possible to isolate the α,β-unsaturated ketone intermediate. However, if the enolate is generated from propiophenone, only the β-hydroxyketone is isolated. Alternative means of generating the enolate are being investigated in an effort to gain some insight into the stereochemistry of the reaction intermediates.

**CHED 1086**

**Impact of cyclopentadienone substitution on the activity of (cyclopentadienone)iron tricarbonyl catalysts**

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Replacing precious metal catalysts with those containing earth-abundant metals has become a major focus of 21st century chemical research. Along those lines, in 2007 Casey and Guan reported that an air-sensitive iron hydride originally synthesized by Knölker’s group catalyzed the reduction of carbonyl compounds through a mechanism similar to that of Shvo’s diruthenium bridging hydride. An air-stable cyclopentadienone(iron) tricarbonyl precursor to the iron hydride, also synthesized by Knölker’s group, has also been shown to be an active catalyst in a variety of organic oxidation and reduction reactions. The cyclopentadienone substitution has been shown to dramatically alter the activity of this class of catalysts, and there have been few studies systematically exploring this impact. In this study, a series of cyclopentadienone(iron) tricarbonyl compounds bearing cyclopentadienones with varying substitution have been synthesized, and the catalytic activity of each compound
has been tested in six organic oxidation and reduction reactions. The impact of steric and electronic variations on catalyst activity will be presented.

CHED 1087

Towards the synthesis of a photocleavable linker for GlcNAc-ligated protein purification

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Proteins routinely undergo post-translational modifications, which are crucial for their optimal function. One such post-translational modification introduces N-acetylglucosamine (GlcNAc) to certain serine and threonine residues. Determining site-specifically where the GlcNAc groups are is important to understanding the role they play in the regulation and function of proteins. Our goal is to synthesize a photocleavable linker that covalently binds to proteins bearing GlcNAc and aids in their purification. Once the proteins are purified, the linker will be removed photochemically before mass spectrometric analysis is done to determine site-specifically which serine and threonine residues bear GlcNAc groups. The photocleavable linker contains three important components: a strained alkyne, a photocleavable group, and an insoluble bead. The focus of our initial efforts has been on synthesizing a model of the targeted linker and exploring its photochemistry. We have found that an aminocoumarin bearing an ester undergoes a relatively clean, reliable photocleavage to afford a carboxylic acid. Our current focus is on introducing the strained alkyne to the aminocoumarin and exploring the behavior of the product. Future work will involve completing the synthesis by introducing the insoluble bead to the aminocoumarin/strained alkyne portion of the linker.

CHED 1088

Synthesis of diepoxo- and triepoxy c-ring analogs of triptolide: An antileukemic, male contraceptive and an anti-inflammatory diterpenoid triepoxide

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Triptolide has been isolated from the Chinese medicinal plant Tripterygium wilfordii Hook f. known as the "Thunder God Vine" that has a long history of medicinal value.

Synthesis of such models will require preparative, chiral HPLC and NMR and they will be a starting point for the development of practical medicinal agents, with variations in stereochemistry and functionality. These could be used to develop a structure-activity
correlation which might help to clarify the mechanism of action and receptor characteristics involved in the biological response.

CHED 1089

Synthesis of HIV-1 capsid protein inhibitors based on SAR analysis

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HIV-1 is the predominate virus responsible for the AIDS pandemic, accounting for greater than 90% of cases globally. The current treatments for the virus are drug cocktails that target the reverse transcriptase and protease enzymes; however, these proteins mutate rapidly through successive iterations making long term treatment difficult. In this project inhibitors are developed to target the HIV-1 capsid protein (CA\textsubscript{N}) through the conserved Phe32 active site at the N-terminus of the virus. Inhibitors were synthesized based on a molecular frame developed through computer modelling, experimental testing, and structural activity relationship analysis. Inhibitors were developed building off of a 3,5-bis(trifluoromethyl) substituted aromatic head in three primary series; one series tests functionality of amino acid tail groups, a second series examines hydrophobic effects of the tail group in binding to a hydrophobic pocket near the Phe32 active site of CA\textsubscript{N}, and a third series explores hydrogen bonding effects of a 2-aminoethanol linker group. 19 novel compounds have been developed and nine new inhibitors have been experimentally tested through \{\textsuperscript{15}N-H HSQC\} NMR titrations, achieving a binding affinity of K\textsubscript{d} of 26 μM.

CHED 1090

Factors affecting the product distribution of substitution and elimination reactions: An experiment for an undergraduate organic lab

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Nucleophilic substitution and elimination reactions are early concepts taught to undergraduate organic students. Various factors influence the product distribution of these reactions including nucleophile strength, leaving group ability, steric crowding, and the type of solvent. During a typical lecture the theories behind the effects of these factors are presented to the students. However, we have found that students have a hard time grasping the influence of these factors on product formation. In the described experiment, undergraduate students will explore the effect of altering reaction conditions on the product distribution of substitution and elimination reactions by altering the reagent to vary nucleophilicity and changing substrate to compare leaving groups and
steric strain. Product distribution will be analyzed by GC/MS, which will enable them to connect the theory to the experimental results.

CHED 1091

Synthesis of phthalocyanine photosensitizers for potential use in photodynamic therapy

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Photodynamic Therapy (PDT) is a novel form of cancer treatment that implements the use of light sensitive molecules called photosensitizers. Once exposed to visible light of a specific wavelength, a photosensitizer becomes activated, causing the formation of reactive, singlet oxygen. Singlet oxygen produces peroxidative reactions, which result in the damage or death of targeted cancer cells. A good photosensitizer should exhibit strong absorbance of red light (>650 nm), as this is where tissue transparency is optimal. In addition, a good photosensitizer should achieve a high quantum yield for singlet oxygen production, as well as exhibit favorable pharmacokinetics and an absence of dark toxicity. By manipulating structural elements such as molecule size, functional groups and rigidity, we were able to synthesize highly fluorescent, quinoxaline starting material. Further experimentation with the quinoxaline afforded a new, symmetric phthalocyanine molecule (EB4). The photosensitizing potential of this molecule was evaluated using UV-Vis and fluorescence spectroscopy, CV electrochemistry and singlet oxygen generation. EB4 shows good photosensitizing potential, as it exhibits strong absorbance of red light (Q-Band, λ_{max}~771 nm) and has a substantial singlet oxygen quantum yield of 0.057. Future research will involve the metalation of EB4, which should further improve its photosensitizing potential.

CHED 1092

Potassium detection using crown ethers

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Potassium plays a vital role in many biological functions. Potassium is a crucial component in the heart, where it aids in the regulation of muscle contraction. It is also common in the nervous system where it is responsible for the charge created across an axon. Potassium is also a cofactor for many enzymes and assists in keeping blood and other bodily fluids at the correct pH by acting as a crucial component in many buffer systems. Current methods for determining the concentrations of potassium ions include atomic absorption spectroscopy, flame photometry, ion sensitive electrodes, and fluorescent spectroscopy via molecular sensors. Many of these methods require large amounts of sample, are destructive, do not allow for continuous monitoring or are expensive. Fluorescent spectroscopy using molecular sensing allows for sensitivity,
selectivity, and can be observed using spectroscopy. Crown ethers have been shown to be useful cation complexing agents. The crown ether’s ability to bind ions varies and depends strongly on the ring size and heteroatoms present. The synthesis of a new molecular sensor that contains a quinoxaline fluorophore bound directly to crown ether was accomplished. The neutral fluorophore exhibits a large Stokes shift making it an ideal biological fluorescent probe. We predict the potassium-bound and -unbound crown ether will display pronounced differences in absorbance and fluorescence spectroscopy. The potassium binding constants will be determined and the utility of the molecule as an effective potassium fluorescent sensor will be evaluated.

CHED 1093

New methyl-imidazolecarboxaldehyde thiosemicarbazones ligands: NMR structural studies and complexation with Pd\(^{2+}\) to form [Pd(MIZCA-TSC)Cl] compounds

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Our research team has synthesized new compounds involving the reaction of methyl-imidazole-2-carboxaldehyde (MIZCA) with several commercially available thiosemicarbazides to form several new methyl-imidazolecarboxaldehyde thiosemicarbazone (MIZCA-TSC) ligands. The new MIZCA-TSC ligands were synthesized in the lab, recrystallized, and analyzed via \(^1\)H NMR and \(^{13}\)C NMR spectroscopy using \(^1\)H detected \(^{13}\)C and \(^{15}\)N Heteronuclear Single Quantum Coherence (HSQC) and Heteronuclear Multiple-Bond Correlation (HMBC) experiments. The NMR spectra show evidence for the proposed structures for the ligands. These ligands have been used to form metal complexes with Cu\(^{2+}\) and Pd\(^{2+}\), and we present the NMR characterization of the d\(^8\) Pd complexes. We have performed anti-proliferative MIC (minimum inhibitory concentration) studies using seven different microbes with the ligands and their Pd complexes in order to determine the anti-microbial properties of each TSC compound synthesized, and have found that the Pd metal complexes of these ligands have significant anti-proliferative activities.

CHED 1094

Utility of C2 substituted imidazolium room temperature ionic liquids in basic reaction media

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Room Temperature Ionic Liquids (RTILs) are known for their use as green organic solvents as well as other applications. They have a wide range of physical properties depending on the structures of the cation and anion. The Baylis-Hillman and Aldol
reactions are two examples of reactions that take place under basic conditions. They both have been done in RTILs with varying degrees of success. It has been revealed that the proton on the C2 position is acidic, making it unsuitable for highly basic reactions. Previous studies have shown that placing a methyl group on the C2 position does not make the RTIL entirely unreactive. This project seeks to expand the pool of available RTILs that are compatible with highly basic reaction conditions. Baylis-Hillman reactions were conducted in 1-butyl-2-butyl-3-methylimidizolium bistriflimide (BBMIM NTf₂) and 2-butyl-1-octyl-3-methylimidizolium bistriflimide (BOMIM NTf₂) and Aldol reactions were conducted in the hydroxide analogs of BBMIM and BOMIM (BBMIM OH and BOMIM OH). The utility of our C2 substituted imidizolium RTILs will be revealed and directions for future research will be discussed.

CHED 1095

Synthesis of dicalix[4]arenes with methylene-bridge flexible linkers

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To prepare a tetrapropoxy-p-tert-butyldicalix[4]arene (5), we began by lithiating tetramethoxy-p-tert-butylicalix[4]arene (1) and treated the intermediate 2 with 1,6-dibromohexane to create the octamethoxy dicalix[4]arene 3. Demethylation of 3 at the lower rim with hydrogen iodide (generated from decomposition of cyclohexyl iodide) yielded the octahydroxy dicalix[4]arene 4. Compound 4 was subsequently fully propylated to give the octapropoxy species 5, which has both calix[4]arene units in the cone conformation. Transformation of the upper-rim tert-butyl groups of 5 to alkylammonium groups could result in a dicalix[4]arene that has the potential to bind in the major groove of DNA.

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The 2-formylcalixarene 3 is accessible through selective deprotonation of a methylene bridge of \( p\)-tert-butyltetramethoxycalix[4]arene (1) followed by treatment of the lithiated intermediate 2 with DMF. With oxygen present, an autoxidative decarbonylation of 3 occurs to yield the 2-oxocalixarene 4; this is facilitated by fluoride ion attacking the formyl group, presumably eliminating carbonyl fluoride. Ketone 4 serves as an attractive entry to 2-alkylidenecalixarenes via the alkylation–dehydration sequence 4 → 5 → 6. The 2-butylidenetetrahydroxycalixarene 7 is generated by demethylation of compound 6 at the lower rim. Compounds 4 and 7 have been characterized by \(^1\)H NMR spectroscopy. Work towards the synthesis and characterization of other alkylidenecalixarene derivatives using similar methods is underway.
Synthesis of calix[4]arenes with a triaryl- or tetraarylalkene group at the 2-position

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The route to an alkene unit installed at a single methylene bridge position of a calix[4]arene began with deprotonation of tetramethoxycalix[4]arene 1 to give lithiated calixarene 2. Subsequent nucleophilic attack by 2 on an aryl aldehyde (4-trifluoromethylbenzaldehyde) or ketone (4,4′-dimethoxybenzophenone) gave, respectively, the secondary alcohol 3 (24%) or tertiary alcohol 4 (36%), each of which
were purified by column chromatography. Alcohols 3 and 4 were dehydrated (POCl$_3$/py or p-TsOH) to alkenes 5 and 6. The crude alkene products have been characterized by $^1$H NMR spectroscopy and require purification by column chromatography. Preliminary investigations suggest that the alkenes fluoresce upon irradiation ($\lambda = 365$ nm).
Synthesis of rhodium(III) azuliporphyrins

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Azuliporphyrins are an important group of porphyrin analogues where one of the pyrrolic subunits has been replaced by an azulene ring. These porphyrinoids exhibit unique characteristics, including intermediary diatropic character, and undergo unusual oxidation reactions. In addition, azuliporphyrins readily form organometallic complexes with Ni(II), Pd(II) and Pt(II). Recently, iridium(III) and ruthenium(III) derivatives have also been reported. In this study, the formation of related rhodium complexes has been investigated. Azuliporphyrin 1 was prepared by the acid catalyzed condensation of a tripyrrane with 6-tert-butylazulene-1,3-dicarbaldehyde. Reaction of 1 with [Rh(CO)₂Cl]₂ in refluxing xylene afforded the first examples of rhodium(III) azuliporphyrins. It was established that not only was rhodium introduced into the inner cavity of the ring, but an axial solvent molecule was also incorporated. The derivatives obtained using o-, m- or p-xylene were characterized by X-ray crystallography. When the reaction was attempted in refluxing chlorobenzene and subsequently treated with acetone, a similar ketone complex was obtained. These results demonstrate that azuliporphyrins are superior platforms for conducting organometallic chemistry.

Study of the substituent effects on the anti-oxidant potential of anthocyanidins: A computational investigation

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A computational chemistry project studying the antioxidant properties of anthocyanidins has been carried out. Anthocyanidins are found in many fruits, berries, and vegetables. The antioxidant properties have been documented in the literature. Health benefits
include free radical scavengers to slow possible carcinogenesis and age-related macular degenerative disease. The substituent effects and the equilibrium structural effects have been studied. The radical quenching strength was determined for two of the four equilibrium structural types of anthocyanidins, the flavylium cation, and the quinonoidal anhydrobase form. The preliminary results of computation indicate that the quinonoidal form has a higher potential to stabilize a free radical species.

Quinonoidal Anhydrobase scheme

**CHED 1100**

**Mechanistic aspects of the photocatalytic peroxidation of squalene on TiO$_2$**

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The photocatalytic peroxidation of squalene on TiO$_2$ particles was investigated using UV-Vis spectroscopy, IR spectroscopy and solid-phase microextraction/gas chromatography-mass spectrometry (SPME/GC-MS). The abstraction of allylic hydrogen atoms to form lipid radicals is facilitated by the photocatalyst, and the resulting lipid radicals undergo molecular rearrangement to form hydroperoxides. UV-Vis spectrophotometric analysis of the reaction mixture shows the appearance of conjugated double bonds arising from molecular rearrangement of squalene radical intermediates. Both IR spectroscopy and headspace SPME/GC-MS confirm the formation of carbonyl products resulting from the decomposition of hydroperoxides. Mechanisms of the photocatalytic peroxidation are proposed.

**CHED 1101**

**Separation of alpha and beta sodium glucoheptonate**

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Approximately five-million tons of alpha-glucoheptonate crystals are produced at the largest plant in the United States every year through the Kiliani-Fischer Mechanism. A side product of this reaction is alpha-glucoheptonate’s isomer companion beta-glucoheptonate. While alpha-glucoheptonate is a white crystal, beta-glucoheptonate has
been described as non-crystalline material contained in the mother liquor of the reaction (US Patent 3679659 A). This presentation outlines the findings of a summer's research on beta-glucoheptonate.

CHED 1102

**Progress toward the synthesis of (S)-curvularin**

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Curvularin and derivatives, isolated from *Curvularia, Penicillium, Aspergillus* and other fungi, have been shown to elicit diverse biological activities including anti-tumor, anti-fungal, anti-nematicidal and anti-bacterial activities. Of particular note has been the demonstration of their ability to act as spindle poisons by binding to tubulin and preventing microtubule polymerization in a fashion similar to colchicine. Further, (S)-curvularin, has been demonstrated to inhibit Janus kinase signaling by inhibiting Tyr701 phosphorylation of STAT1 and subsequently to reduce expression of proinflammatory genes in murine collagen-induced arthritis. Recently, (S)-curvularin and dehydrocurvulain have also been demonstrated to inhibit effects of TGFβ signaling by inhibiting binding of activated Smad2/3 to DNA. Hence, curvularin analogs show promise as agents that may be used in several strategies for treating tumors. Meng has reported the isolation of novel sulfur-containing curvularin derivatives from *Penicillium sumatrense* with increased cytotoxicity in several tumor cell lines. To date these have not been evaluated for toxicity against non-tumorous cells or for mechanisms of action. The progress toward the stereo-and regioselective pathway to toward a class of compounds that display activity as inhibitors against cancer, fungus, and other human ailments has shown the potential to expand beyond this limited scope. This convergent pathway allows for a high throughput analysis of structure versus biological testing. Several of the fragments have been completed and coupling experiments have been initiated.

CHED 1103

**Synthesis of capsaicin analogs**

*Tabatha Slater, tslater@wvstateu.edu, Ethan Higginbotham, Michael W. Fultz. Chemistry, West Virginia State University, Institute, West Virginia, United States*

Capsaicin is the chemical found in peppers that causes a burning sensation when eaten. It is currently used in ointments for treatment of pain and inflammation; however, there are promising studies that show capsaicin could be an effective anti-cancer nutritional agent. Capsaicin is highly selective for several human cancer cells causing apoptosis and cell cycle arrest in those cells but leaving healthy cells untouched. Due to the toxicity level of capsaicin, there was a need for analogs and metabolites to further research efforts into their potential anti-cancer effects. The synthesis of these
analogs from the Capsiconinoid and Capsinoid family has been completed and has
been submitted for further study into its biological activity with local collaborators. The
synthetic effort included synthesizing the benzylic and allylic alcohols to be coupled with
carboxylic acids to form the required esters of the target compounds.

![Chemical structures ofCapsiconinoids and Capsinoids](image)

**CHED 1104**

**Energies and conformational preferences of perfluoronated α-furanoses**

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Fluorinated sugars are widely studied as inhibitors and transporters in biological
systems. The perfluorinated α-D-pentofuranoses were modeled computationally with
B3LYP/6-311G(d,p) and plotted utilizing the Rhoad-Cagg-Carver method. The
conformational preferences of the perfluorinated sugars with respect to the fluoro-
methyl group are gt, with the preferential ring conformation varying greatly with
stereochemistry. Initial attempts to synthesize these molecules were without success.
Current attempts to synthesize with a tosylate intermediate which is reacted with
triethylaminetrishydrofluoride are currently under way.

**CHED 1105**

**Synthesis and purification of aspernigrin A analogs**

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States
Aspernigrin A is a natural product first isolated in 2004 from an Aspergillus niger strain harbored in the Mediterranean sea sponge Axinella damicornis. It was isolated again in 2005 from the endophyte Cladosporidium herbarum obtained from Cynodon dactylon. Aspernigrin A was found to be cytotoxic towards multiple strains of colon cancer, which promotes interest in synthesizing both the compound itself and its analogs. Progress has been made on the synthesis of multiple 6-aryl structural analogs. For example, the TMS enol ether of 4'-methylacetopheneone is converted to 4-hydroxy-6-(4-methylphenyl)-2-pyrone in good yield upon treatment with malonyl dichloride at low temperature. The pyrone is converted to the corresponding 6-substituted 3-carboxy-4-pyridone in a two-step process using dimethylformamide dimethyl acetal followed by methanolic ammonia. Optimization of these reactions have afforded all intermediates in good yield, with several analogs completed and significant progress on related aspernigrin A analogs.

CHED 1106

Efforts toward synthesis of isoindolinone core of muironolide A

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Only 90 µg of muironolide A was isolated from the same marine sponge that produced phorboxazole A. This was only enough to elucidate the structure of muironolide A leaving total synthesis as the only option to explore the biological activity. Our retrosynthetic plan relies on a convergent strategy that delivers three proposed fragments. Thus far, our efforts have focused on the synthesis of the isoindolinone core of muironolide A. After an unsuccessful intramolecular approach, we pursued an intermolecular Diels-Alder reaction leading to the synthesis of the isoindolinone core. This approach relies on the synthesis of an electronically deactivated and sterically hindered diene, but represents potentially straightforward access to the desired isoindolinone core.

CHED 1107

Sequence-specific, nanomolar peptide recognition via the folding and inclusion of neighboring sidechains in cucurbit[8]uril

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This presentation will describe the sequence-specific, nanomolar binding of tripeptides by the synthetic receptor cucurbit[8]uril (Q8), which is large enough to accommodate two guests within its cavity. This uniquely strong and specific recognition is made possible by the folding and inclusion of two neighboring amino acid side chains within the Q8 cavity. The fluorescent dye tetramethylbenzobis(imidazolium) (MBBI) was used
as a sensor component to study the binding of the Q8:MBBI complex to a library of 105 peptides that vary in the N-terminal residue (tyrosine, phenylalanine, and tryptophan) and in the identity of the neighboring residues (varied to 18 amino acids at each position). The fluorescence intensity of Q8:MBBI increased upon treatment with the peptide Tyr-Leu-Ala (YLA), indicating displacement of MBBI from the Q8 cavity, but decreased upon treatment with its sequence isomer Tyr-Ala-Leu (YAL), indicating binding of the tripeptide inside the Q8:MBBI complex. Further studies by 1H NMR spectroscopy, mass spectroscopy, isothermal titration calorimetry, and fluorescence spectroscopy show that Tyr-Leu-Ala binds to Q8 in a 1:1 stoichiometric ratio, with an unprecedented dissociation constant of 7.2 nM, and with >4000-fold specificity versus Tyr-Ala-Leu due to the inclusion of the side chains of the neighboring Tyr and Leu residues in Tyr-Leu-Ala. This novel binding mode was confirmed through the use of Rotating Frame Nuclear Overhauser-Effect Spectroscopy (ROESY) to identify protons that were located proximally though space for the Q8:YLA complex.

CHED 1108

On the reaction of strained alkynes with cysteine thiolates

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Strained alkynes are widely used in chemical biology, most commonly as substrates in the copper-free azide-alkyne cycloaddition. These reagents are often posited to be bioorthogonal and are therefore not reactive with biological molecules. We present an important exception to this bioorthogonality: direct reaction of cyclooctynes with cysteine thiolates. A pH profile of this reaction and other control experiments reveal this reaction may proceed via an ionic mechanism. These results suggest that cyclooctynes should not be regarded as strictly bioorthogonal reagents, and should be employed with caution in scenarios where cysteine proteases and other thiolates are present. Additionally, the direct reaction of cyclooctynes with cysteine motivates further investigation into the use of these strained alkynes as cysteine protease inhibitors for use in chemical biology and cancer research.

CHED 1109

Synthesis of dimethoxyindole-based eumelanin and indigo analogs

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Melanins are some of the least understood biopolymers, but they have the potential to have a significant positive impact in non-biological applications, including as water purification tools and organic semiconductors. Among the three kinds of melanins found...
in humans, our lab has focused on studying the properties of eumelanin, the form of melanin that gives rise to black and brown coloration in hair and skin. Eumelanin is thought to be composed of oligomers of 5,6-dihydroxyindoles. In this project, we are investigating commercially available 5,6-dimethoxyindole (DMI) as a starting material for the construction of synthetic eumelanin analogs. We have investigated the iridium-catalyzed borylation of DMI and tosyl-protected DMI, and have explored conditions for Suzuki coupling reactions of the resulting borylated indoles. During attempted Suzuki reactions, we have observed and isolated a blue product that is likely 5,5',6,6'-tetramethoxyindigo (TMI), a known derivative of the venerable dye, indigo. Previous synthetic routes afford TMI in low yield, and we are currently exploring this serendipitous finding to develop a new synthetic route to TMI. This poster describes our recent studies of modified Suzuki-Miyaura coupling reactions with borylated DMI, toward the goal of constructing eumelanin and indigo analogs.

CHED 1110

Investigation of [5+2] oxidopyrylium cycloadditions

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The Mitchell group focuses on oxidopyrylium [5+2] cycloadditions. In efforts to functionalize the tether in intramolecular variants that could potentially lead to selective ring fracture, we attempted to incorporate a lactone ring within the cycloadduct. Although this was unsuccessful, it has shed light on the criteria necessary to achieve cycloaddition. Another area of research is activation of acetoxypyranones toward oxidopyrylium intermediates. However, instead of forming oxidopyryliums, we have shown that a variety of alcohols can be incorporated via microwave irradiation to construct alkoxypyranones, presumably through an oxocarbenium intermediate.

CHED 1111

Halide inhibition of the copper-catalyzed azide-alkyne cycloaddition: An NMR analysis

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Halides (NaCl, NaBr, and NaI) were all found to inhibit a model copper-catalyzed azide alkyn cycloaddition (CuAAC). Conversions for the reaction of interest were monitored directly by NMR spectroscopy. As the CuAAC is widely employed in chemical biology, materials chemistry, and medicinal chemistry, an understanding of this inhibition is important. In addition to the study of this inhibition, we discuss practical experimental steps that can be taken to accommodate halides when using the CuAAC.
Exploring the rearrangement of complex benzylic trichloroacetimidates to benzylic trichloroacetamides

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The conversion of alcohols to protected amines, such as acetamides, is an important process in synthetic organic chemistry. While this transformation has several solutions, research in this area continues to develop as rapid, environmentally friendly and economical methods are still highly desirable. The goal of this research was to determine if benzylic trichloroacetimidates, which are easily synthesized from benzylic alcohols and trichloroacetonitrile, could be rearranged to benzylic acetamides, which are easily transformed to their corresponding amines. This transformation is known for allylic trichloroacetimidates but usually proceeds through a [3,3] sigmatropic rearrangement, which is unavailable to most benzylic systems. Attempts to directly convert the benzylic trichloroacetimidates to their corresponding trichloroacetamides are described. In the presence of an acid catalyst the reaction proceeded in synthetically useful yields. A number of Lewis and Bronsted acids were screened, and TMSOTf emerged as the catalyst that gave the best yields. The utility and generality of this approach was tested by applying the method to a number of imidates. Progression of the rearrangement was evident in most systems and wide ranges of trichloroacetamides were formed from their corresponding imidates in good to excellent yield. As a control, attempts were made to rearrange the benzylic trichloroacetimidates under thermal conditions (toluene, reflux) without a catalyst. However, under thermal conditions product was only observed in highly reactive systems. This research may be used as a cost-effective, atom-economical, operationally simple protocol to convert benzylic alcohols to their corresponding amines using readily available commercial reagents.

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**Faculty Advisor:** John D. Chisholm, jdchisho@syr.edu

Quantitative assessment of the effect of reaction variables on racemization of alpha-amino acids during amide bond formation

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Fluorenylmethyloxycarbonyl chloride (Fmoc) protected histidine and alanine methyl ester were coupled using ten different solvents and five common coupling reagents to analyze the amount of racemization at the histidine stereocenter. The amount of racemization was quantified by HPLC analysis. Dimethylformamide (DMF) produced high yields (>75%), but the solvent had only moderate affects at limiting racemization. An alternative solvent, isopropyl alcohol (IPA), significantly reduced racemization, but resulted in yields of 61% or lower. In terms of coupling reagents, (Benzotriazol-1-yloxy)tritylloxidinophosphonium hexafluorophosphate (PyBOP) was the most successful at retaining stereochemistry in all solvents, but the only solvent that resulted in high yield was DMF with a yield of 81%.

CHED 1114

Preliminary assessment of volatile organic compounds (VOCs) in indoor parking facilities in the greater Houston area

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Automobiles have been widely known as sources of VOC emissions in outdoor environments; however, the impact of these emissions indoor has not yet been studied in detail and needs to be developed. Two different types of indoor parking facilities have been assessed for the VOC concentrations, which include residential attached garages and commercial ground garages. For this assessment, Houston, Texas, a representative big city, was chosen because of its high dependency on private cars by its citizens, the numerous petrochemical industries emitting VOCs, and the several days each year that it experiences a high ozone level. These factors significantly increase Houstonians’ exposure to VOCs. Indoor air samples were collected using 6-L stainless steel canisters for 24-h period and analyzed using a modified version of EPA Method TO-15, which is TSU-TO15 with GC-MS coupled to cryogenic pre-concentrator. The eight most abundant VOCs were identified in each sample. Six out of the eight VOCs identified are classified as hazardous air pollutant (HAPs) based on EPA regulations. This research found the concentrations of VOCs are higher in attached residential garages following ground commercial garages.

CHED 1115

Progress toward the total synthesis of hemerocallisamines

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The hemerocallisamines are a family of compounds isolated from the Daylily plant which is used in traditional medicine as a sleep aid. Efforts to synthesize two members
of this family through a convergent route that is well-suited to the preparation of analogues. The route starts from furfuryl alcohol and involves an Achmatowicz rearrangement and amine condensation.

Hemerocallisamine I

CHED 1116

Synthesis of antioxidants: Modified arginine derivatives

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It has been reported that modified arginine compounds, particularly methylglyoxal-derived hydroimidazolones (MH) have shown antioxidant properties, but also that its oxidation leads to the formation of non-beneficial elements for the good functioning of cells. The synthesis and analysis of a modified compound that is designed to be more metabolically stable is underway. This derivative replaces the hydroimidazolone heterocycle with an amino-imidazoline, deleting the hydrolyzable amide bond. The synthetic plan and progress, and evaluation of the anti-oxidant properties of these derivatives will be presented.
Natural (A) and synthetic (B) anti-oxidants derived from arginine.

**CHED 1117**

**Continued efforts toward the total synthesis of solomonamide B**

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The reported isolation of cyclic peptides solomonamides A and B from the marine sponge *Theonella swinhoei* was reported in 2011 by Zampella and coworkers.\(^1\) Solomonamide A was shown to have in vivo anti-inflammatory activity. However, the amount of solomonamide B available hindered its biological evaluation. Due to the interesting structural features and lack of the authentic natural product, we have begun a total synthesis effort to obtain sufficient quantities of solomonamide B for evaluation. Here we give an account of our progress toward solomonamide B.


**CHED 1118**

**Utilization of monohalogenated alkyl halides in copper-catalyzed atom transfer radical addition (ATRA) at elevated temperature**

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Catalyst regeneration in atom transfer radical addition (ATRA) in the presence of a reducing agent has significantly reduced the amount of catalyst needed, thus creating a
“greener” process. This method was first applied in the addition of polyhalogenated alkyl halides to various alkenes, and was extended to the utilization of monohalogenated substrates such as bromoacetonitrile (BrACN), 2-bromopropionitrile (BrPN), and 2-ethylbromophenylacetate (EBrP). The single carbon-halogen bond formed from the monohalogenated alkyl halides is more expedient for further organic transformations. After optimizing the reactions in NMR tubes, it was found that significantly higher yields were achieved when performed in pressure tubes with BrACN, BrPN, and EBrP, allowing reaction temperature to exceed the boiling point of the solvent; solvents with lower boiling points may be utilized. ATRA reactions in pressure tubes were generally much faster than those in NMR tubes. The reactions were performed using BrACN, BrPN, and EBrP as the monohalogenated alkyl halides with alkenes such as 1-octene, styrene, methyl acrylate, and methyl methacrylate.

CHED 1119

Determination of products formed by the photolysis of 2,4,6-trinitrotoluene in seawater

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Munitions constituents, such as 2,4,6-trinitrotoluene (TNT), can enter the marine environment through the corrosion of unexploded ordnance casings at shooting ranges or dumping grounds. Exposure of these dissolved compounds to sunlight can cause some of them to degrade into products that are more toxic than the parent compound. In this work, some of the products formed by photolysis of TNT in seawater were separated and identified. Solutions containing TNT were exposed to simulated sunlight. After irradiation, the product mixtures were extracted on C-18 solid phase extraction cartridges and sequentially eluted using water, acetonitrile and methanol. The extracts were analyzed using a liquid chromatography system equipped with a UV/Vis detector and a mass spectrometer. The products isolated from the product mixture, including trinitrobenzene, were identified by matching the retention time using absorbance at 254 nm and the characteristic mass fragmentation pattern by negative ion mode atmospheric pressure chemical ionization mass spectrometry.

CHED 1120

Oximes derivatives from ferrocenyl chalcone as potential antibacterial agents

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Ferrocene derivatives have numerous applications in chemical sensing, asymmetric catalysis, material science and medical chemistry. Among them, ferrocenyl chalcones
derivatives, obtained from the Claisen-Schmidt reaction of acetylferrocene has been paid much attention for their synthetic versatility. The chalcones could be transform into oximes derivatives. Oximes have different applications, such as conversions into nitriles, nitro compounds, nitrones, amines, antibacterial and anti-inflammatory applications and are useful in the preparation of fungicides and herbicides. Our hypothesis is that oximes derivatives from ferrocenyl chalcones will exhibit an enhanced antibacterial activity. This research is focused on three specific aims: (a) develop an efficient methodology for the synthesis of oxime derivatives from ferrocenyl chalcones (substituted with electron-withdrawing and electron-donating groups), (b) spectral and electrochemical characterization, and (c) collaborative-based biological testing for S. saprophyticus, B. cereus, S. aureus, K. pneumoniae, E. coli, and P. aeruginosa bacterias. The synthetic methodology, characterization, electrochemistry and preliminary bioassays results of these compounds will be elaborated.

CHED 1121

Improving the efficiency of fluorescein diether cytochrome P450 substrates

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Fluorescein diether derivatives are stable masked fluorophores that have been shown to exhibit very low background fluorescence before an unmasking chemical reaction takes place. This makes them ideal candidates as substrates to investigate cytochrome P450 activity, but the derivatives are generally hydrophobic and the enzyme oxidation of the ether moiety can be sluggish. To address these issues, we are synthesizing a library of compounds starting from 2',7'-dihalogenated 5-carboxyfluoresceins (1). Through a common leuco-dye intermediate (2), we can obtain a variety of diether substrates 3 to investigate cytochrome P450 activity.

CHED 1122

Designing an efficient and practical polarity assay for xanthene dyes
The open–closed equilibrium of xanthene dyes like rhodamine B is a key characteristic of fluorescence to understand and compare in novel probes. Rhodamine B and related compounds are pH insensitive over a significant range, making comparison difficult. However, the local environment, including the polarity of the solvent, can affect the equilibrium between the closed, nonfluorescent state (2) and the open, fluorescent state (1). We have developed an efficient polarity assay to characterize and compare structurally unique rhodamine B derivatives and have optimized the assay for more general use to investigate novel probes.

CHED 1123

New frontiers in organizing crystals by molecular shape

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The property of molecular shape is highly dependent on the framework and pendant functional groups of the molecule in question. Molecular shape is especially important to the areas of drug design and molecular chirality, where the spatial alignment of complementary molecules is one structural feature responsible for favorable drug-receptor docking. Seemingly inconsequential changes to the structure of these chiral molecules often result in drastically different material properties, as illustrated by the compounds carvone and thalidomide. Despite the critical importance of molecular shape, a set of criteria has yet to be developed that is capable of describing the impact of the spatial arrangement of atoms on the organization of molecules. This study seeks to explore the effect of shape on molecular recognition, and ultimately chemical reactivity, by preparing a family of homologous arylsulfonamides. Our recent investigations show these compounds and secondary additives, such as bipyridine and bipyridine-N-oxide, cocrystallize to form tetrameric motifs linked by hydrogen bonds and complementary shapes. Though these components were designed to form inversion related motifs, our initial results showed many of these systems lacked the prescribed centrosymmetric alignment. This group of compounds and their crystal structures offer
important access to shape directed motifs that will provide a unique view of the origins of best-fit scenarios involving molecular topologies. Additionally, insight from this study has been applied to photochemical transformations in the solid state as a means to control the spatial orientation of neighboring reactive centers. By studying systems that differ in R groups in an attempt to correlate the group with the observed symmetry, gaining a better understanding of the role of chirality and molecular shape to engineered and functional crystalline motifs is possible.

CHED 1124

Nucleophilic [4+4] cyclodimerization of cyclopropenylmethanol derivatives to 4,9-disubstituted-2,7-dioxatricyclodecanes

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It has been shown that a number of different nucleophiles can be added to cyclopropanes with high diastereoselectivity. Cyclopropanes with nucleophilic moieties can dimerize. One method to perform cyclodimerization of numerous cyclopropenylmethanol derivatives with high diastereoselectivity is discussed.

CHED 1125

Synthesis of precursors of aromatic diamidines: Bisnitriles and hydroxilamine with ether and amide as linkers

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Aromatic Diamidines (ADs) have pharmacological properties that have been studied for many years. The interest in synthesizing these compounds comes from their potential therapeutic properties against microbial and parasitic diseases. Some diseases have been treated with diamidines, such as the first stage of Trypanosoma brucei gambiense, sleeping sickness, that cause human trypanosomiasis, with pentamidine. Pentamidine is also used in other treatments like leishmaniasis and Pneumocystis Carinii Pneumonia, mostly in AIDS patients. Bisnitriles are the first step in the synthesis pathway to generate different ADs with a linker between two aromatic rings that are believed to have some interactions with the minor groove of the DNA. This work involves the synthesis of the precursors of the AD: bisnitrile and a hydroxylamine with an amide as linker. Also, the hydroxylamine having a ether as a linker was synthesized. Thin Layer Chromatography (TLC) was used to confirm the reactions completion and to partially characterize the compounds, melting point (mp) and infrared spectroscopy (FT-IR) were performed. After characterizing these compounds with an elemental analysis and NMR spectroscopy, these hydroxylamines will be reduced to their corresponding ADs.
CHED 1126

Synthesis, characterization, and kinetic application of tris-(2-aminoethyl)amine (TREN) ligand derivatives

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Atom transfer radical reactions of haloalkanes and α-halocarbonyls to α-olefins have emerged as some of the most atom economical methods for simultaneously forming C–C and C–X bonds, leading to the production of more attractive molecules with well-defined compositions, architectures, and functionalities. Halide functionality incorporated in the monoadduct can be very beneficial as it can be easily reduced, eliminated, displaced, or converted into a Grignard reagent. The reaction mechanism has a conspicuous kinetic component and is governed by many steps and rates. For most optimized reactions incorporating active catalysts and fast initiators, the activation step occurs too quickly to be monitored by common instrumentation, rendering direct measurement of the activation rate constant ($k_{act}$) very difficult, if not impossible. Herein, we describe a method that can be used to calculate $k_{act}$ values in reactions that incorporate highly active copper complexes with fast initiators. This was achieved utilizing a new class of modified tris[2-(amino)ethyl]amine (TREN) based ligands that generated analogous copper complexes capable of slowing down the activation process to allow monitoring by UV/Vis spectroscopy.

CHED 1127

Library synthesis of novel Xanthoglow fluorophores

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Fluorophores are becoming increasingly more popular to visualize cellular biology and are commonly used to tag cellular components, used as probes, and used to track cellular events such as mitosis. A recently described dipyrrinone derivative, termed Xanthoglow, shows promising leads as a biologically compatible fluorophore. For example, xanthoglow fluorophores do not possess a fixed positive or negative charge and can pass readily through cellular membranes. However, the previously described xanthoglow fluorophores absorb light at ~440 nm and emit ~530 nm and tend to be a bit energetic for cells. In attempt to red-shift xanthoglows, we have developed an 8 step synthesis of a bromoxanthoglow scaffold that can be modified through cross coupling reactions to extend the π-bond conjugation. This poster illustrates the synthetic steps used to construct the bromoxanthoglow scaffold as well as some key reactions that will be used to construct a library of novel xanthoglow fluorophores.
S$_{\text{N}}$Ar reactions utilizing iterative decomposition of formamides

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The current methods used to substitute relatively small hindered amines onto aromatic rings through S$_{\text{N}}$Ar typically utilizes extreme conditions, such as high temperatures and pressures. Often, these conditions can result in the degradation of sensitive substrates and require specialized equipment. In particular, the substitution of dimethylamine can be difficult as reaction rates are often slow and the compound at atmospheric pressure is a gas. We have developed an optimized method that uses iterative decomposition of N,N-dimethylformamide (DMF) through heating in basic solution to install dimethylamino groups onto aromatic compounds with varying electron withdrawing and leaving groups. This method allows for the consistent generation of dimethylamine, keeping the volatile nucleophile in high concentration throughout the course of the reaction. The reaction follows typical S$_{\text{N}}$Ar trends where stronger electron withdrawing groups such as nitro and nitriles gave relatively fast reaction times (typically $<4$ h) and high yields (typically 70 - 97%). Substituted benzaldehydes, benzamides, and acetophenones also cleanly gave substitution products in moderate to high yields (65 – 97%) albeit the reaction rates were slower (typically 2 – 12 h). In addition, the electronegativity of the leaving group was proven significant in the reactivity of the substrate. Similar to traditional S$_{\text{N}}$Ar, fluorine substitutes with dimethylamine most rapidly, while larger halogens such as bromine or iodine proved to be unreactive under the conditions used. Therefore, this method also allows for a chemoselective approach to substituting halogenated aromatic rings.
CHED 1129

Study of the photodimerization of 4-vinylbenzylthymine and 4-vinylbenzyl trialkyl ammonium chloride using UV-Vis spectrophotometry and gel permeation chromatography

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4-Vinylbenzyl thymine (VBT), a synthetic monomer designed with the ability to photodimerize was copolymerized with a positively charged, water-soluble monomer, 4-vinylbenzyl trialkyl ammonium chloride (VBA), resulting in VBT/VBA copolymer. Due to the thymine moiety in VBT, the copolymer has the ability to photo-crosslink upon irradiation with short-wavelength ultraviolet light, and due to VBA, it is water-soluble. One of the main applications of the VBT/VBA copolymer is as a photoresist that can be used to manufacture semiconductors. In this study, first, the molecular weights for VBT/VBA copolymers with 1 to 4 ratios were determined via Gel Permeation Chromatography (GPC). Second, the photo-induced immobilization process of the VBT/VBA copolymer was monitored using both UV-Vis Spectrophotometry (UV-VIS) and GPC to determine the gel point of the copolymer at which optimal crosslinking is achieved.

CHED 1130

Polymer bound Wittig reaction under solvent free ball milling conditions

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In the Mack lab a form of mechanochemistry called high-speed ball milling is used in order to avoid harmful solvents, which are a major source of hazardous waste. Over 3 billion pounds of solvent waste was produced in 2012 according to the EPA, which
accounts for almost 25% of all chemical waste produced that year. Chemical waste is detrimental to the Earth’s environment. If we are able to run a reaction without using these harsh solvents a decent portion of the total waste would be eliminated. After any reaction, we must separate the product mixture. Normally wet column chromatography would be used. Since that requires the use of harmful solvents, the goal is to find an alternative to this separation process. In order to avoid chromatography altogether, a functionalized polymer is incorporated into the experiment. This functionalized polymer can be separated from the product mixture by simple filtration using a green solvent. This method was tested using the Wittig reaction. In order to carry out the Wittig reaction, one needs an alkyl halide, an aldehyde, triphenylphosphine, and a base to yield desired alkene products plus triphenylphosphine oxide. In order to bypass the inconvenience of separating triphenylphosphine oxide from the desired alkene products, a polymer-bound triphenylphosphine was used. This led to the byproduct being attached to the polymer that remained in the filter paper after the isolation process. Our system was successful in producing alkenes from various aldehydes in good yield.

Test Reaction

CHED 1131

Investigations of the conjugate hydrocyanation of α,β-unsaturated aldehydes in organic synthesis

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Cyanide is a useful one-carbon nucleophile that readily participates in conjugate addition reactions with α,β-unsaturated ketones and esters to form β-cyano carbonyl compounds. However, cyanide does not readily react with α,β-unsaturated amides to form the desired β-cyanoamides. Herein we describe a novel two-step approach to prepare β-cyanoamides via the conjugate hydrocyanation of α,β-unsaturated aldehydes. To date we have demonstrated proof-of-concept for the synthesis of Weinreb amide 3 starting from the simple substrate 1-cyclohexene-1-carboxaldehyde (1). We are currently
optimizing reaction conditions for the conjugate hydrocyanation of compound 1 using GC-MS analysis of reaction aliquots, and the results of this work are presented.

![Chemical Reaction Diagram]

CHED 1132

Synthesis of nonsymmetric ferrocene derivatives from 1,1'-diacetylferrocene

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An active research area is the use of the organometallic compound, ferrocene and its many analogues, for medicinal applications and stability. Some of its characteristics are neutrality, chemical stability, non-toxicity and ability to cross cell membranes giving a wide potential of biological activity. Many reports have demonstrated that some ferrocenyl derivatives are highly active against several diseases, including cancer. The design motif in ferrocene-based architectures plays the most important role to deliver the targeted property, those in which the ferrocene unit is appended with having unsaturated side-arms π-conjugated to the cyclopentadienyl ring, are of significant interest. As a result, they have gained prominence as new generation molecular materials, π-conjugated multi-metallic systems and as redox-switchable receptors. Previous studies reported that a mixture of products of the di-condensation, monocondensation and cyclization are obtained when 1,1'-diacetylferrocene is reacted under Claisen-Schmidt conditions. The focal point of this investigation is develop an efficient methodology to control the reaction products of condensation of the 1,1'-diacetylferrocene to favor the nonsymmetric ferrocene. Until now we have found that variation of temperature, solvent, stoichiometry and substitution of the benzene ring influence the ratio of the desire product. The synthetic methodology, characterization, and electrochemistry of these compounds will be elaborated.

CHED 1133

Determining the benefits of alternative haircare conditioning practice
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There has been a significant shift in health and beauty practices in favor of more all-natural solutions. Among these shifts is the use of alternative conditioners, such as raw food items. These foods include, but are not limited to, the use of bananas, avocados, and honey, in lieu of traditional, commercial conditioners. By observing physical changes at the microscopic level, measuring initial and final hair thickness, and determining initial and final tensile strength, this research aims to validate anecdotal claims, which support the use of alternative conditioning agents.

CHED 1134

Microwave-enhanced synthesis involving aliphatic alcohols & other compounds

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Aliphatic alcohols tend to be compounds more difficult to work with in terms of practical synthesis within a laboratory setting. An example of a particularly cumbersome reaction involved with aliphatic alcohols is the Williamson Ether Synthesis. The standard synthesis requires a 60-70 minute reflux time frame to allow for this reaction to run until completion; however, the ability to reduce this reaction time via microwave radiation has become increasingly prominent in organic synthesis. The conventional means of Williamson Ether Synthesis is also not ideal for optimal purity or speed, thus microwave synthesis of this compound was investigated. In order to obtain the greatest yield in the shortest amount of time, multiple reactions were run in order to optimize time and temperature parameters for the synthesis of 3 different ethers. 1-dodecanol was used as the aliphatic alcohol of choice to synthesize 1-ethoxydodecane, 1-propoxydodecane, and 1-butoxydodecane—all aliphatic ethers. To investigate the synthesis of these compounds, each individual parameter was changed while all other parameters were held constant. Purity was assessed via $^1$H NMR, $^{13}$C NMR, and IR spectroscopy. Other classes of reactions associated with usage of aliphatic alcohols and other functional groups as reagents are currently being investigated.

CHED 1135

Progress toward the synthesis of $N$-methyl improgan

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Imporgan is a synthetic drug which appears to be a powerful pain reliever without addictive properties. The goal of this research is to synthesize a brain penetrating improgan analogue. The progress towards the synthesis of $N$-methyl improgan will be
described in detail. The synthesis produces intermediates with methylation occurring at the \( \tau(N-1) \) or \( \pi(N-3) \) positions. The separation of the tautomers will be further elaborated.

![Chemical structure](image)

CHED 1136

**Synthesis and investigation of sila-allyl anions**

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Resonance has a central role in organic chemistry as it is used to understand the relative reactivity and selectivity of many intermediates in reactions. We are investigating the relative importance of resonance to silicon versus resonance to carbon by synthesizing and investigating sila-allyl anions. In this poster we will present our efforts at preparing two new precursors to the sila-allyl anion, a vinyl silole and a vinyl-dimesitylsilane. We will also present the results of our calculations of the structures of these molecules.

CHED 1137

**Trends observed in solvent studies of 2-ethylhexyl chloroformate**

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Primary alkyl chloroformates like 2-ethylhexyl chloroformate are precursors for alcohols, amines, esters and long carbon chains. This substrate is important in the Quantitative High Throughout Screening (qHTS) assay of hormone receptor inhibitors and activators since it identifies the hormones that catalyze multiple enzymatic pathways. We followed the specific rates of reaction of 2-ethylhexyl chloroformate in a constant temperature water-bath (kept at 25.0 °C). Using the acid-base titration method we studied its acetolysis and alcoholysis in a variety of pure and mixed aqueous alcohols. The indicator used was lacmoid (resorcinol blue) in acetone. Our results indicate that the
two-step carbonyl-addition pathway is dominant.

This undergraduate project was sponsored by the Delaware INBRE program with an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences - NIGMS (8 P20 GM103446-14) at the National Institutes of Health (NIH). Katelyn Null received a Cannon Scholar scholarship from an NSF S-STEM grant (NSF-DUE 1355554).

CHED 1138

Kinetics and mechanism of cyclohexyl chloroformate

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Cyclohexyl chloroformate is known to explode if heated. It decomposes into CO₂ and cyclohexyl chloride at temperatures slightly above room temperature.

Because of convenient rates of reaction at temperatures close to ambient, the specific rates of solvolysis of cyclohexyl chloroformate are analyzed using the extended Grunwald-Winstein equation. Previous research from this laboratory has shown that isopropyl chloroformate solvolyses via a dominant addition-elimination channel and only in the more ionizing and least nucleophilic solvents does the principal reaction channel involve an ionization-fragmentation process. Hence, it will be of interest to see if cyclohexyl chloroformate, a secondary chloroformate, also follows similar pathways.

Research reported in this poster was supported by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number 8 P20 GM103446-14, and a National Science Foundation (NSF) Experimental Program to Stimulate Competitive Research (Delaware-EPSCoR) grant EPS-0814251. Both Laura and Catherine have received an AY 2014-2015 Cannon Scholarship from an NSF S-STEM program (NSF-DUE 1355554).

CHED 1139

Polyphenolic compounds from an acetone extract of Hypericum pyramidatum

Emily Fortier, fortier@susqu.edu, Dalyna K. Ngo, Jean Heneks, Rebecca Force, Shui Ling Chen, Geneive E. Henry. Susquehanna University, Selinsgrove, Pennsylvania, United States

Studies of several species of the Hypericum genus, including H. perforatum, have identified a wide range of biologically active natural products from the naphthodianthrone, acylphloroglucinol, flavonoid and xanthone classes. Several members of these classes of natural products show anti-HIV, anticancer, antioxidant, antibacterial, anti-
inflammatory, and antidepressant activities. In a recent study, the hexanes extract of leaves of *H. ascyron* ssp. *pyramidatum* afforded four new spirocyclic acylphloroglucinol derivatives, pyramidatones A-D. In the current study, the acetone extract was purified to afford polyphenolic compounds including xanthones and flavonoids. The compounds were obtained by a combination of normal phase silica gel column chromatography and reverse-phase HPLC. The structures were determined on the basis of 1D and 2D NMR spectroscopic data.

CHED 1140

**Xanthones and a caffeic acid ester from an acetone extract of *Hypericum stragulum***

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The *Hypericum* plant genus has attracted widespread attention owing to the antidepressant and wound-healing properties of St. John’s wort (*H. perforatum*). Phytochemical studies of several members of the *Hypericum* genus, including *H. perforatum*, have yielded a number of structurally diverse and biologically active secondary metabolites from the acylphloroglucinol, flavonoid, and xanthone classes. The range of biological activities exhibited by these compounds include anti-HIV, anticancer, antioxidant, antiviral, antibacterial, anti-inflammatory, and anti-depressant effects. As part of an ongoing study to discover new bioactive compounds from *Hypericum* species growing in Pennsylvania, an acetone extract of the leaves of *H. stragulum* was investigated. The crude acetone extract was fractionated by silica gel column chromatography, and the medium polar fractions were further purified by reversed-phase HPLC. Two new xanthones and two known xanthones were obtained, together with a caffeic acid ester. The structures were elucidated on the basis of 1D and 2D-NMR spectroscopic data.

CHED 1141

**Flavonoids and stilbenes from an acetone extract of *Hypericum stragulum***

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The *Hypericum* plant genus consists of over 450 species distributed in warm-temperate regions throughout the world. The *Hypericum* genus is widely known as a source of biologically active natural products including xanthones, flavonoids, naphthodianthrones and acylphloroglucinol derivatives. As part of an ongoing project to characterize biologically active compounds from *Hypericum* species growing in Pennsylvania, United States, *H. hypericoides* ssp *multicaule* (*H. stragulum*) was selected for study. An acetone extract of the leaves of the plant was fractionated by silica gel column chromatography. Polar fractions obtained from initial silica gel chromatography were
subjected to further column chromatography with silica gel and Sephadex LH 20, followed by reversed phase HPLC purification. Flavonols and flavonol glycosides including quercetin, quercitrin and isoquercitrin were obtained, together with two stilbenes, resveratrol and piceatannol. The structures of the isolated compounds were determined based on 1D and 2D-NMR spectroscopic data.

CHED 1142

Chemical constituents of *Scirpus atrovirens* leaves

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The *Scirpus* plant genus (family: Cyperaceae) consists of approximately 120 species, but only a few of these species have been studied to determine their chemical constituents. Resveratrol, piceatannol and their dimers constitute the major compounds isolated from the genus so far. These compounds exhibit a wide range of biological effects including antimicrobial, antioxidant, anti-inflammatory and cytotoxic activities. In the current study, purification of the acetone and methanol extracts of the leaves of *Scirpus atrovirens* by silica gel column chromatography and reversed-phase HPLC have yielded a number of natural products. The structures of the compounds were determined based on $^1$H-, $^{13}$C-, and 2D-NMR spectroscopic data.

CHED 1143

Synthesis of indole derived fluorine-containing amino acids

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Synthesis of trifluoromethyled amino acids derived from indole is described. Commercially available starting materials were used as basic building blocks, and the synthesis of proposed compounds was achieved by aminoalkylation of indoles with trifluoromethylated imines to form trifluoromethylated-indole amino esters which on further hydrogenolysis provided the corresponding acids.

CHED 1144

Lewis acid-catalyzed decarboxylative addition of keto acid to trifluoromethyl imines

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Decarboxylative Mannich reaction employing B-keto acids with trifluoromethyl imines catalyzed by a lewis acid catalyst has been described. The desired amino ketones were obtained in good yields under mild reaction conditions.

CHED 1145

Use of Langlois' reagent in the synthesis of CF₃-containing bicyclic aromatic compounds

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The application of trifluoromethylating agents can aid in the synthesis of many complex organic molecules, especially in pharmaceuticals. In the present study we utilized Langlois' trifluoromethylating agent with various allyl phenyl ether substrates. The goal of performing these reactions was to create bicyclic-trifluoromethylated aromatic compounds.

CHED 1146

Selective oxazole and thiazole formation from a common intermediate

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The thiourea, N-(2-hydroxyethyl)-N'-phenylthiourea, can be synthesized at high yield and has demonstrated reaction condition-dependent cyclization to selectively form an oxazole or thiazole. This selective cyclization shows great promise as a synthetic tool due to its ability to create two synthetically useful ring structures from a common parent compound. We will discuss optimal conditions for selective cyclization of N-(2-hydroxyethyl)-N'-phenylthiourea as a means for selectively synthesizing oxazole and thiazole ring structures from a common intermediate.

CHED 1147

Methodology for trifluoromethylation

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The goal of this project is to develop an alternative and cost-efficient methodology for the addition of a trifluoromethyl group to alkenes. Radical oxidants were utilized to initiate the formation of CF₃. The scope and limitations on alkene substrates was evaluated using the optimized conditions.
Ozonolysis of silyl enol ethers: Synthesis of 3-silyloxy-1,2- and 3-alkyl-3-silyloxy-1,2-dioxolanes

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Silyl enol ethers are important synthetic intermediates and are widely used in a variety of reactions. Though reported ozonolysis reactions of these substrates are relatively uncommon, they typically provide the expected carbonyl cleavage product. However, silyl enol ethers are structurally and electronically related to enol ethers, which have been shown to undergo anomalous ozonolysis reactions to generate 3-alkoxy-1,2-dioxolane products. We have shown that silyl enol ethers do undergo similar reactions to enol ethers, providing 3-silyloxy- and 3-alkyl-3-silyloxy-1,2-dioxolane products in moderate to excellent yield. These dioxolane products can be further reacted to generate a variety of novel silyl protected products.

Organic synthesis of novel SSRI analogs

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The serotonin transporter protein (SERT), a member of the neurotransmitter sodium symporter family (NSS), functions as a homeostatic regulator via reuptake of serotonin from the synaptic cleft into the presynaptic cell. The inhibition of SERT function is of primary interest in the treatment of depression and anxiety disorders. There is no documented high-resolution crystal structure of SERT to date. As such, the crystalline structure of the bacterial homologue of SERT, LeuT, was utilized in the development of a protein-based pharmacophore. Virtual screening (VS) of a small molecule structural library using this generated SERT computational model yielded a novel selective serotonin reuptake inhibitor (SSRI) candidate ligand, SM11. Novel synthesis schemes for SM11 analogs are developed in order to yield high purity compounds. Analog binding affinity is then evaluated via competitive membrane binding assays. Results of the binding assay are used to elucidate the drug-binding site.
Figure 1. SSRI binding to SERT. Two proposed binding pockets in SERT (S1, S2) based on the crystal structure of bacterial homologue, LeuT.

Figure 2. Preliminary NMR analysis of dichloro SM11 analog.
Quorum sensing in *P. aeruginosa*: Synthesis of natural derivatives

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*Pseudomonas aeruginosa* is a bacterial strain that utilizes Quorum Sensing (QS) to produce biofilms which increase antibiotic resistance, as well as to produce virulence factors that cause tissue damage within a host. *P. aeruginosa* is most often found in hospitalized immune-deficient patients, and thousands of infected patients die each year. Finding small molecules that regulate QS through binding to the LasR receptor, a well-studied receptor that is known to initiate the entire QS pathway of *P. aeruginosa*, may lead to therapeutics which limit the harmful effects of an infection. 3-oxododecanoyl-homoserine lactone (3O-C12-HSL) is the natural autoinducer that binds to this receptor. The goal of this project is to improve the synthesis of 3O-C12-HSL, as well as 3-oxo-dodecanoyl-homocysteine thiolactone (3O-C12-HTL); a compound with a very similar shape and binding affinity to 3O-C12-HSL that can also induce QS activity. The synthesis of both of these compounds presently suffer from low yields and require HPLC purification. Optimization of the synthesis is currently underway. These compounds are to be used in an *E. coli* LasR GFP reporter assay to analyze QS regulation by a variety of small molecules.

Synthesis and evaluation of symmetrical biphenyltetrols as aggregation inhibitors for Alzheimer’s amyloid-β peptide

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Inhibition of amyloid-beta peptide (Aβ) aggregation is one therapeutic target for prevention and treatment of Alzheimer’s disease. We have previously demonstrated that biphenyl-3,3′,4,4′-tetrol (3,4-BPT) effectively abrogates Aβ aggregation at stoichiometric concentrations. To investigate this molecular architecture and determine how the positioning of the hydroxyl hydrogen-bond donors impacts inhibitor efficacy, we have synthesized five additional symmetrical biphenyltetrols (2,3-, 2,4- 2,5- 2,6- and 3,5-BPT). Congo red and Thioflavin T dye-binding assays were employed to monitor Aβ aggregation as a function of time and determine inhibitor IC₅₀ values for reducing equilibrium levels of aggregation. The six characterized isomers exhibit a range of IC₅₀ values spanning more than one order of magnitude. Circular dichroism and transmission electron microscopy measurements, in progress, will enable comparison of secondary structural transitions and aggregate morphologies in the presence and absence of inhibitors. Collectively, these results will aid in the design of unsymmetrical biphenyltetrols and related inhibitor architectures.
In search of objective measures of molecular structural similarity

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Federal and several state laws attempt to control the influx of new potentially dangerous non-scheduled synthetic drugs that are in part, allegedly “substantially similar” in molecular structure to reference Schedule I and II controlled substances. The qualifying phrase “substantially similar in structure” used by several laws is neither defined nor is it quantifiable by any current scientific methods. This study develops objective scientific methods to quantify and suggest a definition for the important “substantially similar” structural parameter. Two Tanimoto coefficient calculations, the chemical fingerprint (CF) and atom-pair (AP) will be compared as a potential objective measures of structural similarity and propose what may possibly qualify as substantially similar in structural comparisons between test and reference molecules.

Survey of bracket and crust fungi for the presence of monacolin K and citrinin

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Oyster mushrooms, OM, Pleurotus ostreatus, have been used in traditional medicines for over 3000 years. Among the many purported health benefits is its apparent antilipidemic effect. OM are reported to contain the statin monacolin K, also known as mevinolin or lovastatin. While surveying commercially available Red Yeast Rice supplements for the presence of monacolin K and possible contamination by the mycotoxin citrinin, a commercial sample of dried oyster mushrooms and a specimen of false turkey-tail fungi, Stereum ostrea a crust fungi were analyzed. As expected, the OM sample did contain monacolin K, somewhat unexpectedly, the false turkey-tail fungi also contained appreciable quantities of monacolin K. Suprisingly, both samples also contained citrinin. We have expanded our survey to evaluate bracket or shelf fungi including Pleurotus ostreatus species, as well as crust fungi for the presence of lovastatin and citrinin.

Survey of pesticide presence in local honey compared with migratory bee keepers
Losses in bee hives over the winter months are regularly anticipated but the unsustainable reduction of the European honey bee, *Apis Mellifera* over the last decade has come to be known as colony collapse disorder (CCD). Although no specific single factor has been determined to be the cause of CCD, honey bees’ exposure to pesticides has consistently been at the top of the list. This research project focuses on the analysis and comparison of pesticides found in honey obtained from different parts of the country using a liquid-liquid extraction procedure as well as the analysis of whole bees and foundation wax using a modified QuEChERS method. The samples were analyzed using a Perkin Elmer Clarus 580 gas chromatography and Clarus 560S mass spectroscopy (GC/MS). Pesticide standards were first purchased and analyzed prior to running the samples. Thus far, we have been able to detect the presence of the organophosphate type pesticide Dichlorvos and the carbamate based Pirimicarb. These two pesticides are insecticides used on agricultural crops. Dichlorvos has been classified by the EPA as group B2, probable human carcinogen and was proposed for cancellation in 1995 for all home uses, and for many commercial and industrial uses. Other pesticides within these two classes were detected at lower trace levels in the honey samples. The next phase of this project involves the determination of the actual levels of pesticide residues in the honey samples by building calibration curves for both classes of pesticides.

**CHED 1155**

**Evaluating the leaching of phthalates and bisphenol A from children’s drinking cups**

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European and United States government regulatory agencies restrict the use and amount of certain phthalates and bisphenol A in children’s products. These chemicals are not bound to the polymer matrix and are able to leach out of the material even during their designed use. Phthalate free and BPA free baby bottles are now the standard and the evaluation of these products for chemicals of concern has been an active area of study. However, children’s plastic “sippy” cups have not received the same level of attention and evaluation for these potential endocrine disrupting chemicals. These chemicals of concern are suspected endocrine disruptor which may disrupt the hormonal development of children and can lead to early puberty, reproductive defects, and other health problems. These problems can even occur due to low level exposure and little is known of the problems associated with constant exposure at low levels. This paper will report our results on using the techniques of sonification and Soxhlett extraction to remove the analytes from children’s plastic drinking cups. These relatively mild methods mimic the actual use of these products by children. The extraction samples were then concentrated and analyzed by gas
chromatography mass spectrometry (GC/MS). Quantification of the analytes was generated by using calibration curves generated by running standards and compared with recent literature studies and US requirements.

CHED 1156

Comparison of BPA migration levels from polycarbonate food storage containers subjected to detergents, dishwasher, and microwave use

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Polycarbonate based food storage containers contain Bisphenol A which is one of the monomers used to make these polymeric materials. BPA migrates out of the polymer matrix during use, over time, and has been a target of regulation by the United States Food and Drug Administration. It is a suspected endocrine disrupting chemical that has recently been banned from plastic products designed for use by infants. It remains a chemical of concern for humans of all ages and little is known about the effects of low dose exposure over extended periods of time. This project aims to model the changes in migration levels of BPA from these plastic containers over time during designed use. The polycarbonate containers were subjected to simulated use by being washed with detergents at room temperature, in a dishwasher at elevated temperature, and to microwave treatments. The plastic was then cut into pieces, subjected to Soxhlett extraction, and liquid-liquid extraction. The analytes were then treated with bis(trimethylsilyl)trifluoroacetamide to derivative the BPA and concentrated for analysis by gas chromatography mass spectrometry (GC/MS) using single ion monitoring. Quantification of the analytes was done by using calibration curves generated by running standards for comparison.

CHED 1157

Antibiotic compounds isolated from fungal endophytes

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A study was completed to isolate and identify secondary fungal metabolites in search for novel antibiotic compounds. The fungal endophytes were isolated from a variety of plant species. The fungal cultures were grown in a nutrient broth for several months to promote the production of secondary metabolites. The secondary metabolites were then extracted using ethyl acetate, and the extracts were tested for antibiotic activity using the Kirby-Bauer disc diffusion method. Extracts that presented antibiotic activity were further fractionated to isolate the bio-active components.

CHED 1158
Synthesis of flavanones from 2-hydroxychalcones using 1H-1-hydroxy-5-methyl-1,2,3-benziodoxathiole 3,3-dioxide

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In this investigation various 2-hydroxychalcones were converted in moderate to high yields to flavanones by treatment with catalytic amounts of 1H-1-hydroxy-1,2,3-benziodoxathiole 3,3-dioxide (HMBI) in conjunction with Oxone® as the stoichiometric oxidant. The reduced materials are easily removed from the reaction mixture by liquid-liquid extraction. The flavanones were isolated and purified by recrystallization or preparative thin layer chromatography.

CHED 1159

Derivatives of ferulic acid

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Aspergillus flavus is a pathogenic fungus that affects many different agricultural crops in the United States including grains, legumes, and tree nuts; and can cause Aflatoxin in higher organisms such as livestock and sometimes human beings. There are few countermeasures to avoid the growth of A. flavus on grains and even protective means for trees. The goal of this study is to develop novel compounds derived from Ferulic acid as possible fungicides to treat A. flavus growth. A series of compounds were synthesized via a two-step process that includes reduction and replacement reactions. All products were purified by Flash Column Chromatography and structures were determined using Nuclear Magnetic Resonance Spectroscopy (NMR). Collaborators at the USDA-ARS Plant Mycotoxin Research group in California will evaluate these novel compounds for fungicidal activity.

CHED 1160

Synthetic modifications of hypervalent iodine reagents

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The current impetus in hypervalent iodine compounds is two-fold. New reagents including ‘engineered’ versions of those already in use are widely studied in the literature. Secondly, the scope and reactivity of these reagents are constantly being explored. In this investigation we have endeavored to study synthetic modifications of
hypervalent iodine compounds. Our focus in this study is modifications of the betaines based on 2-[(aryl)iodonio]benzenesulfonates, while maintaining the iodonium moiety intact. Reactions we have studied include electrophilic aromatic substitution, ligand exchange and modifications of the sulfonate moiety.

CHED 1161

Oxidative-substitution reactions of polyaromatic hydrocarbons with BF$_3$-activated iodonium ylides of 1H-1-hydroxy-5-methyl-1,2,3-benziodoxathiole 3,3-dioxide

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The treatment of polyaromatic hydrocarbons with bis(carbonyl)methylides of 1H-1-hydroxy-1,2,3-benziodoxathiole 3,3-dioxide formed in situ in the presence of Et$_2$O-BF$_3$ leads to bis(carbonyl)alkylation of the aromatic nucleus. The recovered reduced iodine compound is easily recovered by aqueous extraction and can subsequently be recycled and reused. This chemistry allows the facile functionalization of polyaromatic hydrocarbons, well known to be carcinogenic and mutagenic pollutants, as feedstock for organic synthesis.

CHED 1162

Computational analysis of monomethylated and dimethylated Hückel and Möbius [12]-, [14]-, and [16]annulenes

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Many research groups have taken interest in the nature of π-electron bonding, and the extent of aromatic character in large Hückel and Möbius [4n+2] and [4n] annulenes. The overarching goal of this research is to computationally characterize a stable, neutral, Möbius aromatic hydrocarbon that is more stable than its Hückel counterpart. Various mono- and dimethylated conformers and isomers of [12]-, [14]-, and [16]annulene were studied using DFT (M06-2X/6-31G*) in order to search for preferential stabilization of Möbius minima and transition states. For at least one [16]annulene configuration, the lowest energy mono-methylated system may be a weakly aromatic Möbius molecule.

CHED 1163

Electronic characterization of organic materials
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Donor-acceptor columnar liquid crystals (DACLCs) have exciting potential to serve as organic semiconducting materials for molecular electronics, including photovoltaic applications. These materials are composed of electron rich and electron poor aromatic molecules which self-assemble to form columnar structures capable of transporting charge. These materials have several advantageous optical properties, however the electronic properties of DACLCs are currently poorly understood. Presented here is the initial electronic characterization of these materials. By investigating the electronic behavior of DACLCs, those materials with superior electronic properties can be identified and better understood, thus allowing for the development of more effective organic semiconducting materials.

**CHED 1164**

Synthesis of small molecule inhibitors of LOX using BAPN and its derivatives

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Lysyl oxidase (LOX) is a protein that plays a role in the spread of cancer within the body when upregulated by tumor cells. There have been findings that demonstrate that the inhibition of LOX can stop and prevent the spread of cancer. It has also been shown that β-aminopropionitrile (BAPN) is an effective inhibitor of LOX. However, since BAPN is highly reactive and toxic, this project will focus on synthesizing molecules that selectively release BAPN, and derivatives of BAPN, in the hypoxic environment of tumors. These molecules will be tested against LOX and the results will then be used to design a more effective inhibitor.

BAPN and its derivatives

**CHED 1165**

Progress towards N-alkylbenzamides as potential antimalarials

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Artemisinin-resistant strains of malaria are becoming increasingly frequent, and this constitutes a need for antimalarials that exhibit dissimilar modes of action. Recently Medicines for Malaria Venture, together with GlaxoSmithKline released articles outlining a series of compounds that are potential candidates for the next line of antimalarials. We selected a specific N-alkyl-N-imidazoylbenzamide compound from a refined listing and began investigating several synthetic approaches to synthesize the target, in hopes of conducting efficacy tests. Herein we outline the synthetic progress achieved in preparing both the parent N-alkyl-N-imidazoylbenzamide and several of its analogs.

CHED 1166

Preparation of trifluoromethylated vanillins for preparation of new curcumins

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Curcumin, a constituent of the widely used natural product turmeric, has been shown to possess significant biological properties including anti-cancer, antioxidant, and anti-inflammatory activity. It suffers significantly from poor bioavailability, however, and often requires huge dosages to obtain significant medicinal benefit. Progress towards the synthesis of selectively trifluoromethylated curcumin analogues is reported. Replacing one or more hydrogens with a trifluoromethyl group has become an increasingly common and beneficial approach to seeking enhanced bioavailability in pharmaceuticals. We describe our attempts to prepare various trifluoromethylated vanillins, as key building blocks in the total synthesis of curcumin analogues bearing one trifluoromethyl group on each ring providing a way to attempt to make the well-documented properties of curcumin more accessible.

CHED 1167

Environmentally conscious one pot synthesis of isoxazolines in aqueous media

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Heterocyclic ring systems such as isoxazolines have a broad application to pharmaceutical and pesticide control agents. The synthesis of isoxazoline derivatives contribute in stability and function as a new source of medicinal properties. While current synthesis methods of isoxazolines employ solvents toxic to the environment, we are developing a reaction to synthesize isoxazolines using environmentally benign solvents. Additionally, our modified reaction utilizes SDS as a surfactant for an efficient one-pot synthesis of isoxazolines. This research aims to determine the optimal conditions for a high yield synthesis of isoxazolines in a one-pot reaction using SDS in
aqueous media. Thus far, 0.4 mmol SDS with 6.0 mmol bleach at 0 °C has provided yields comparable to literature values that utilize toxic methods of synthesis.

![Diagram of Isoxazoline synthesis]

Modified one-pot synthesis of Isoxazoline in aqueous media

**CHED 1168**

**Reduction of nitrobenzene derivatives using crystalline polymorphs of cobalt(II) sulfide and sodium borohydride**

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This study focuses on the ability of several commercially available cobalt(II) sulfide polymorphs to catalyze the reduction of nitrobenzene derivatives. Three crystalline polymorphs (CoS, CoS$_2$, and Co$_6$S$_5$) were studied and compared with previous results using amorphous Co$_3$S$_4$. The reduction using CoS and Co$_6$S$_5$ was only partial, with approximately 30% of the corresponding nitrobenzene derivative recovered unreacted. Preliminary results suggest that complete reduction to aniline derivatives is obtained using CoS$_2$. However, the isolated yields were lower compared to the use of amorphous Co$_3$S$_4$. The correlation between crystalline structure and reactivity will be presented.

**CHED 1169**

**Preparation and NMR studies of 2-benzoyl-1-naphthols**

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This project focuses on the preparation and NMR characterization of substituted analogs of 2-benzoyl-1-naphthols. These compounds are prepared via 1-naphthyl benzoate esters that are subsequently subjected to the photo-Fries rearrangement. The analogs consist of two series where X or Y are varied from –OCH$_3$, -CH$_3$, -H, -Br, -Cl, and -NO$_2$. NMR studies focus on a Hammett analysis of the effect of $\sigma$ on the $^1$H chemical shift of the phenolic proton and $^{13}$C shifts of certain naphthalene carbons.
CHED 1170

General route to C-nucleosides

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Nucleosides are the essential carriers of information in organisms and like other components in cells undergo chemical modifications. Cancer and other diseases have characteristic and detectable effects on cell turnover rates, the activity of modifying enzymes and ultimately RNA and DNA modifications. This in turn causes cancer patients, who might otherwise still be symptom-free, to excrete elevated amounts of modified nucleosides. Consequently, the detection of these biomarkers in biological fluids is becoming an important diagnostic tool for the early detection of malignant tumors. The urinary excretion of pseudouridine (Ψ), a modified C-nucleosides found in RNA and one of our model compounds, is increased in cancerous patients. A general and convergent synthetic route to modified C-nucleosides is being investigated. Our synthetic approach starts with protected riboses and substituted uracils or related heterocyclic systems; a key step is the stereocontrolled establishment of the C-glycosidic bond. While procedures for the synthesis of nucleosides including C-nucleosides are available, a versatile methodology to establish β–glycosidic bonds is being investigated. The formation of the desired anomer is supported through an appropriate protecting group strategy.

CHED 1171

Synthesis and purification of cyclohexylphosphoserine for application as a potential phosphatidylserine analog

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Phosphatidylserine (PS) is a negatively charged phospholipid that serves as an important component of cellular membranes. PS binds to Ca(II)-protein complexes that are involved in important biological processes such as apoptosis (programmed cell death) and blood coagulation. PS can also serve as a receiver in Targeted Drug Delivery systems because of its location on the outer cellular membrane in tumor cells. The overarching goal of this project is to synthesize cyclohexylphosphoserine for use as a potential PS analog for use in phospholipid-metal ion-protein binding studies. A four-step synthetic scheme was utilized in the successful synthesis of cyclohexylphosphoserine. $^1$H and $^{31}$P NMR spectroscopy was used to confirm the synthesis of the target molecule. The current focus on the project is the optimization of the purification and scaling up the reactions to synthesize sufficient cyclohexylphosphoserine to perform metal and protein binding studies.

CHED 1172

Formation of a protected carbobenzyloxy-L-serine-benzyl ester cyclohexyl H-phosphonate diester towards the synthesis of cyclohexylphosphoserine as a potential phosphatidylserine analog

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The goal of this project is to reduce reaction time and byproduct formation for synthesis of protected carbobenzyloxy-L-serine-benzyl ester cyclohexyl H-phosphonate diester (CBZ-L-Ser-PH-cyc) for use towards the synthesis of cyclohexylphosphoserine to serve as a phosphatidylserine (PS) analog. PS is a phospholipid that is located in cellular membrane and participates in cell functions such as apoptosis and nutrient transportation. The starting material, carbobenzyloxy-L-serine-benzyl ester H-phosphonate monoester (CBZ-L-Ser-PH), a white powdery solid, was converted to the target compound CBZ-L-Ser-PH-cyc, an off-yellow oil. The reaction was tracked using $^{31}$P NMR spectroscopy, with the product forming signals consistent with the expected diastereomer formation. The reaction occurred fastest and most selectively with a 1:3 molecular ratio of starting carbobenzyloxy-L-serine-benzyl ester H-phosphonate monoester to pivaloyl chloride. Current work is focused on scaling up the reaction and optimizing purification.

CHED 1173

Synthesis of a potential phosphatidylserine analog: Cyclohexyl diphostosserine

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Phosphatidylserine (PS)-Ca(II) structures are challenging to structurally characterize due to micelle formation, and functional knowledge is essential to maximizing our understanding of this biological functions of this phospholipid. PS is has key structural
and functional roles in the blood coagulation cascade and cell apoptosis. Synthesis of a representative analog for PS will reduce difficulties in structural characterization due to structure simplification while maintaining its functionality. To achieve this, phosphoserine is being anchored to a cyclohexane ring to simplify the aliphatic structure and permit regio- and stereocontrol of the phosphoserine substituents. A preliminary monosubstituted PS analog was synthesized and a disubstituted analog is now being synthesized to observe structural binding effects related to typical PS-Ca(II) ion binding affinities. Characterization of the analog will provide more detailed understanding of function and the biological role of PS with proteins and Ca(II).

CHED 1174

Extraction of N-methylcytisine from *Caulophyllum thalictroides* (blue cohosh)

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*Caulophyllum thalictroides*, or blue cohosh, roots have been used for centuries by Native Americans and midwives to induce or augment labor. Despite this long history, literature on the use of blue cohosh gives mixed assessments on its effectiveness. Experiments using rat uterine tissue show that aqueous extracts of blue cohosh root do causes contractions of the uterine tissue, though the active ingredient is unknown. However, the current hypothesis is that the alkaloid family of compounds present in blue cohosh are responsible for the contractile response. Isolation of these alkaloids and determination of their role in the contractile response will aid in providing further information as to the implications of using blue cohosh as a natural remedy. The purpose of this research is to develop a method for rapid purification of N-methylcytisine, the most abundant alkaloid in blue cohosh, and to determine its role in the physiological response. Preliminary results using synthetic N-methylcytisine have shown that this alkaloid does contribute to the contractile response but is not solely responsible. While this result needs to be confirmed using isolated N-methylcytisine our research has expanded to developing methodologies for the extraction and purification of anagyrine and baptifoline, two additional alkaloids that may play a role in the physiological response. The purification methodologies will be worked out using a GRACE Reveleris® X2 flash chromatography system and identification of the alkaloids will be analyzed using a JEOL ECS-400MHz NMR spectrometer.

CHED 1175

Synthesis of homoleptic bismuth(III) sulfonylimide complexes

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While bismuth(III) complexes of alkoxides and phosphates are well-known, few examples of sulfonylimide Bi(III) complexes have been reported. Herein we report
progress towards the synthesis and characterization of a novel bismuth sulfurylimide complex, tris(1,1′-binaphthyl-2,2′-bis(sulfurylimide)Bi(III). This complex offers potential as an inexpensive, non-toxic, green catalyst. Furthermore, this type of complex may find utility as a chiral Lewis acid catalyst.

CHED 1176

**Rapid synthesis of N-(4-chlorobenzyl)-N-methylformamide**

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Recently, we developed a rapid procedure for the synthesis of substituted N-benzyl-N-methylformamides. Interestingly, in the reaction conducted on piperonal (3,4-methylenedioxybenzaldehyde), a large amount of a by-product, N-methyl-N,N-dipiperonylamine was produced as the main product with an isolated yield of 51.4%. We hypothesized that the reaction conducted on benzaldehydes with electron-withdrawing substituents may produce lower yields of the by-products (substituted N,N-dibenzyl-N-methylamines) and higher yields of the main products, substituted N-benzyl-N-methylformamides. In this work the hypothesis was tested by conducting the reaction on 4-chlorobenzaldehyde. The reaction was conducted on 10 mmol scale at 175 °C. Column chromatography was used for the isolation of the products of the reaction. NMR-spectroscopy and elemental analysis were used to determine the structures of the products. The reaction was fully completed in 10 minutes and produced N-(4-chlorobenzyl)-N-methylformamide as the main product with an isolated yield of 52.0%. N,N-di-(4-chlorobenzyl)-N-methylamine was produced as the main by-product with an isolated yield of 31.3%. The reaction provides a new rapid method for the synthesis of N-(4-chlorobenzyl)-N-methylformamide. This work was supported by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103442.

CHED 1177

**TPEN and TPEN* ligands and ATRA in polar aprotic solvent system**

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Atom Transfer Radical Addition reactions have been traditionally performed using TPMA (tris(2-pyridylmethyl)amine) in a methanol solvent system. Structurally similar multidentate ligands TPEN (N,N,N',N'-tetrakis(2-pyridylmethyl)ethane-1,2-diamine) and TPEN* (methyl groups in 3,5 and methoxy on 4 positions of the pyridine rings) were predicted to catalyze the ATRA more efficiently than previous catalysts. The low halidophilicity of both TPEN and TPEN* in methanol contributed to the previously poor
performance of the two ligands, but the values increased when the complexes were examined in the polar aprotic solvent acetone. The $K_x$ of TPEN * increased from 12 ± 2 in methanol to 16000 ± 4000 in acetone, with TPEN acting similarly. ATRA was then performed with the TPEN and TPEN* complexes in varying ratios of acetone and methanol solvent systems with a variety of alkene reagents, including methyl acrylate, methyl methacrylate, octene, styrene, and hexene, in catalyst loadings between 0.002 and 0.0001 compared to alkene.

CHED 1178

Microwave promoted synthesis of diethyl phenylmalonate

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Arylated malonates are key synthetic intermediates for the preparation of medicinally relevant compounds, such as barbiturates. Many of the methods for their preparation involve transition metal-catalyzed processes. As an alternative to those conditions, malonate arylation was accomplished using bromobenzene, potassium tert-butoxide, and microwave irradiation. GC-MS analysis helped facilitate optimization of these reaction conditions. Diethyl phenylmalonate prepared through this methodology was used as an intermediate to prepare more complex compounds.

CHED 1179

Synthesis of tetrabenazine via visible light photoredox catalysis

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Tetrabenazine was synthesized in six steps from commercially available materials. The carbon framework for tetrabenazine was assembled rapidly in two steps, which involved the Michael addition of a tetrahydroisoquinoline to the Baylis-Hillman adduct of isobutyraldehyde and methyl vinyl ketone. The key step in this work, annulation of the final ring, was achieved through photoredox catalysis. Solvent choice in the photoredox cyclization was critical. Use of methanol led to the formation of a mixed ketal, whereas acetonitrile/water (10:1) led to the direct formation of the desired ketone.

CHED 1180

Visible light photoredox catalysis: Synthesis of $N$-heterocycles

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Azabicyclic ring systems, such as indolizidines and quinolizidines, frequently appear in secondary metabolites that are biologically active. Our group is using visible light photoredox catalysis to prepare these heterocycles through the oxidative cyclization of tertiary amine substrates. To these ends, N-alkyl pyrrolidine and piperidine substrates were prepared from a common intermediate. Photoredox cyclizations of these substrates were monitored by GC-MS, which provided useful information for reaction optimization.

CHED 1181

Microwave promoted malonate arylation: Regioselectivity

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Our group has been developing a microwave promoted malonate arylation that employs diethyl malonate, bromobenzene, and potassium tert-butoxide. The regiochemical outcome of arylation reactions with several unsymmetrically substituted arylhalides was studied to provide evidence for whether they involve the formation of a reactive benzyne intermediate. Furthermore these reactions provide key information about the scope and limitations of this arylation method.

CHED 1182

"Click" synthesis of triazole-based cefotaxime derivatives

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Cefotaxime is a powerful, third-generation cephalosporin that contains favorable properties for treating bacterial infections, as it has the ability to inhibit bacterial cell wall synthesis in both Gram-negative and Gram-positive species. A high-yielding methodology known as click chemistry was performed to link cefotaxime to 2-ethynylanisole, creating a potentially extended-spectrum drug that may also exhibit fluorescence upon light activation. In theory, creating an antibiotic that possesses useful properties for both the treatment and study of bacterial infections is an indispensable tool in clinical settings. This application of click chemistry is therefore an important advancement in the antibiotics design field. The first phase of this study was to substitute the acetate at the C3 position of cefotaxime with an azide. This allowed for the completion of the second phase, which was to “click” together cefotaxime with 2-ethynylanisole in addition to other prospective anti-microbial compounds.

CHED 1183

Acetamide as a solvent in the rapid synthesis of N-(2,4-dichlorobenzyl)formamide
Recently, we developed a rapid procedure for the synthesis of various benzylformamides. We also investigated acetamide as an alternative solvent for the reaction. Interestingly, in the reaction conducted on 4-chlorobenzaldehyde, \(N\)-(4-chlorobenzyl)formamide was produced only as a minor product. The use of acetamide resulted in a substantial shift towards \(N,N\)-di-(4-chlorobenzyl)formamide and \(N,N,N\)-tri-(4-chlorobenzyl)amine that were produced with the isolated yields of 33.5% and 12.4%. \(N,N\)-di-(4-chlorobenzyl)formamide appeared to be the main product of the reaction. We hypothesized that the successful formation of the dibenzyl and tribenzyl products should correlate with electron density on the nitrogen atom of the respective benzylformamides. Therefore, the reaction conducted on benzaldehydes with electron-withdrawing substituents should result in a less pronounced shift towards dibenzyl and tribenzyl products. In this work, this hypothesis was tested on 2,4-dichlorobenzaldehyde. The reaction was conducted on 10 mmol scale at 198\(^\circ\)C. Column chromatography was used for the isolation of the products of the reaction. NMR-spectroscopy and elemental analysis were used to determine the structure of the products. The reaction was fully completed in 1 minute. It produced \(N,N\)-di-(2,4-dichlorobenzyl)formamide and \(N,N,N\)-tri-(2,4-dichlorobenzyl)amine with the yields of 22.6% and 5.6%, respectively. \(N,N\)-(2,4-dichlorobenzylidene)-bis-acetamide appeared to be the major product of the reaction with the yield of 36.1%. As expected, electron-withdrawing substituents reduced the shift towards the dibenzyl and tribenzyl products. Research reported in this publication was supported by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103442.

CHED 1184

**Rapid synthesis of \(N,N\)-dipiperonylformamide**

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Recently, we developed a rapid procedure for the synthesis of various benzylformamides. We also investigated acetamide as an alternative solvent for the reaction. Interestingly, in the reaction conducted on 4-chlorobenzaldehyde, \(N\)-(4-chlorobenzyl)formamide was produced only as a minor product. The use of acetamide resulted in a substantial shift towards \(N,N\)-di-(4-chlorobenzyl)formamide and \(N,N,N\)-tri-(4-chlorobenzyl)amine that were produced with the isolated yields of 33.5% and 12.4%. \(N,N\)-di-(4-chlorobenzyl)formamide appeared to be the main product of the reaction. We hypothesized that the successful formation of the dibenzyl and tribenzyl products should correlate with electron density on the nitrogen atom of the respective benzylformamides. Therefore, the reaction conducted on benzaldehydes with electron-donating
substituents should result in even larger shifts towards dibenzyl and tribenzyl products. In this work the hypothesis was tested by conducting the reaction on piperonal (3,4-methylenedioxybenzaldehyde). The reaction was conducted on 10 mmol scale at 200°C. Column chromatography was used for the isolation of the products of the reaction. NMR-spectroscopy and elemental analysis were used to determine the structure of the products. The reaction was fully completed in 1 minute and produced \( N,N \)-dipiperonylformamide as the main product with the isolated yield of 34.1%. \( N,N,N \)-tripiperonylamine, was produced in substantially larger amount with the isolated yield of 20.0%. The combined yield of the dibenzyl and tribenzyl products was 54.1%, significantly higher than the combined yield of the dibenzyl and tribenzyl products in the 4-chlorobenzenzaldehyde reaction (45.9%). The reaction provides an important step towards a new rapid method for the synthesis of \( N,N \)-dipiperonylformamide. Research reported in this publication was supported by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103442.

**CHED 1185**

Rapid synthesis of \( N,N,N \)-tri-(4-t-butylbenzyl)amine

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Recently, we developed a rapid procedure for the synthesis of various benzylformamides. We also investigated acetamide as an alternative solvent for the reaction. Interestingly, in the reaction conducted on 4-chlorobenzaldehyde, \( N \)-(4-chlorobenzyl)formamide was produced only as a minor product. The use of acetamide resulted in a substantial shift towards \( N,N \)-di-(4-chlorobenzyl)formamide and \( N,N,N \)-tri-(4-chlorobenzyl)amine that were produced with the isolated yields of 33.5% and 12.4%. \( N,N \)-di-(4-chlorobenzyl)formamide appeared to be the main product of the reaction. We hypothesized that the successful formation of the dibenzyl and tribenzyl products should correlate with electron density on the nitrogen atom of the respective benzylformamides. Therefore, the reaction conducted on benzaldehydes with electron-donating substituents should result in even larger shifts towards dibenzyl and tribenzyl products. In this work the hypothesis was tested by conducting the reaction on 4-t-butylbenzaldehyde. The reaction was conducted on 10 mmol scale at 200°C. Column chromatography was used for the isolation of the products of the reaction. NMR-spectroscopy and elemental analysis were used to determine the structure of the products. The reaction was fully completed in 1 minute and produced \( N,N,N \)-tri-(4-t-butylbenzyl)amine as the main product with the isolated yield of 29.8%. \( N,N \)-di-(4-t-butylbenzyl)formamide, was produced with the isolated yield of 22.3%. The combined yield of the dibenzyl and tribenzyl products was 52.1%, significantly higher than the combined yield of the dibenzyl and tritribenzyl products in the 4-chlorobenzaldehyde reaction (45.9%). The reaction provides an important step towards a new rapid method for the synthesis of \( N,N,N \)-tri-(4-t-butylbenzyl)amine. Research reported in this
CHED 1186

Rapid synthesis of \( N,N,N \)-tri-(1-naphthylmethyl)amine

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Recently, we developed a rapid procedure for the synthesis of various benzylformamides. We also investigated acetamide as an alternative solvent for the reaction. Interestingly, in the reaction conducted on 4-chlorobenzaldehyde, \( N-(4-\text{chlorobenzyl}) \)formamide was produced only as a minor product. The use of acetamide resulted in a substantial shift towards \( N,N \)-di-(4-chlorobenzyl)formamide and \( N,N,N \)-tri-(4-chlorobenzyl)amine that were produced with the isolated yields of 33.5% and 12.4%. \( N,N \)-di-(4-chlorobenzyl)formamide appeared to be the main product of the reaction. We hypothesized that the successful formation of the dibenzyl and tribenzyl products should correlate with electron density on the nitrogen atom of the respective substituted benzylformamides. Therefore, the reaction conducted on electron rich benzaldehydes should result in even larger shifts towards dibenzyl and tribenzyl products. In this work the hypothesis was tested by conducting the reaction on 1-naphthylcarboxaldehyde.

The reaction was conducted on 10 mmol scale at 200ºC. Column chromatography was used for the isolation of the products of the reaction. NMR-spectroscopy and elemental analysis were used to determine the structure of the products. The reaction was fully completed in 1 minute and produced \( N,N,N \)-tri-(1-naphthylmethyl)amine as the main product with the yield of 40.9%. \( N,N \)-di-(1-naphthylmethyl)formamide, was produced with the yield of 31.5%. The combined yield of the dibenzyl and tribenzyl products was 72.4%, significantly higher than the combined yield of the dibenzyl and tribenzyl products in the 4-chlorobenzenaldehyde reaction (45.9%). The reaction provides a new rapid method for the synthesis of \( N,N,N \)-tri-(1-naphthylmethyl)amine. Research reported in this publication was supported by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103442.

CHED 1187

Rapid synthesis of \( N,N' \)-(4-chlorobenzylidene)-bis-formamide

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Recently, we developed a rapid procedure for the synthesis of substituted \( N \)-benzylformamides. We also found that the reaction typically produces three minor byproducts, specifically, substituted \( N,N \)-dibenzyllformamides, substituted \( N,N,N \)-
tribenzylamines, and substituted $N,N'$-benzylidene-bis-formamides. It was interesting to investigate if the procedure could be modified towards the selective production of any of these by-products. We hypothesized that using oxalic acid as a catalyst may lead to a selective production of substituted $N,N'$-benzylidene-bis-formamides. In this work the hypothesis was tested by conducting the reaction on 4-chlorobenzaldehyde. The reaction was conducted on 10 mmol scale at 133°C. NMR-spectroscopy and elemental analysis were used to determine the structure of the products. The reaction was fully completed in 1 minute and produced $N,N'$-(4-chlorobenzylidene)-bis-formamide as the main product with the isolated yield of 67.4%. The reaction provides a new rapid method for the synthesis of $N,N'$-(4-chlorobenzylidene)-bis-formamide. Research reported in this publication was supported by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103442.

**CHED 1188**

*Synthesis of 1,1'-ferrocenyl chalcones derivatives as potential biological active compounds*

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Ferrocene and its derivatives fascinated the scientist’s attention with its numerous uses and applications. Our interest is primarily focused in ferrocenyl chalcones that exhibit remarkable stability in their structure and excellent biomedical properties. These ferrocenyl chalcones properties promise treatments to human diseases, and as synthetic precursors for other biological active compounds. Using a solvent free approach for the Claisen–Schmidt reaction, our laboratory has synthesized twelve symmetric ferrocenyl chalcones from 1,1-Diacetylferrocene with shorter reaction times and moderate to good yields. We have characterized these compounds by spectroscopic techniques (NMR, IR, UV/visible) and some of them by X-Ray crystallography. Moreover, we have conducted a study of their electrochemistry and some bioassays. The synthetic methodology, characterization, and results of preliminary bioassays of these compounds will be elaborated.

**CHED 1189**

*Synthetic approach toward attaching a pyridine based cation receptor to solid support*

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The Marcellus Shale region is known for the vast supply of natural gas imbedded in the shale rock. Although the whereabouts and quantity of natural gas have been known for decades, it is only recently that hydraulic fracturing made accessing this natural resource a reality. Unfortunately, hydraulic fracturing is not without a significant impact on the environment and the quality of the Marcellus Shale freshwater supply. Drilling in the Marcellus Shale requires millions of gallons of freshwater. Using this method of drilling produces massive amounts of wastewater containing excessive amounts of cations that cannot be disposed of using traditional methods of wastewater purification. This investigation will explore attaching a known pyridine based cation binder on a solid surface to be used as a renewable cation scavenger. This research focuses on using synthetic chemistry to develop an appropriate linker for attaching the pyridine based molecule to a solid support.

CHED 1190

Diastereoselective dipolar cycloadditions for the synthesis of pyrazoline and pyrazolidine pharmacophores

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Pirazolines and pirazolidines are a very important class of five-membered, nitrogen-containing heterocycles. These pharmacophores are essential for the biological properties of many drugs and natural products. Thus, there is a continuous demand for the development of more efficient and systematic methods to access these key scaffolds. We have found an efficient and convergent method for the synthesis and isolation of Cbz and Boc protected diaziridine synthons. These molecules have shown to undergo cycloaddition reactions with alkynes and alkenes across the C-N bond in the presence of a transtion-metal catalyst to form pyrazolines and pyrazolidines. This study would provide reliable and selective route towards the synthesis of highly functionalized pyrazolines, pyrazoldines and more complex cycloaddition adducts.

CHED 1191

Blue copper protein models: Characterization of copper (I/II) complexes of the N₂S₂ macrocycle 1,8-dithia-4,11-diazacyclotetradecane and derivatives

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Proteins containing copper in their active sites represent a large and significant class of metallobiomolecules.¹ The Type 1 Blue Copper Proteins (BCP) are fundamentally important for their ability to transfer electrons and exhibit unusual spectroscopic and
The ligand 1,8-dithia-4,11-diazacyclotetradecane (14[ane]N₂S₂) is a synthetic target analogous to the active site of BCP. Analysis of ligand L₁ using X-ray Crystallography, Cyclic Voltammetry (CV), Electron Paramagnetic Resonance (EPR) and Ultra-Violet/Visible Spectroscopy (UV/Vis) are presented. X-ray analysis confirmed square planar geometry in CuⅡ and distorted tetrahedron in CuⅠ. UV-Vis showed three absorption bands at 295, 350 and 550 nm with a binding constant of 9.34 X 10² M⁻¹ at pH 5. The ligand is quasi-reversible with a redox potential of +119 mV vs Ag/AgCl, which indicates the stabilization of the CuⅠ species. EPR is consistent with the square planar geometry observed in the X-ray structure. Due to the alternating N-S heteroatoms in L₁, reaction with dibromoethane to afford L₂ will provide insight into the reversibility and stability of CuⅡ/I complex when the flexibility is restricted. This presentation will focus on the synthesis of the ligands along with a detailed explanation of the results.

References

Fig. 1: The N₂S₂ macrocycle L₁ and derivative L₂

CHED 1192

Mass scale-up of pyrazolidinones and N-alkylation tests

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This research attempted a mass scale-up of workups conducted on a smaller level. The model experiment used 4-methyl cinnamic acid and excess hydrazine under thermal conditions and then a hot vacuum. The experiment was conducted on a 100mmol scale up. Once the scale up was completed successfully. Some N-alkylation tests were conducted during the second scheme of the procedure. Previous experiments have
shown this to work with benzaldehyde or benzyl bromide. The procedure was tested with several other alkyl halides in benzyl bromide's stead.

CHED 1193

Palladium cross-coupling reactions enhanced with aromatic co-catalysts

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Palladium catalyzed cross-coupling reactions of electron-rich (deactivated) aryl chlorides are known as inherently slow reactions. It is desirable to find ways to improve the efficiency of these reactions, as aryl chlorides are relatively cheap and abundant as materials for cross-coupling. Proposed here is a general approach to enhancing the coupling reactions of deactivated aryl chlorides by use of an electron-poor aromatic co-catalyst. The relevant $\pi$-$\pi$ interactions will be promoted by the hydrophobic effect in water, also a green solvent for these reactions. Here is described work done in synthesizing water-soluble reagents for study of the coupling reactions. Additionally, research was done in determining an appropriate technique for coupling reaction analysis using gas chromatography.

CHED 1194

Hydrodehalogenation of aryl halides using sodium borohydride

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The hydrodehalogenation of aromatic halides has been achieved using a wide variety of methods. In our system, aromatic halides are dehalogenated using a sodium borohydride reducing agent and catalytic palladium-on-carbon under ambient conditions. High conversion yields are seen within an hour for many substrates in this heterogeneous reaction system. Solvent effects and catalyst variations have been studied to provide optimized conditions. Reactivity is best with aryl iodides and aryl bromides, although chlorinated and fluorinated compounds have also shown promising results.
Preparation of a simple acetylenic poly(aryl ether)

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Poly(Aryl Ethers) (PAEs) are high-molecular weight polymers that contain diphenyl ether links and can be synthesized by nucleophilic aromatic substitution ($S_{\text{NAr}}$). In 1993, Hayes and coworkers demonstrated that alkynyl groups were sufficiently activating to allow for $S_{\text{NAr}}$ reactions. They also showed that bis-(4-fluorophenyl)acetylene (BFA) could react with bisphenols, such as bisphenol-A (BPA) to form acetylenic PAEs. My research looked at using bis(4-hydroxyphenyl)acetylene as a comonomer with BFA to form the PAE, poly(oxy-1,4-phenyleneethynylene-1,4-phenylene). The resulting PAE was reacted with aqueous acid to form a poly(aryl ether ketone) and with bromine to form a brominated PAE. Additionally, the potential for thermal crosslinking of the PAE’s triple bonds was investigated. The products were characterized by $^1$H NMR, C-13 NMR, and GPC-MALS.
Synthesis and characterization of novel boron cluster carboxylic acids

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Derivatives of the 1-carba-closo-dodecaborate(1-) carborane anion (closo-CB11) have potential uses in medicine, industry, optics, and electronics. However, few simple and efficient synthetic techniques have been developed for boron-substituted derivatives of CB11. We prepared the mono and dicyanated derivatives, 12-CN-CB$_{11}$H$_{11}^-$ and 7,12-(CN)$_2$-CB$_{11}$H$_{10}$, in a simple two-step procedure via an iodinated intermediate with yields of over 80%. Hydrolysis of the nitrile groups gave the corresponding carboxylic acid derivatives, 12-COOH-CHB$_{11}$H$_{10}^-$ and 7,12-(COOH)$_2$-CB$_{11}$H$_{10}^-$. These compounds were characterized by NMR, IR, MS, and X-ray diffraction. Titration studies indicate that the boron-substituted carboxylic acids in these compounds are significantly less acidic than typical organic carboxylic acids. 7,12-(COOH)$_2$-CB$_{11}$H$_{10}^-$ is the first example of a CB11 cluster with a B-COOH group and the only X-ray structure of a boron cluster that contains an adjacent pair of these groups. The synthesis and characterization of these compounds will be discussed.

Liquid-liquid extraction and analysis of the antioxidant, resveratrol, from various red and white wines
The objective of this study was to extract, isolate and analyze the antioxidant, resveratrol from various red and white wines. Three different companies of vineyards were chosen for the study. The three vineyards include Gallo Family, Barefoot and Woodbridge. Merlot from each vineyard was selected as the red wine and chardonnay was selected as the white wine. The extraction and quantification of resveratrol was conducted in order to compare the amount of this antioxidant found in the different red and white wines. In order to extract resveratrol liquid-liquid phase techniques were implemented. The concentration of the antioxidant was quantified using ultraviolet/visible spectroscopy at a wavelength of 310 nm. High Performance Liquid Chromatography was also used to isolate and identify the active ingredient from each wine after extraction. The analysis of the data collected from this study will suggest which type of wine contained the most resveratrol.

CHED 1198

Soxhlet extraction and analysis of capsaicin from various pepper flesh

The objective of this study is to extract, isolate and analyze the active ingredient, capsaicin, from various types of pepper flesh. Soxhlet techniques were used to extract the capsaicin from the flesh of each type of pepper using 95% ethanol. Ultraviolet/Visible (UV/Vis) spectroscopy was used to evaluate and quantify the total amount of capsaicin extracted from each type of pepper. High Performance Liquid Chromatography (HPLC) was also used to verify the quantity of the active ingredient in the extraction solvent. Most recently, capsaicin was found to have antioxidant properties. In this study, the amount of capsaicin isolated from each pepper has some correlation to the amount of heat the pepper contains based on the Scoville scale for the hotness of peppers. Therefore, the hotter the pepper the more capsaicin it contains and the more antioxidant potential.

CHED 1199

Electrophilic aromatic substitution reactions with naphthalene and guaiazulene using ionic liquids

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This investigation will involve the preparation of several ionic liquids containing the 1-hexyl-3-methyl-imidazolium cation coupled to various anion systems. These ionic liquids can be substituted for typical organic solvents and used in the electrophilic aromatic substitution reactions of naphthalene and guaiazulene to produce several interesting products. There are many advantages for using these ionic liquids over organic solvents in synthesis reactions. Ionic liquids are recyclable, they can stabilize intermediates better than traditional solvents and the product yield is typically much higher. The ionic liquids can also be used for synthesis at lower temperatures and are a less toxic alternative to typical organic solvents.

CHED 1200

Synthesis of four putrescine analogs using 95% and 100% ethanol

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This investigation will involve the synthesis of several putrescine analogs produced using 95% and 100% ethanol as the solvents. These nucleophilic substitution reactions with alkyl or acyl halides will produce bis(propyl), bis(butyl), bis(pentyl) and bis(benzyl) putrescine. In this study, 95% or 100% ethanol were used as the reaction solvents. Which allowed for production of the polyamine analogs to proceed in a greener solvent. There are many advantages for using alcohols over traditional volatile organic solvents in synthetic reactions. Alcohols are preferred solvents as they are more environmentally friendly, can be reclaimed or recycled, and reactions are run at lower temperatures. It was also found, in this work that the use of 100% ethanol increased the product yield dramatically over other more toxic alcohol solvents used for previous studies in our laboratory.

CHED 1201

Synthesis of five spermidine analogs using 95% and 100% ethanol

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This investigation involves the synthesis of several spermidine analogs produced in 95% and 100% ethanol as the solvents. These nucleophilic substitution reactions with alkyl or acyl halides produce bis(ethyl), bis(propyl), bis(butyl), bis(acetyl) and bis(benzyl) spermidine. In this study, 95% or 100% ethanol solvents were used, allowing for the "greener" production of the polyamine analogs. There are many advantages for using alcohols over traditional volatile organic solvents in synthetic reactions. Alcohols are preferred solvents as they are more environmentally friendly, can be reclaimed or recycled, and reactions are run at lower temperatures. It was also found in this work that
the use of 100% ethanol increased the product yield dramatically over other more toxic alcohol solvents used in previous studies in our laboratory.

CHED 1202

4,4’- Bis(bromomethyl) diphenyl ether as a monomer for a new poly(arylene) ether

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Poly(arylene) ethers (PAEs) have many useful properties such as good thermal stability, moisture absorption, and resistance to solvents. We wondered whether 4,4’-bis(bromomethyl) diphenyl ether (1) could do an S_N2 reaction with a bisphenol such as hydroquinone under basic conditions to produce a new AB copolymer, poly(oxy-p-phenyleneoxymethylene-p-phenyleneoxy-p-phenylenemethylene) (2). This polymerization method would directly integrate preformed aryl ether bonds into the backbone of the polymer. We also reacted 1 with p-cresol to form 4,4’-bis(p-tolyloxymethyl) diphenyl ether (3) as an aid in spectral interpretation of the polymer and for determining optimum conditions for the bisphenol polymerization reaction.

CHED 1203

Hydrogenation using palladium nanoparticle catalysts: Functional group survey

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Coffee is an effective reductant for the preparation of palladium nanoparticles supported on polycarbonate membranes. These same supported palladium nanoparticles catalyze alkene hydrogenations. A series of alkenes, aldehydes, ketones and nitriles have been
exposed to identical catalytic hydrogenation conditions to begin to explore the extent and limitations of this reaction.

CHED 1204

Synthesis of symmetrical biphenyls using phenylboronic acids and manganese(III) acetylacetonate

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Arylboronic acids react with manganese(III) acetylacetonate to produce the corresponding coupled biaryl compounds. A series of experiments was conducted using substituted phenylboronic compounds to determine the efficacy of this homocoupling reaction with substituents in the ortho, meta and para positions.

CHED 1205

Drug delivery systems utilizing modified nucleobase hydrogelators and polyamines: Synthesis of polyamines

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Tumorous cancer cells have shown to have elevated levels of polyamine transport systems attached to the cell surface versus normal cells. In order to maintain an effective drug delivery system, we aim to attach polyamines to the nucleic acid base (nucleobase) guanosine. Guanosine is preferred due to its biocompatibility and high magnitude of packed molecules that produce hydrogels. The work developed for this project involves synthesis and protection of polyamines for appendage to functionalized nucleobases. The development of this drug delivery system will allow for the guanosine: polyamine compounds to specifically target cancer cells via the polyamines transport systems.

CHED 1206

Utilization of nucleobase interactions to develop supramolecular polymer hybrids

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Our research is designed to utilize hydrogen bonding motifs in guanosine and cytidine nucleobase pairings to assemble supramolecular polymers. This is relevant to the
development and functionalization of nanomaterials. To accomplish this, cytidine will be appended with vinyl ester, acrylate, azide, and acrylamide derivatives which will be attached to a larger polymer backbone. The positions that will mainly be altered are the 2', 3', and 5' positions as well as the amine. The cytidine precursors will undergo RAFT polymerization so the size, length, and other physical properties can be controlled. In the future, the cytidine polymers will be paired with guanosine polymers to determine new supramolecular polymeric structures.

CHED 1207

Drug delivery systems utilizing modified nucleobase hydrogelators and polyamines: Synthesis of modified nucleobases

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Guanosine is a biocompatible nucleobase that can form a G-quartet system which is a tightly packed structure; numerous quartets form quadruplexes that result in significant hydrogel formation. When combined with various polyamines, these quadruplexes can be used to form a drug delivery system that is used to detect tumorous cancers with elevated polyamine transport systems on their cell surface. The aim of our research is to stabilize the molecule and the G-quartet/quadruplex systems by adding various aromatic rings on the 8-position of guanosine and append polyamines to the 5'-position of the ribose sugar. The development of this drug delivery system will allow us to specifically target cancer cells with increased potency.

CHED 1208

Multiple methods for analysis of organic materials using the GC/MS

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The use of instrumentation is an integral part for the analysis of compounds. Gas Chromatography/Mass Spectrometry (GC/MS), in particular, identifies different types of compounds present in a mixture through separation and subsequent identification based on specific chemical properties. Advances in GC/MS instrumentation allow for a larger range of chemicals to be analyzed due to its improved design and increased sensitivity. These enhanced parameters allows for the investigations of more volatile samples. The direct insertion probe (DIP), a feature on some GC/MS instruments, permits the analysis of low volatile organic species by directly inserting them into the MS ionization chamber. The objective of this research was to determine appropriate methods for the analysis of organic materials using traditional GC/MS and DIP techniques. Such methods focus on the analysis of known materials and applying them
to new materials not yet fully characterized. Specifically, these new materials of interest include benzodithiophenes - an important class of organic materials used in a variety of electronic devices. The preliminary results of our method development suggested that unoxidized benzodithiophenes can be analyzed by GC/MS while oxidized molecules required DIP analysis.

CHED 1209

Diastereoselective dipolar cycloadditions for the synthesis of imidazoline and imidazolidine pharmacophores

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Imidazolines and imidazolidines are highly conserved five-membered ring nitrogen-containing pharmacophores in the field of medicinal chemistry. These heterocyclic molecules are key scaffolds in several blockbuster drugs and natural products. Thus, there is a continuous demand for the development of more efficient and systematic methods to access them. Our lab has developed simple and inexpensive reaction conditions for the synthesis and isolation of a series of robust benzyl protected diaziridine synthons, which upon exposure to a series of transition-metals undergo diastereoselective cycloadditions across the N-N bond to access a wide variety of stereochemically-dense imidazolines and imidazolidines. This study would provide efficient and continuous access to complex highly functionalized heterocycles from simple scaffolds, which will facilitate the engineering of convergent approaches towards more complex heterocyclic pharmacophores.

CHED 1210

Synthesis of hydrazide heterocycle for development as an organocatalyst

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The development of new catalysts capable of enantioselective induction is an ongoing effort at the forefront of organic chemistry. We are interested in developing catalysts that can be used in water. Organocatalysts are a catalyst type that is more likely to display catalytic behavior in water compared to Lewis acids. However, solubility of organic molecules can be a source of problems. Hydrazides are highly hydrophilic and could potentially fulfill these goals if displayed in an organic molecule. There is evidence in the literature that other hydrazides have behaved as catalysts and readily form iminium ions. Platinum catalysis was used to promote cyclization of a hydrazide to synthesize a proline-like potential organocatalyst. The structure has some promising features that could lead the molecule to behave as an effective organocatalyst. The
acetamide substituent of the structure supports the formation of an iminium ion because of increased nucleophilicity due to the α-effect of the N-N bond. These studies explore the ability of the catalyst to induce diastereoselectivity in reactions such as the Diels-Alder.

CHED 1211

Investigating the stereoselectivity of magnesium Oppenauer oxidations

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Stereoselectivity was investigated for addition of dialkyl magnesium Grignard reagent and postliminary magnesium Oppenauer oxidation with gas chromatographic methods. The oxidation, facilitated by magnesium alkoxide salts formed in-situ, involved hydride transfer to various hydride acceptors that were added after the alkoxides were formed. The system of diastereomers formed from alpha-chiral alcohols demonstrated different rates of hydride abstraction. The rates of hydride transfer were found to be influenced by solvation and the nature of the hydride acceptor.
Ionic liquids (ILs) can be used as solvents for biopolymers due to unique chemical and physical properties that enable mobilization and disruption of the hydrogen bonding.
present in the biopolymer structure. Chitin is a biopolymer known to have natural antimicrobial properties that can help aid in wound healing. It also has the ability to absorb heavy metal contaminants in water, which could be used for water purification. The goal of this work is to functionalize a composite cotton yarn or cloth with chitin biopolymer, in order to exploit the bio-active properties of chitin, while maintaining the intrinsic physical and chemical properties of cotton yarn. The method used to reach this goal is known as Natural Fiber Welding (NFW). NFW is the process of full or partial dissolution of a biopolymer substrate and the regeneration using Ionic liquids, such as 1-ethyl-3-methylimidazolium acetate. Using this process, chitin is able to be permanently adhered and chemically hydrogen bonded to the outer and inner surface of the native yarn. Changing factors, such as ionic liquid solution composition (introducing DMSO), temperature, and time alters the degree of biopolymer mobilization which influences what properties the composite yarn displays. In this presentation we will show results for chitin and cotton composite yarns. We will present data characterizing the physical, chemical, and biochemical properties of these composites. Data from tensile testing, confocal fluorescence microscopy (CFM), and SEM imaging as well as antimicrobial studies will be shown.

CHED 1213

Production of methyl-ester (biodiesel) using oleic acid and methanol and lipase B Candida antarctica

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Biodiesel will be the main alternate to petroleum in coming years. At present many researches for the production of biodiesel are in progress around the globe. The main reaction everyone is following is the esterification - reacting oil of fat + alcohol in the presence of catalysis to get glycerol and ester (biodiesel). This research aims at producing biodiesel in a clean and eco-friendly way. Two catalyst systems have been employed in this research: the natural biologically important organisms, such as bacteria and fungi, and tin(II) bromide. Oleic acid is used as the fat of oil because it has almost the same carbon chain as soybean oil. Methanol was chosen as the alcohol, and lipase B Candida antarctica, an enzyme, and tin(II) bromide as the catalysts. The main focus of this research project was to compare two esterification reactions using two different catalysts, list their pros and cons, and determine which catalyst is better and more ecofriendly.

CHED 1214

Stereoselective synthesis of fluorinated β-lactams

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We have explored the reaction of fluorinated enolates with imines. This reaction produces a mixture of erythro and threo β-lactams and β-amino esters. The conditions have been varied to determine the effects on the erythro/threo ratios as well as β-lactam to β-amino ester ratios. Methodology involving the Zn enolate gives a 5:2 threo to erythro β-lactam ratio. Methodology involving a ketene silyl acetal intermediate has proven to increase this to a 5:1 ratio. Under anhydrous conditions, this reaction gives a 3:2 β-lactam to β-amino ester ratio. Under non-anhydrous conditions this reaction gives a 2:3 β-lactam to β-amino ester ratio.

CHED 1215

Synthesis, characterization, and phototoxicity studies of paraben derivatives

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Parabens are anti-microbial preservatives found in topical therapeutic agents and cosmetic products. Methylparaben, butylparaben and isopropylparaben are used in order to preserve products applied to the skin, such as body lotion, sun block and eye shadow powder. It has recently been shown that parabens may be toxic to mammalian cells by acting as hormone agonists or antagonists or cellular enzyme inhibitors, or due to analgesic or anesthetic effects. This poster will describe efforts to synthesize, purify, and characterize new derivatives of parabens whose properties, and potential health risks, have been modified through steric and/or electronic modifications. Current efforts include attempts to increase the hydrophobicity of the paraben compounds via conversion to long-chain or ring-containing esters, as well as the introduction of bulky substituents and electron-withdrawing and electron-donating groups to the phenolic ring. Additionally, this poster will describe experiments designed to study the toxicity and phototoxicity of the synthetic paraben derivatives, and will compare those results to those obtained from the commercial paraben products.

CHED 1216

Progress toward the synthesis of fluorinated antimalarial analogs

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Malaria is an infectious disease caused by protozoan parasites of the genus plasmodium that are transmitted by the female Anopheles mosquito. Chloroquine is perhaps the most commonly known antimalarial belonging to the 4-aminoquinoline class of antimalarials. The emergence of a chloroquine-resistant parasite has made its use obsolete. Amodiaquine and tebuquine (also 4-aminoquinolines) are active against chloroquine-resistant strains of malaria. However, their use has been limited due to
harmful side effects resulting from the *in vivo* oxidation of the aminophenol functionality which is a structural alert for hepatotoxicity as it forms highly reactive and toxic quinone imines (Scheme 1a). Replacement of the OH by a similar group that cannot be oxidized is thus desirable. We hypothesize that substitution of OH by CF$_2$H should eliminate *in vivo* oxidation to toxic metabolites thereby eliminating the dangerous side-effects (Scheme 1b). Herein, we propose a seven step synthetic route for the new series of CF$_2$H analogs and the progress we have made thus far. Once these analogs are synthesized they will be assayed for anti-malarial activity.

**Scheme 1.** a) Bio-activation of amodiaquine to Toxic Quinone Imines and b) Substitution of OH by CF$_2$H

**CHED 1217**

*Synthesis of the benztropine derivative as a precursor of fluorescence labeled analogs to be used in dopamine transporter binding affinity assays*  

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4,4'-Dichlorobenztropine and its demethylated analog were synthesized. These compounds will be linked to a small but potent fluorescent tag to be used as an alternative to radioactivity in traditional dopamine transporter (DAT) binding affinity assays. The benztropine derivative was selected as a template due to its high affinity binding and selectivity at the site of the DAT. The development of fluorescent labeled molecule allows for a decrease in both hazard and cost in the process of studying the structure and function of the DAT, potentially increasing DAT-related research output.

**CHED 1218**

*Synthesis of molecular electronic components for self-assembly onto metal electrodes*
Molecular electronics encompasses the synthesis and study of single-molecule electronic devices. Such devices have the potential to be smaller and more efficient than their silicon-based analogs. Our present goal is to design and synthesize a carbon-based molecular diode. Current work is centered on molecules bearing an electron-rich dimethoxybenzene donor ring and an electron-poor quinone acceptor ring separated by a single bond. We have successfully synthesized a template molecule, dibromohemibiquinone – which can then be converted to aminohemibiquinone – that will allow for the substitution of functional groups at its attachment sites. The purpose of such groups is bonding to metal electrode surfaces. Through deprotonation and acylation at the amino site of aminohemibiquinone, it is possible for attachment groups to be added to the hemibiquinone framework. Some particularly useful groups for bonding to metal surfaces are nitriles and thiols. A benzyol nitrile moiety has been incorporated via cyanobenzoyl chloride. In order to append a thiol group, we have prepared 4,4'-dithiodibenzoic acid. Transformation of the acid into the acid chloride then allows for acylation of the aminohemibiquinone molecule. Once this substitution is completed, surface studies will be conducted on both the nitrile- and thiol-containing compounds in order to determine the geometry of a monolayer of self-assembled molecules on a gold surface. Monolayer geometry is essential, since the purpose of the diode is to allow unidirectional electron flow between two surfaces via attachment to each. Ideal surface geometry would be near perpendicular. In addition, derivatives of the hemibiquinone backbone have been synthesized for electrochemical and spectral comparison with the hemibiquinones.

CHED 1219

Thiosemicarbazone-derivatives from ferrocenyl chalcones as potential antibacterial and antimalarial agents

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Chalcones and their derivatives are some of the many occurring natural products. They can be found in fruits, vegetables, spices, tea and soy. These compounds are well known for their broad range of biological activities, specifically for their antimalarial, antibacterial, antitumor, antioxidant, and anti-HIV activity. It is known that replacing one of the aromatic rings of a chalcone with a ferrocenyl group results in greater biological activity, presumably due to the lipophilicity of the ferrocenyl group and resulting bioavailability. Some chalcone derivatives are also known to exhibit greater biological activity than their corresponding chalcone core, as is the case for the thiosemicarbazone derivatives. This research is focused on thiosemicarbazone derivatives. We pursue three specific aims: (a) develop an efficient methodology for
their synthesis from ferrocenyl chalcones, (b) spectral and electrochemical characterization, and (c) collaborative-based biological testing for malaria and a series of bacteria. The synthetic methodology, characterization and preliminary biological assays of these compounds will be elaborated.

CHED 1220

Synthesis of (2-fluorophenyl)methanol followed by an investigation of hydrogen bonding via $^1$H-NMR

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Investigation on the properties of fluoro-organic compounds has increased in recent years due to their important applications in the pharmaceutical and agricultural industries. An open question is whether the fluorine atom can form a hydrogen bond with a suitable donor. To investigate this issue I will synthesize (2-fluorophenyl)methanol in three steps: attachment of the Boc protecting group to 2-(hydroxymethol)phenol, fluorination of alcohol, and deprotection of Boc-group. This compound will be used to examine the strength of hydrogen bonding via $^1$H-NMR spectroscopy.

CHED 1221

Synthesis of novel GLP-1 stimulants

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Diabetes mellitus is a chronic disease resulting from elevated blood glucose levels. Arising for various reasons, diabetes affects 8.3% of the US population and has become a growing epidemic. During the summer of 2013, a compound with potential antimicrobial properties was synthesized in the Ippoliti lab. After showing no antimicrobial activity, the compound was sent for testing at Eli Lilly Open Innovation Drug Discovery and was found to have a strong effect in stimulating the release of glucagon-like peptide-1 (GLP-1). GLP-1 is a peptide capable of lowering high blood glucose levels by increasing the body’s response to insulin. By modifying various functional groups of the original structure, the current study aimed to determine the functionally active substituents and maximize the compound’s biological effects on GLP-1, with the intent of creating a novel GLP-1 stimulant. Thus far, ten analogs have been synthesized using a three- or four-step synthetic scheme. Full characterization of each new compound was performed using nuclear magnetic resonance and mass spectroscopy. The analogs will be sent to Eli Lilly for testing of their biological effects.
CHED 1222

Synthetic investigation of Diels Alder reactions with α-β unsaturated ketones

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α-β unsaturated ketones can be used as starting materials to form highly substituted cyclohexene compounds, which have various applications ranging from antimicrobials and pain relievers, to preservatives. The goal of this research is to develop innovative synthetic methods for these compounds using inexpensive and readily available materials. In our work, we have demonstrated that 3-penten-2-one can be successfully used as a reactant to form a highly substituted cyclohexene compound. As such, we are investigating the synthesis of similar cyclohexene compounds using trans-methyl crotonate and mesityl oxide as reactants. The progress of our work will be discussed in detail.

CHED 1223

Synthesis and characterization of new oxadiazole-containing compounds

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We have prepared a set of derivatives that contain an oxadiazole core attached to an aromatic group with an alkoxy chain that ranges from 4 to 12 carbons in length. This combination of a rigid core and a flexible tail may allow for liquid crystalline properties. The multi-step synthesis of these compounds as well as the characterization of the intermediate and final products will be presented. Preliminary results from microscopy and thermal analysis may also be discussed.

CHED 1224

Synthesis of a novel blue light-emitter for use in organic light emitting diodes (OLED's)

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OLED's have the ability to produce large, flexible image displays that rival LED's in efficiency and cost effectiveness. For OLED's to produce a full color display, red, green, and blue light-emitters are needed, but the production of stable and efficient blue light-emitters has been problematic. The aim of this research is to synthesize a family of novel blue light-emitting molecules that demonstrate high stability and pure blue light emission. The parent molecule is comprised of three subunits: Diphenylacetylene (DPA), Carbazole, and a Dendron, each chosen specifically to ensure stability and
effective blue light-emission. Each subunit has been individually synthesized and the terminal DPA subunit has been borylated in order to be coupled to the central carbazole subunit. The reaction conditions for the final Suzuki-Miyaura coupling reactions to complete the parent molecule are being investigated and optimized. Upon synthesis of the parent molecule, study of its light emitting and electronic properties as well as stability tests in solution and in thin film form will be performed.

CHED 1225

Synthesis of fluorescent bisimidazole sensors for heavy metals

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A series of aryl-substituted 4,4'-bisimidazoles are being investigated as sensors for heavy metal ions. The sensor molecules are synthesized in four steps from phenylacetylene and benzoylnitromethane. The metal-specific fluorescence response to various metal ions will be reported.

CHED 1226

Synthesis of an alkyne-containing isoprenoid mimic for the investigation of the role of substrate length on prenyl transferase activity

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Protein farnesyltransferase (PFTase) has been attributed to the cell division cascade, making it an interesting target of study for cancer research. PFTase site-specifically transfers isoprenoid-containing groups to proteins ending in the specific amino acid sequence CVIA via farnesylation. This farnesylation process can be studied through the synthesis of non-natural substrates that can be modified post-prenylation to express characteristics of interest such as fluorescence. Here an alkyne-containing isoprenoid mimic is reported that can be enzymatically phosphorylated and incorporated into CVIA proteins. This mimic contains one more carbon than previously reported alkyne substrates. This will allow for future study on the role that isoprenoid length has on prenyl transferase activity.

CHED 1227

Formylation of substituted phenols using microwave irradiation

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The Duff reaction is commonly used to introduce a formyl group to an aromatic ring with hexamethylenetetramine (HMTA) as the carbon source. The purpose of this project is to efficiently produce mono- and dialdehydes by the Duff reaction from substituted phenols under microwave irradiation. The reaction was performed in a sealed tube placed in a CEM microwave reactor and identification of the products was completed using NMR. The substituents of the phenols tested varied from the highly electron donating methoxy group to the highly electron withdrawing nitro group. Monoaldehyde formation with 4-methoxyphenol and 4-t-butylphenol produced high yields with only five minutes in the reactor. Monoaldehyde formation with 4-nitrophenol had yields of 56% and 57% for five and 15 minutes in the reactor. The dialdehyde formation reactions were done in the presence of a large excess of HMTA and reactions with 4-methoxyphenol produced a mixture of the mono- and dialdehyde. The results of the reaction using a large variety of starting materials will be presented. Monoaldehyde formation via the Duff reaction in the microwave reactor is very successful while the dialdehyde formation is more difficult.

CHED 1228

Progress towards the synthesis of a norbornene containing substrate for the enzyme protein farnesyltransferase

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Protein farnesyltransferase (PFTase) is an enzyme that incorporates farnesyl groups into proteins and peptides that end in a certain amino acid sequence. Previously, non-natural substrates have also been transferred by PFTase. These substrates contained azide and alkyne moieties that could subsequently undergo bioconjugation reactions via copper catalyzed click chemistry. However; because of copper’s cytotoxicity, these substrates were not compatible with many in vivo applications. Here progress toward the synthesis of an norbornene containing isoprenoid diphosphate is reported. Different protecting group strategies are highlighted in two possible synthetic routes for this target. One route includes an acetyl protection of an alcohol while the other includes THP protection. Once synthesis is complete this norbornene containing PFTase substrate will allow for subsequent bioconjugation of functionalized tetrazines without the use of copper catalysts. In end this will allow for the study of the prenylome inside living systems.

CHED 1229

DNA binding affinity and cleavage of aryl sulfoxides

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Radical-initiated DNA cleavage is an important mechanism in cancer therapy. When exposed to ultraviolet light, aryl sulfoxides have the ability to cleave DNA by means of
Four aryl sulfoxides containing polyaromatic ring systems, 1-methylsulfinylanthracene, 9-methylsulfinylphenanthrene, 1-methylsulfinylnaphthalene and 2-methylsulfinylnaphthalene, were synthesized. Using an ethidium bromide displacement assay, the DNA binding affinities of these compounds were determined. DNA cleavage assays were performed on 1-methylsulfinylnaphthalene and 2-methylsulfinylnaphthalene. These compounds exhibited greater DNA binding affinity and cleavage than phenyl sulfoxide and methyl phenyl sulfoxide.

CHED 1230

Transesterification of hypophosphorous esters: The tales of secondary alcohols

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The Deepwater Horizon explosion in the Gulf of Mexico released oil into the ocean causing damage to many ecosystems. To help alleviate the spill, drastic measures were taken and the gulf region was treated with millions of liters of chemical dispersants, to allow for a rapid breakdown of the oil. Our objective is to synthesize original phosphorous based surfactants to help make the oil spill clean-up more environmentally friendly. The first step of our synthetic scheme is the silicon-based (tetraethyl orthosilicate (TEOS)) transesterification of ethyl hypophosphite with a cyclic alcohol to serve as a model for long chain ester synthesis. A one pot one-step synthesis of cyclohexanol, concentrated H₃PO₂ and TEOS all mixed at once in CH₃CN and refluxed for 2 hours, generated³¹P crude NMR yields from 41 to 64% depending on the number of equivalent of alcohol used. Similarly, 3-pentanol displayed crude yields ranging from 42 to 60%. The moderate yields can be linked to the alcohol replacement competition and steric hindrance of the secondary alcohols used. In an effort to optimize our percent yields, we varied the sequence of the esterification/transesterification synthesis to a one pot two-step synthesis, where the esterification was conducted first for 2 hours, and then the transesterification was initiated for 2 hours. The results show that four equivalence of alcohol in acetonitrile or toluene produced the cyclohexyl ester in 63 and 64% respectively. No significant yield increase was observed compared to the previous method but we are currently continuing our study with linear secondary alcohols such as 3-pentanol and 2-octanol to better understand the impact of the molecule’s geometry on the reaction’s efficiency. Future directions include yield optimization and hydrophosphinylation of the esters synthesized under Pd or Ni catalyzed conditions.

CHED 1231

Polymeric melamine-metal catalysts in Suzuki-Miyaura couplings and azide-alkyne cycloadditions
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Melamine has been shown as an effective ligand for palladium in homogenous Suzuki-Miyaura cross-coupling; the melamine-palladium complex provides high yields and tolerates a wide range of functional group substitution. The melamine-palladium catalyst system can be cross-linked with formaldehyde to provide a heterogeneous analog for use in water-based reactions. The use of water is an important advance in green chemistry, and the heterogeneous catalyst system offers advantages in catalyst recovery and reuse.

In this research, a polymerized melamine-copper catalyst system is prepared using a procedure based upon that of the melamine-palladium catalyst. The use of glutaraldehyde as a cross-linking agent was also investigated, since a change in cross-linking density has an effect on metal ligation and steric hindrance near the reaction site. This catalyst system was shown to be active in the azide-alkyne cycloaddition.

Immobilization of these catalysts on a solid support allows for flow chemistry applications. The use of copper and palladium catalyst chambers in tandem provides the opportunity to easily synthesize products that would be difficult to produce in a batch setup. Prospects in this application are discussed.

References:

CHED 1232

1H NMR analysis of the methylation of acetic acid catalyzed by tin (II) bromide: A kinetic study

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Biodiesel made from waste cooking oil is a popular substitute for petroleum diesel. However, due to its high content of free fatty acids (FFA), waste oil must undergo an initial acid catalyzed esterification. This process typically employs concentrated H2SO4 but we chose a milder Lewis acid, tin (II) bromide, as our catalyst. Our investigation is part of a larger project which employs acetic acid, and tin (II) bromide as catalyst at various temperatures to verify computationally derived activation energy and mechanistic data acquired from a collaborator. The computational data suggest the formation of a methanol-tin complex as the acidic species in this reaction. This poster
will present our interpretation of the data and how it supports the preference of one mechanism over the other for the esterification reaction.

CHED 1233

Synthesis of biphenyl urea derivatives related to 3-iodothyronamine

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The Thyroid hormone (TH) is known to actively participate in many biological processes including vertebrate metabolisms, cardiovascular function, brain development and growth. Decreases in TH production by the body can lead to hypothyroidism and result in cognitive lost. Inversely, elevated TH levels, hyperthyroidism, can lead to severe heart and bone problems if untreated. Because hormone biology is not completely understood, there are minimal treatment options available. Recently, 3-iodothyroamine (T1AM) was demonstrated to act on the trace amine associated receptors (TAAR) to induce physiological effects in opposition to those of TH, including hypothermia and cardiac depression in mice. Further studies have developed a structure activity relationship for T1AM mediated TAAR regulation. The development of urea based derivatives has been the focus of our laboratory. The project herein examines the synthesis of biphenyl urea derivatives with varying the substitution patterns. Exploring the effects of these urea derives as TAAR regulators may have pharmaceutical applications, especially for those patients with thyroid hormone irregularities.

CHED 1234

Asymmetric design and synthetic studies of monoterpene indole alkaloid analogs

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Monoterpene alkaloids represent an abundant family of natural products frequently exhibiting pharmacological activity. Due to their structural complexities and therapeutic potential, considerable synthetic interest has been dedicated to monoterpene alkaloids, and specifically, monoterpene indole alkaloid scaffolds. Indole alkaloids, which are
derived biologically from the amino acid, tryptophan, are found in a multiplicity of organisms including fungi, animals, and plants. Previously, synthetic strategies focusing on asymmetric control have been effective in the manipulation and production of indole alkaloid scaffolds. Because structure-activity relationships are often contingent on stereochemical arrangements of atoms, it is increasingly important to develop methodologies addressing the complexities of asymmetric synthesis. Herein, we investigate the asymmetric total synthesis of monoterpene indole alkaloids and their analogues.

CHED 1235

Reaction of O-silylated cyanohydrins with epoxides as an alternative for the enantio- and diastereoselective preparation of aldols

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The aldol addition is an important carbon-carbon bond forming reaction in chemical synthesis. The reaction occurs between an aldehyde or ketone and a second enolized aldehyde or ketone, forming a β-hydroxycarbonyl. The reaction can result in the formation of up to two new chiral centers, and the stereochemistry of the product can be challenging to control. Modern variations of the reaction that utilize chiral auxiliaries allow for significant enantio- and diastereoselectivity but are encumbered by poor atom economy and the additional synthetic steps required for auxiliary introduction and removal.

An alternative potential route for the enantio- and diastereoselective preparation of aldols is the reaction of O-silylated cyanohydrins anions with epoxides. This method takes advantage of the many available asymmetric epoxidation procedures, providing an efficient stereoselective method.

The method was developed by preparing the tert-butyldimethylsilyl (TBS) ether of mandelonitrile. The substrate was deprotonated using LiHMDS and alkylated with 1,2-epoxybutane as the electrophile. The initial adducts were desilylated with tetrabutylammonium fluoride (TBAF) to expel cyanide and form the desired aldol product. After optimized conditions were determined, the scope and limitations of the method were investigated with respect to the epoxide structure. Yields up to 90% for the two-step process (alkylation-desilylation) could be achieved. Monosubstituted epoxides generally give higher yields than either geminally or vicinally disubstituted epoxides. Epoxides possessing larger aliphatic chains also gave higher yields.
CHED 1236

Synthesis of enaminones using copper as a catalyst

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Enaminones are synthetic intermediates in organic synthesis that contain the N-C=C-C=O functional group. These compounds are useful in the development of pharmaceuticals. Although the biological activity of enaminones is not well-documented, enaminones have currently come under investigation because of their therapeutic potential. Recently, our research group has found a ruthenium catalyzed method for the synthesis of enaminones that requires ruthenium for catalysis. This project uses a copper catalyzed method for the synthesis of enaminones. Copper (II) Bromide was investigated for the coupling of a diverse group of thioamides (1) and diazo compounds (2). Temperature and time were screened and the catalyst was found to give 100% conversion of several thioamides into the corresponding enaminones (3) at 90 °C using dichloroethane as a solvent. Copper (II) Bromide shows a broad scope in the synthesis of enaminones. By using a copper catalyzed method, the reaction has become more economical.

CHED 1237

Diversity oriented synthesis of an alkaloid-like library via cyclotrimerization of easily accessible aminonitriles

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Alkaloid and terpenoid natural products display an extensive array of chemical frameworks and biological activities. However such scaffolds remain underrepresented in current screening collections and are, thus, ideal targets for the synthesis of natural product-based libraries. We have established a highly efficient route for the synthesis of a large array of complex aminonitriles. These synthons are perfect templates for transition-metal mediated cyclotrimerization reactions. Our initial efforts have shown that highly complex aza- and diaza- indoles and indolines can be obtained with high efficiencies from our simple aminonitriles. The completion of this project will provide access to a wide array of alkaloid-like small molecules for high throughput screening (HTS) and foster the discovery of new therapeutic applications for underexploited biological targets.

CHED 1238

Cross-coupling reactions of fluorinated aryl chlorides and aryl chloride acetals with 1-hexylmagnesium bromide

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Previous research by Furstner has shown that Fe(acac)₃ catalyzed cross-coupling reactions between an aryl chloride and a Grignard reagent are most successful when the aryl chloride contains electron-deficient substituents¹. Several Fe(acac)₃ catalyzed cross-coupling reactions between various fluorinated aryl chlorides and 1-hexylmagnesium bromide were conducted in order to gather data on the effectiveness of fluorine at promoting the cross-coupling of an aryl group and a Grignard reagent. It was discovered that fluorine promotes the greatest coupling conversions when in the meta position to the chlorine. 4-chlorobenzaldehyde bis trifluoroethyl acetal was successfully synthesized. The trifluoroethyl acetal protecting group both prevented the aldehyde from reacting with the Grignard reagent and promoted nearly complete conversion to 4-n-hexylbenzaldehyde bis trifluoroethyl acetal. Thus, highly efficient cross-coupling between chlorobenzaldehyde derivatives and a Grignard reagent is now possible using this acetal.

Summary of the three major types of reactions investigated.

CHED 1239

Synthesis of highly substituted anthraquinone derivatives via microwave assisted self-condensation of benzoic acids
Highly substituted anthracene derivatives are a class of three-ringed aromatic molecules with promising properties for a variety of applications, from dye imaging to organic electronics. Additionally, they can serve as donor components in Donor-Acceptor Columnar Liquid Crystals (DACLCs), a relatively new type of organic material. Exploring the structure-function relationships in anthracene-based DACLCs requires the synthesis of new derivatives. Presented here is the development of new methodology towards the general synthesis of a variety of highly-substituted anthraquinones as immediate precursors to new anthracene derivatives. The investigation of microwave assisted Friedel-Crafts acylation on substituted benzoic acids in strongly acidic conditions will be discussed.

CHED 1240

GC-MS analysis of phytosterol content of dried mushrooms

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The goal of this research was to determine the phytosterol content of dried mushrooms and compare the results to that previously reported by others for fresh mushrooms. Ergosterol is particularly important due to its role as a light-activated precursor of vitamin D2. Dried mushrooms (Pleurotus ostreatus and Morchella) were Soxhlet extracted with petroleum ether, saponified (1M NaOH in EtOH), extracted again with petroleum ether, dried over Na$_2$SO$_4$, and derivatized as TMS-ethers, which were analyzed by GC-MS.

Our results suggest similar sterol content for dried and fresh mushrooms. However, ergosterol was found to be significantly less abundant in dried mushrooms (oyster = 67%, morel = 19 ± 2%) than in fresh mushrooms (oyster = 84%, morel = 30-40%). An unknown sterol previously reported in fresh morel mushrooms was confirmed to be present in dried morels and identified as 24-methylenecholesterol.
CHED 1241

Preparation of functionalized dendrimers and their effectiveness in organocatalytic reactions

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Dendrimers (highly branched macromolecules) present an attractive option for use as a catalytic framework because of their large size and their availability for functionalization. In addition, the use of organocatalysts to form asymmetric products has become an increasingly studied field in the pharmaceutical industry. Organocatalyst terminally functionalized dendrimers present the possibility of both increased catalytic utility and recovery in MacMillan-type asymmetric reactions. For this project, terminal sites of generations two, three, and four PAMAM dendrimers have been functionalized with the MacMillan group’s (2S, 5S)-5-benzyl-2-tert-butyl-3-methyl-imidazolidin-4-one catalyst. These functionalized PAMAM dendrimers were characterized by NMR and MALDI-TOF MS analysis. The organocatalyst functionalized dendrimers are being screened for their effectiveness and recoverability in MacMillan-type organocatalytic reactions.

CHED 1242

Direct esterification of H₃PO₂: A Dean Stark methodology

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The 2010 BP oil spill in the Gulf of Mexico left a raft of ecosystems harmed and endangered. In the interim efforts have been made to remove the harmful chemical agents left behind in hopes to proliferate the damaged ecosystems. This clean-up has been approached utilizing various methodologies; one includes, but not limited to the use of dispersants. In our study we propose a novel surfactant that is phosphorus based. The synthesis of this phosphorous surfactant involves three steps, the first of which we are currently focusing on. This step entails the synthesis of a hypophosphite ester from hypophosphorous acid and an alcohol. Previous studies in our lab have proved adequate formation of the hypophosphite ester through transesterification. Recently we have found a more efficient route to synthesize our desired product. Utilizing the Dean Stark apparatus we are able to directly esterify the hypophosphite ester. Preliminary results have shown desirable product yields that are comparable to the transesterified product. Reacting hypophosphorous acid with our alcohol of choice we have yielded 68%, 54%, and 90% for heptanol, nonanol, and dodecanol respectively. Moving forward with our results we seek to synthesize the hypophosphite ester using other primary alcohols. After obtaining desirable yields we will continue onto the next step in synthesis of our phosphorous based surfactant: palladium-catalyzed hydrophosphinylation with brominated olefins.

CHED 1243

Synthesis of α-chalcones and derivatives via a microwave Knoevenagel condensation

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We have recently developed a facile approach to generate α-substituted chalcones. This methodology allows for the generation of these biologically active compounds and derivatives with little to no purification. We have successfully expanded the methodology to generate a variety of substituted groups on the α-carbon yielding α-cyano, ester, nitro, and fluoro chalcones. We will also report our most recent progress by successfully implementing aliphatic substituted species to the methodology. Additionally, when these synthetic conditions are applied to α-chloro and bromo chalcones, an unexpected oxide product is generated, where an epoxide forms between the chalcones’ α and β carbons.

CHED 1244

Diversification of thiol phosphonamidates

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We have developed a synthetic route featuring ring-closing metathesis to form a thiol phosphonamidate, a seven-membered heterocycle containing sulfur, phosphorus, and
nitrogen. This path allows for modification of the thiol phosphonamidate by utilizing various amino acid starting material derivatives. Herein, we report on two diversification strategies, one which diversifies the heterocycle externally at the nitrogen, and another which results in diversification within the heterocycle via a substituted allyl amine. By employing these synthetic routes, we can develop an array of heterocycles whose potential biological activity can be further explored and exploited.

CHED 1245

Characterization of α-substituted chalcones

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A facile methodology for inducing a Knoevenagel condensation utilizing microwave irradiation has yielded chalcone products. The reaction has been optimized and expanded to generate diverse substitution on the α-carbon, including cyano, nitro, ester, and fluoro groups. Herein, the crystal structures of the α-substituted chalcones are presented, and we can see that the α-substitution decreases the pi bond overlap of the conjugated system thereby disrupting the expected planarity. The solid state bond orientations suggest that the differences in steric influence of the α-groups dictate the resulting s-cis or s-trans conformation. Additionally, two unexpected products were formed during the synthetic exploration—an uncondensed chalcone and an epoxide product—which are included in the crystal structure analysis.

CHED 1246

Purposeful biofilm disassembly with unnatural alkyl and aromatic D-amino acids

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Biofilms are incredibly complex structures manufactured by microorganisms in locations that are intermittently wet. They are primarily composed of a complex mixture of exopolysaccharides, extracellular DNA, and proteins collectively called the extracellular polymeric substance or EPS. Bacteria use the enantiomers of natural L-amino acids known as D-amino acids for cell wall assembly and as the signal for biofilm dissociation. Because biofilms are responsible for 65-80% of human infection, D-amino acids with various side chain attachments could serve as the next class of effective antimicrobial compounds. Non-natural D-amino acids were synthesized from Glycine using the chiral auxiliary, S,S-pseudoephedrine. Glycine was then subject to alkylations with different alkyl halides. The hydrolysis of the alkylated products was the library of new D-amino acids for analysis. The compounds will then be exposed to the biofilm forming gram-positive bacterium Staphylococcus epidermidis. The effectiveness of the compounds will be verified using bacterial biofilm assays.

Faculty supervisor: Dr. Michael Bertucci
Manipulation of n to π* orbital interactions in the hydrolysis of para-substituted N-acyl homoserine lactones

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N-Acyl Homoserine Lactones (AHLs) are molecules found in gram negative bacteria used for a chemical communication process known as quorum sensing. Modulation of quorum sensing is controlled by hydrolysis of the lactone component of the molecule. A critical n to π* orbital interaction of the butyrolactone has been hypothesized to attenuate hydrolysis. In our study, para-substitution of the benzoyl-AHL derivative was explored to understand how electron donating and withdrawing groups affect hydrolysis. Substituted benzoyl groups were chosen to specifically study the potential influence of inductive and resonance effects on the n to π* interaction. The n to π* orbital interaction of the butyrolactone leading to hydrolysis was affected by these substitutions. HPLC was used to examine the variation in rates of hydrolysis to calculate relative rates and assess how electron donating and withdrawing groups affect hydrolysis.

Intramolecular oxazolium salt/azomethine ylide cycloaddition reactions with varying dipolarophile tether position

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Pyrroles and pyrrolidines are heterocyclic compounds that are particularly useful for medicinal purposes. They can be found in an assortment of biological contexts, such as cofactors and secondary metabolites, and are present in a range of drugs that treat everything from cardiovascular disease to cancer. Engineering these compounds can be accomplished through a multitude of ways, but a 1,3-dipolar [3+2] cycloaddition may prove to be beneficial in producing lucrative pyrroles or pyrrolidines. This research aims to expand the scope of the known oxazolium salt/4-oxazoline/azomethine ylide route to these important investigate the assembly of five member heterocycles. via azomethine ylide formation through a nucleophile-mediated opening of an oxazolium salt. This methodology generates the reactive Formation of the azomethine ylide under mild conditions that allow in this manner is milder, allowing sensitive functional groups to be preserved. However, only . The 5-substituted and 2,5-disubstituted oxazoles are known to undergo this transformation.ring-open under these conditions Further, only substrates with the di with tethered and un-tethered dipolarophiles. However, Dipolarophile tethered at the five position have been shown to undergo an intramolecular cyclization. Thus, we are focusing our efforts on varying the position of the dipolarophile tether to the position two carbon and position three nitrogen. To tether at position 2, we have used DCC and EDC coupling reactions to prepare keto-amides
from the appropriate carboxylic acids and alpha-amino-ketones (e.g., from a protected 4-hydroxy butyric acid and 2-amino-acetophenone). These compounds were then subjected to typical oxazole-forming conditions, using reagents such as triphenylphosphine. From here, the alcohol is deprotected, converted to the aldehyde, and treated with a lithiated alkyne to install the tethered dipolarophile that is ready for the [3+2] cycloaddition sequence. To tether the dipolarophile at position 3, 6- and 7-iodo-2-alkynoates have been prepared that are being used to alkylate the oxazole nitrogen, thus forming the oxazolium salt that is employed in the cycloaddition sequence. Preparation of all intermediates and progress to date will be reported.

CHED 1249

Microwave accelerated deprotections of aryl silyl ethers

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The ability to utilize microwave irradiation to accelerate the deprotection of aryl silyl ethers was investigated. t-Butylphenol protected with a TBS group was used to find the ideal reaction conditions for this deprotection. By altering the temperature, the molar quantities of the reactants, and the length of time of the reaction, the ideal conditions were found to be 150°C for 30 minutes, using 0.2 molar equivalents of LiOAc. By comparison, conventional heating requires reaction times of up to 24 hours. Once the reaction conditions were found, different silyl protecting groups were tested, including TBDPS, TES, and TIPS. Finally, the ability to perform selective deprotection reactions with these conditions was explored. The microwave proved effective at successfully mediating the deprotection of silyl ethers with high yields in greatly reduced reaction times and selectivity in the removal of silyl groups on phenolic oxygens.

CHED 1250

Look at biodiesel produced using *Chlorella vulgaris* microalgae

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The purpose of this research project is to investigate the cloud point and heat of combustion of biodiesel samples produced from chlorella vulgaris microalgae and compare them to biodiesel samples made from vegetable oil feedstock, and petroleum diesel. In an attempt to alter the cloud point and heat of combustion, biodiesel will be synthesized with the strong base catalyst potassium hydroxide (KOH), and the alcohols: methanol, ethanol, isopropanol, and tert-butanol. At the completion of this project the data will be summarized to determine which alcohol/feedstock combination produced the biodiesel with the lowest cloud point temperature and the highest heat of combustion.
Structural elucidation of pyrrolizidine alkaloids from *Arnoglossum plantagineum*

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Pyrrolizidine alkaloids (PA) are potentially toxic naturally occurring secondary products, found in the plant family Asteraceae. As a member of the family, *Arnoglossum* is expected to contain PA’s. Examination of the GC-MS data has shown that the major alkaloids in this species are otonecine based seco-PA’s, including otonecine, florosenine, floridanine, and floricaline. It was difficult to quantify the amount of florosenine due to its co-elution with floridanine. A second compound, also at m/z 441 was observed and trivially named arnoglossine, this compound appears to be isomeric to floridanine. We will focus on chromatographic isolation and structural elucidation of minor *Arnoglossum* PA’s using NMR analysis.

Studies on "under air" direct arylation

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The purpose of this research was to find conditions to run direct arylation reactions under air. This was done by varying the ligands and catalysts used in the reactions. The mechanism of direct arylation reactions is very similar to that of Suzuki-Miyaura cross-coupling reactions. With that in mind, the focus of the research was to see if air stable ligands used in Suzuki-Miyaura reactions would also work in direct arylation reactions. Further studies showed that most did not work. One ligand, however, was found to be very successful under air. This ligand, S-Phos, comes from a group of ligands called the Buchwald ligands. S-Phos was used with palladium acetate as the catalyst to yield high amounts of product in just two hours. These findings may now be used as an under air direct arylation reaction for undergraduate lab courses.

Reactions of the highly pyramidalized alkene pentacyclo[4.3.0.0²,4.0³,8.0⁵,7]non-4-ene

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We have previously shown that pentacyclo[4.3.0.0^2,4.0^3,8.0^5,7]non-4-ene (2) may be generated via dehalogenation of 4,5-diiodopentacyclo[4.3.0.0^2,4.0^3,8.0^5,7]nonane (1) with alkyllithiums. The resultant pyramidalized alkene may be trapped as its Diels-Alder adduct with diphenylisobenzofuran (3) and other conjugated dienes. Recently, we have been investigating new methods for the synthesis of 4,5-diiodopentacyclo[4.3.0.0^2,4.0^3,8.0^5,7]nonane (1) as well alternative approaches toward pentacyclo[4.3.0.0^2,4.0^3,8.0^5,7]non-4-ene (2), and we will report our progress in this area including the reactions of this highly pyramidalized alkene.

CHED 1255

Studies toward the synthesis of altersolanol P

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We recently initiated synthetic studies toward the synthesis of altersolanol P (AP), a naturally occurring tetrahydroanthraquinone recently isolated from forest leaf litter collected at the Caribbean National Forest in Puerto Rico. AP has displayed broad-spectrum Gram-positive antibacterial activity and strong activity against the Gram-negative bacteria, Haemophilus influenza. Antithetic analysis led us to explore the possibility of a regioselective Diels-Alder reaction as a method to produce a synthetic intermediate containing the complete carbon framework of the target molecule. From the desired adduct, AP could conceivably arise from a sequence of alkene isomerizations followed by dihydroxylation. Currently, we are synthesizing a series of isoprene and juglone derivatives for a methods study that will allow us to examine the regioselectivity of potentially useful Diels-Alder reactions. Our long-term goal is to craft an efficient route to altersolanol P, and its derivatives, so that its biological activity can be further explored.

CHED 1256

Studies toward the synthesis of Hunanamycin A and its derivatives
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We have recently initiated studies toward the synthesis of Hunanamycin A (HA). HA is a natural product first isolated from *Bacillus hunanensis*. It exhibits antibacterial activity for various pathogens such as *Salmonella* and *E. coli*. At the onset of this research project, conceivable synthetic routes to HA were designed based on related literature precedents for each planned reaction of the route. Currently, test reactions (e.g. nitration, reductive amination, and amine alkylation) are being optimized on model systems to explore multiple pathways of producing the target product, along with structurally similar derivatives, via chemical synthesis. Once an efficient synthetic route is elucidated, further biological testing of synthetic HA, and related derivatives, could allow for a calculated modification of the antibacterial properties displayed by this class of molecules. Our most progressive route to date employs a reductive amination method to provide a prenylated amine intermediate in moderate yield over multiple steps from commercially available and relatively inexpensive starting materials.

CHED 1257

**Microwave synthesis and cytotoxicity studies of novel amino-substituted chalcones**

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The microwave synthesis and characterization of novel amino-substituted chalcones has been carried out. Chalcones are model compounds based on Combrastatin A4, a natural product of the African willow tree. Attempts were then made to couple the novel amino-chalcones to fluorescein isothiocyanate (FITC). The coupling of 3’-amino-4-hydroxychalcone with fluorescein isothiocyanate characterized. The fluorescein-chalcone derivative allows for fluorescence and microscopic detection of whether the chalcones are selectively taken up by cells and perhaps may even provide *in vivo* clues to the (tubulin) binding location. Finally, the cytotoxicity of these the amino-chalcones and the fluorescein-chalcone materials will be discussed. The cytotoxicity was examined with and without light exposure. The concentration dependence of phototoxicity and whether the phototoxicity of the chalcone materials is due to activation of apoptosis will also be discussed.

CHED 1258

**Synthesis and characterization of a reversible carceplex**

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A carceplex is a macromolecule formed by the joining of two bowl shaped structures, carcerands, first proposed by Professor Donald Cram. The goal of this study is to synthesize a reversible carceplex capable of encapsulating smaller molecules. The carceplex proposed is the association of an acid and amine carcerand together through an acid base reaction; thereby forming ionic bonds. The ionic bonds give the carceplex the ability to open and close; thereby making a reversible structure. Alternately, a reversible carceplex can be formed through hydrogen bonding of two acid carcerands. The hydrogen bonds are weak bonds and can be broken and formed more easily than an ionic bond. The synthesis of the carcerands will be presented as well as their physical properties.

CHED 1259

Construction of the Choi framework

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New technology allows for the direct alpha-amination of ketones, esters, and aldehydes via copper catalysis. This technology has improved synthetic opportunities and is the key step in a possible stereoselective synthesis of 2-carboxy-6-hydroxyoctahydroindole (Choi). This compound is found in natural products and has been produced both biologically and synthetically, although thirteen of the sixteen stereoisomers have yet to be observed in nature. A five-step synthesis has been proposed using direct alpha-amination for the final cyclization to yield the Choi framework and may be used to investigate the stereoisomers that have not been observed in nature. Progress toward the synthesis of this conformationally constrained amino acid will be reported.

CHED 1260

Progress towards the synthesis of 2-amino-1,3-dihydroxyphosphonates via oxazolidinone phosphonates

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This research involves the synthesis of two diethyl amino-dihydroxy butyl phosphonates (4) which could potentially serve as anti-fungal and anti-microbial agents. The first step of this research involves epoxidation of the phosphate-containing olefins (1) made using the Arbuzov procedure with cinnamaldehyde and crotonaldehyde. The second step synthesizes an oxazolidone (3) using benzyl isocyanate to open the epoxide (2) and cyclize the compound. Hydrolysis of the oxazolidones is performed for the production of the 1, 2 amino alcohols in the third stage. This step synthesizes the amino-phosphonates. The preparation for the first step, as well as the first step itself
has been completed. Upon successful retrieval of the oxazolidones, the alcohols can be synthesized. The oxazolidones will also be manipulated to produce phosphonosugars. Throughout the exploration of these compounds, stereo-chemical manipulation on the epoxides and their resulting products will also be investigated.

CHED 1261

Progress on the synthesis of a fluorescent lead(II)–trapping coumarocryptand

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Research in the Baar lab involves the synthesis of a fluorescing Pb(II)-trapping coumarocryptand to act as a more sensitive clinical method for detecting low lead levels in blood and water. This six-step synthesis employs a converging synthetic strategy where 6,7-di-(2'-trifluoromethanesulfonyloxy)-4-methylcoumarin undergoes an SN2 ring closure with 2,2'-(ethylenedioxy)bis(ethylamine) to produce 2,3-(4-methylcoumaro)-1,4,10,13-tetraoxa-7,16-diazacyclooctadecane. A second ring closure with N,N'-bis(2-chloroethyl)-N,N'-dimethylthelyenediamine should produce 5,6-(4-methylcoumaro)-4,7-dimethyl-4,7,13,16-tetraoxa-1,10-21,24-tetraazabicyclo[8.8.8]hexacosane whose bicyclic macroheterocyclic portion is selective for Pb(II) and whose fluorescent coumarin portion allows for its detection. Five steps have been completed, with current work focusing on the final ring closure and optimizing earlier steps. Once the synthesis is completed, the coumarocryptand's fluorescence will be investigated.
Antiaromatic dications containing sulfur: Dications of sulfur analogues of tetrabenzo[5.5]fulvalene

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Spurred by a generous gift of the monothiophene derivative of fluorenone, 1, by Dr. Craig Hawker, we began the synthesis of precursors to antiaromatic dications 2-4, for comparison with the previously reported dication of bifluorenylidene, 5. As can be seen by the nucleus independent chemical shift values, shown below the dications, substitution of S for CH can have a dramatic effect on the antiaromaticity of these species. Approaches to the synthesis of the precursors to 2-4 will be discussed.

\[
\begin{align*}
1 & \quad 2 \quad 3 \quad 4 \quad 5 \\
\text{264.9} & \quad \text{394.5} & \quad \text{114.1} & \quad \text{394.1}
\end{align*}
\]

Relationship between delocalization and antiaromaticity in 5,5’-bisindenylidene dications
Antiaromatic species should resist delocalization to minimize antiaromaticity; dications should seek delocalization to disperse the positive charge. We are examining the tension between these factors in 5,5'-bisindenylidene dications, 1. By careful placement of a phenyl substituent we should be able to modify the pattern of delocalization and therefore the antiaromaticity of the species. The nucleus independent shift calculations, shown below dications 2-4 support this approach. We will report our progress in the synthesis of precursors to 2-4.

CHED 1264
Exploring and optimizing new palladium-catalyzed reactions

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Palladium is known for its efficient and versatile reactivity in the synthesis of a variety of interesting molecules. Recently, a new oxidative intramolecular palladium-catalyzed reaction has been explored that allows for the synthesis of α,β-unsaturated lactones by the addition of a carboxylic acid and aryl group across a carbon-carbon bond. The reaction design could be used to substitute for more dangerous, inefficient, or hazardous procedures that would otherwise be utilized in the synthesis of the lactone products. Starting materials were synthesized by the efficient combination of glyoxylic acid and aromatic compounds followed by allylation. The palladium-catalyzed reaction was optimized through careful study of parameters such as oxidant, reaction time, solvent, palladium source, and concentration to yield optimized conditions. Products were confirmed by NMR spectroscopy and IR. Further studies into the substrate scope and the chemical mechanism are underway.
Optimizing the purification of diarylacetic acid derivatives

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Diarylacetic acids are a class of molecules with interesting structure and properties. In line with our goals to design a greener synthesis of these molecules, we sought to optimize their isolation and purification following synthesis in a manner that reduces hazardous waste and increases efficiency. Acid-base extraction with aqueous sodium carbonate solution was found to be superior to other basic solutions for the more polar derivatives, providing 2,2-bis-(4-methoxyphenyl)acetic acid in greater than 95% yield consistently on a multiple gram scale. The more nonpolar derivatives formed emulsions under these conditions, requiring an alternate procedure for purification. Column chromatography was used to purify and isolate 2,2-bis-(4-methoxy-3-methylphenyl)acetic acid to a 65% yield and 2,2-bis-(2-methoxy-5-methylphenyl)acetic acid to a 97% yield. Research presented will include studies into the purification of more nonpolar derivatives and investigations into the separation of regioisomers.

Synthesis and characterization of curcumin ferrocenyl analogs

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Curcumin has many medical properties like anti-bacterial, anti-inflammatory, antioxidant, chemopreventive, and chemotherapeutic activity. Also, studies have shown that this natural chalcone, present in the turmeric, exhibit activity against cardiovascular, neurodegenerative, pulmonary, and many other diseases, including the inhibition of cancer, because of its potential as anti-oxidant and anti-inflammatory activity. However, it presents some limitations: its bioavailability is very poor because it has poor absorption, limited tissue distribution, short half-life, and is metabolized fast, creating metabolites that are not effective as curcumin is. It has been reported that adding the lipophilic ferrocenyl group, in many cases, improved the bioactivity. With this in mind and to overcome these limitations, this research is focussed on the synthesis of ferrocenyl chalcones analogous to curcumin from acetyl- and 1,1'-diacetylferrrocene and explore their biological activity toward malaria and some bacterias. The analogous were synthesized in moderate yield and proved to be biologically active. The methodology, characterization, and preliminary results of the bioassays will be discussed.
Factors affecting aggregation of beta-sheets

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In order to better understand the formation of protein structures, small hydrogen bonding amides were synthesized. Hydrogen-deuterium studies and NMR concentration studies were used to probe the effect of structural differences on hydrogen bond strength. These differences include replacing oxygen with sulfur as a H-bond acceptor, changing hydrogen bonded ring size, and the position of the hydrogen bond acceptor on the amide. In addition, the propensity for polypeptides to aggregate was investigated by manipulating the side chains of tri-peptide dimers. The alanine of an effectively neutral hydrogen bonding peptide was replaced with serine in an effort to block the exterior hydrogen bonding face of the dimer. Comparing these mimics to the small molecules that act as controls, we can distinguish what might contribute to more or less robust beta-sheets.

Hydrogen bonding principles and synthetic beta-sheet mimics

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Naturally occurring beta-sheets are a common structural motif appearing in complex biological molecules. The laboratory synthesis of beta-sheet mimics allows us to isolate and probe their intramolecular hydrogen bonding tendencies. We hope to strengthen the next generation of beta-sheet mimics by optimizing rigidity and hydrogen bonding affinity. The premium placed on these structural attributes can provide a layer of difficulty to the synthetic trajectory. Additionally, smaller control molecules were synthesized that exhibit the potential to form intramolecular hydrogen bonds. These smaller molecules allow us to develop a foundational understanding of the same hydrogen bonding principles that are applied in larger molecules, such as our mimic.

Benzyldieneanilines and benzonitrile oxides: Solid-state structure and reactivity studies

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We are using single-crystal X-ray diffraction to examine how molecular structure influences crystal structure and solid-state reactivity. Our focus is on two families of
nitrogenous organic compounds: the benzylideneanilines (R-CH=N-R', R = aryl) and the benzonitrile oxides (R-CN=O, R = aryl). Among the benzylideneanilines we have identified pairs of molecules we have designated bridge-flipped isomers, molecules that differ only in the orientation of a bridge of atoms connecting two major parts of the molecule (R-CH=N-R' vs. R-N=CH-R'). Bridge-flipped isomeric benzylideneanilines that are isomorphous (that assume identical molecular packing arrangements in the solid state) should be capable of solid solution formation over a wide range of component ratios; those that are not isomorphous may be capable of serving as seed crystals that could initiate the growth of a new polymorph of each isomeric compound in the pair. We have been investigating the role of the nitrile (CN) group in defining molecular packing patterns in crystals; its versatility in participating in a range of commonly occurring intermolecular interactions such as halogen-nitrile contacts and C-H…:NC contacts lends it significance in crystal engineering. We have thus prepared and determined the crystal structures of two nitrile-bearing benzylideneanilines: 4'-cyanobenzylidene-2-methylaniline and 2'-cyanobenzylidene-4-cyanoaniline. Although we have not yet obtained crystals of the bridge-flipped isomer of the methyl compound, our previous determination of the crystal structure of the bridge-flipped isomer of the dicyano compound shows that these two are not isomorphous. In contrast, the methyl compound is isomorphous with the corresponding iodo compound but not with the corresponding bromo and chloro compounds. In a parallel investigation, we are investigating the relationship between ring substitution and solid-state reactivity in benzonitrile oxides. To that end, we have prepared 4-bromobenzonitrile oxide and 3-nitrobenzonitrile oxide and have been investigating their potential solid-state dimerization to one of three possible dimers.

CHED 1270

Effects of molecular structure on crystal structure and solid-state reactivity of some nitrogenous organic compounds

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We have been using single-crystal X-ray diffraction to investigate the structures and properties of compounds from two families of nitrogen-containing organic compounds: the benzonitrile oxides (R-CN=O, R = aryl) and the benzylideneanilines (R-CH=N-R', R = aryl). In solution, benzonitrile oxides dimerize to form three possible products: one head-to-head dimer (the furoxan) and two head-to-tail dimers (the dioxadiazine and the oxadiazole-N-oxide). We are examining the course of solid-state dimerization of benzonitrile oxides to determine which dimer is formed in the crystal and whether or not the product of solid-state dimerization can be predicted on the basis of the molecular packing arrangement of the benzonitrile oxide. We are also investigating the possibility that different dimers could be formed from different polymorphs of a given benzonitrile oxide. We have now prepared 4-chlorobenzonitrile oxide and have determined its crystal structure. Our previous work has shown that the solid-state dimerization product is the head-to-head dimer, but the closest intermolecular distances between reactive
sites in this crystal are found to be between inversion-related molecules. This result is consistent with calculations indicating that the transition state leading to the head-to-head dimer is centrosymmetric. We intend to determine how the close intermolecular oxygen-halogen contact we observe in this structure might also occur in the 2- and 3-chloro isomers and influence their solid-state molecular packing and reactivity. In a parallel investigation, we are examining the role of intermolecular contacts involving halogens in establishing the crystal structures of bridge-flipped isomeric benzylideneanilines, isomers related by the reversal of the bridge (R-CH=N-R' vs. R-N=CH-R'). To determine whether close intermolecular contacts of the type X-R-CN:···X-R-CN: occurring in both members of a bridge-flipped pair will encourage their isomorphism (identical packing arrangements), we have prepared and determined the crystal structure of 4'-cyanobenzylidene-2-bromoaniline. In this structure, space-filling considerations apparently dominate, and no nitrile/halogen contacts occur.

CHED 1271

Solid-state structures and reactivity of some nitrogen-containing organic compounds

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We are investigating the solid-state structures and reactivity of two families of nitrogenous organic compounds: the benzylideneanilines (R-CH=N-R', R = aryl) and the benzonitrile oxides (R-CN-·O·, R = aryl). The benzylideneanilines provide examples of pairs of molecules we have designated bridge-flipped isomers, molecules differing only in the orientation of a bridge of atoms connecting two major parts of the molecule (R-CH=N-R' vs. R-N=CH-R'). Bridge-flipped isomers that are isomorphous (possessing identical solid-state molecular packing arrangements) should be capable of forming solid solutions over a wide range of component ratios; bridge-flipped isomers that are not isomorphous may be capable of serving as seed crystals for solutions of the isomeric compound and facilitating its crystallization into a new packing arrangement identical to that of the seed. We have been preparing benzylideneanilines bearing both a halogen substituent and a nitrile substituent to determine whether or not similar Lewis acid-base contacts of the type X-R-CN:···X-R-CN: occurring in both isomers could encourage their isomorphism. To that end, we have prepared 3'-chlorobenzylidene-2-cyanoaniline and are determining its crystal structure by X-ray diffraction. Although we have not yet obtained the crystal structure of its bridge-flipped isomer, we are pursuing that compound and can already compare our current structure with the previously determined bromo analogues. In a parallel investigation, the benzonitrile oxides provide the opportunity to examine the influence of molecular structure on solid-state reactivity. We are determining which of three possible dimers might form in the solid-state dimerization of these compounds and are examining 4-fluorobenzonitrile oxide as part of that study. An additional property of sterically hindered nitrile oxides is their potential rearrangement to isocyanates, so we have prepared the nitrile oxide derivative of
piperonal to determine which route, dimerization or rearrangement, might be followed in a solid-state reaction occurring in this case.

CHED 1272

Structures and reactivity of some nitrogenous organic solids

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Our work is focused on the relationship between molecular structure and crystal structure in organic compounds and its implications for solid-state reactivity. As part of that work, we have been examining two families of nitrogen-containing organic compounds, the benzylideneanilines (R-CH=N-R’, R = aryl) and the benzonitrile oxides (R-CN=O-, R = aryl). We define bridge-flipped isomeric benzylideneanilines as those pairs that differ only in the reversal of the orientation of the imino linkage: R-CH=N-R’ vs. R-N=CH-R’. The relatively small size of the bridge hydrogen atom and the common occurrence of end-for-end disorder of the molecules in benzylideneaniline crystal structures suggest to us that isomorphism (identical solid-state molecular packing arrangements) should be possible for bridge-flipped isomeric benzylideneanilines. We are examining benzylideneanilines substituted with both halogen atoms and nitrile groups to determine whether similar intermolecular X-R-CN:·X-R-CN: Lewis acid-base interactions occurring in both members of a bridge-flipped pair can encourage their isomorphism. We are also preparing bis-benzylideneanilines capable of assuming centrosymmetric molecular conformations to determine whether or not the tendency of centrosymmetric molecules to occupy crystallographic centers of symmetry can encourage isomorphism. Our studies of crystalline benzonitrile oxides concern the solid-state reactivity of these compounds as a function of their ring substitution pattern. Which of three possible solid-state dimers may form and how readily they form are questions being explored. As part of that study, we have begun monitoring the solid-state reactivity of 3-bromobenzonitrile oxide and 4-nitrobenzonitrile oxide by infrared spectroscopy and are pursuing an X-ray crystal structure determination of one of the possible 3-bromobenzonitrile oxide dimers, the bis-(3-bromophenyl)furoxan.

CHED 1273

Synthesis of aziridinomitosene anticancer analogs that vary at the C6/C7 positions

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Mitomycin C (MC) is a naturally occurring anti-cancer therapy that has historically seen extensive use as a treatment for a wide variety of cancer types. However, MC’s utility has been greatly diminished as a result of severe side effects, such as delayed
myelosuppression. We have prepared and studied structurally similar compounds, called aziridinomitosenes (AZMs), that have similar anticancer activity but may be operating by a mechanism different than that of MC. Both MC and AZMs alkylate DNA to form interstrand cross-links (ICLs) that inhibit DNA replication and lead to cell death. In contrast to MC, the AZMs contain electrophilic centers at the C6 and/or C7 positions that are thought to play a role in the observed increased cytotoxicity in a number of cancer cell types. The present study aims to investigate the importance of these sites by preparing analogs that have methyl, ethyl, butyl, phenyl, or benzyl groups at one or both of these positions. The synthesis of each target molecule relies upon the preparation of a 2,5-disubstituted oxazole that is converted to the AZM tetracyclic core via an oxazolium salt/azomethine ylide cycloaddition sequence. To prepare the cycloaddition precursors, readily available 1,2-diols or butyrolactones are converted over a one to three step sequence that generates appropriately substituted esters or lactones. These are subsequently treated with lithiated methyl isocyanide to facilitate oxazole formation. Assembling the remainder of the cycloaddition precursors involves addition to a serine-derived aldehyde, which forms an amino alcohol that is closed to form the required aziridine ring. After this, a lithiated propargyl alcohol is used to install the tethered dipolarophile, which is subjected to the oxazolium salt/azomethine ylide cycloaddition sequence that leads to the final tetracyclic core. Following cycloaddition, oxidation state manipulation and carbamate addition result in the desired AZM analogs. Herein, we will report on our progress to date on all substrates, including steps that have focused on optimization of reactions to form the early stage esters/lactones, intermediate stage cycloadditions, and late stage carbamate installations.

CHED 1274

Developing a synthesis of α-diazoamides

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Carbenes that are stabilized by an anionic β-heteroatom display unique nucleophilic reactivity. While carboxylate carbenes have been synthesized and studied, the analogous amidate carbenes have not yet been realized. This body of research reports a three-step synthetic strategy that allows the synthesis of α-diazoamides, the immediate precursors of amidate carbenes, from acyl cyanides. The development and optimization of this strategy will be reported.

CHED 1275

Transition metal-catalyzed coupling of organic sulfonates and metal azides

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Organic azides are recognized for their usefulness in organic synthesis as well as for their function as energetic compounds. It is perhaps due to this second property that synthetic methods that afford organic azides have seen limited development and can suffer from lower yields. This research project aims to develop a palladium-catalyzed cross-coupling method that allows the mild synthesis of organic azides from vinyl and aryl sulfonates. With the synthesis of four families of sulfonate starting materials, high-throughput screening is used to identify catalysts and conditions that will promote product formation. The development of a starting material library and the results of the reaction screening will be reported.

CHED 1276

Studies toward total synthesis of axinelloside A and its analogs

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Sulfated saccharides mediate a myriad of physiological processes, including primary steps of bacterial and viral pathogenesis, tumor growth and progression, and angiogenesis. Out of the subset of bioactive. A well-studied lipopolysaccharide within this class of saccharides is Axinelloside A. Axinelloside A is a unique target for chemical synthesis due to its distinct structural features, and its potent inhibitory activity against human telomerase (IC$_{50}$ 2 mg/mL). In this communication we will present recent progress toward total synthesis of Axinelloside A and its analogs; specifically, we will discuss the application of dehydrative glycosylation method to preparation of truncated fragments of this highly sulfated lipopolysaccharide and the impact of sulfation on its biological activity.

CHED 1277

Synthesis of core-substituted naphthalene diimide derivatives

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Donor-Acceptor Columnar Liquid Crystals are a combination of electron rich and electron poor aromatics that stack in alternating columns which enhances the π-π stacking and its light absorption. Naphthalene Diimides (NDIs) are planar electron deficient aromatic molecules that exhibit a low-lying LUMO that could be tunable through addition of electron withdrawing groups off of its core. Brominated naphthalene diimides were synthesized and they were then used as intermediates for addition of electron withdrawing groups such as trifluoromethyl group that make them excellent components in Donor-Acceptor Liquid Crystals. This derivative is particularly important due to its low-lying LUMO and is expected to stack similarly to naphthalene diimide due to the size of the fluorine atoms. Further synthesizing core-substituted naphthalene
diimide derivatives is in progress through the addition of various electron withdrawing groups and analyzing their properties.

CHED 1278

Surface orientation analysis of naphthalene diimides using infrared spectroscopy

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The surface orientation of Naphthalene Diimides (NDI) on silicon surfaces is important to understanding the charge transfer that occurs along these semiconducting crystals. The NDI molecule is deposited on the silicon surface and then analyzed using IR Spectroscopy. The polarized ATR IR technique used looks at two different polarized angles that allow us to determine the orientation of the NDI with proficiency. We found that the molecule’s orientation and ordering is dependent on the thickness of the NDI layer deposited on the silicon surface. We also found that the molecule’s orientation changes when heat is applied to the surface. The change in the molecules orientation due to heat is dependent on the thickness of the NDI layer on the silicon crystal. The NDI on the silicon surface can be affected by film thickness and cooling rate. This leads us to believe that the ordering of the NDI is due to the silicon surface driving the orientation of the molecule. Further analysis of the NDI’s surface driven orientation is progressively being tested by using techniques that modify the silicon crystal’s surface.

CHED 1279

Investigations of green and microscale methods in the synthesis of several flavones

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The goal of this investigation was to improve yields in the synthesis of different flavones by controlling both the amount of time spent on the initial esterification as well as the organic solvents. Flavones are a naturally occurring sub group of flavonoids (found in many plant tissues) which are centered on a 2-phenyl-1-benzopyran-4-one backbone. Flavones have been indicated as having possible applications in medicine including anticancer properties, neurogenesis promotion, antimicrobial and antiviral activities. A three step, green synthesis using microscale techniques began with the esterification of 2-hydroxyacetophenone using various benzoyl chlorides, followed by an intramolecular Baker-Venkataraman rearrangement to β-Diketones, and finally an acid catalyzed synthesis producing the flavones. In the esterification reactions of 2-hydroxyacetophenones with the benzoyl chlorides, the amount of time spent on synthesis and recrystallization was varied producing different yields. Results indicate
that these methods improve yields and are suitable for an undergraduate organic second semester lab.

CHED 1280

Computational study on the high temperature isomerization of phenanthrene

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Previous experimental work by Necula and Scott has characterized the isomerization of polycyclic aromatic hydrocarbons (PAHs) under flash vacuum pyrolysis (FVP) conditions.¹ Four mechanisms were proposed for the FVP of phenanthrene, but no one mechanism was deemed favorable. One mechanism describes the simultaneous removal of two bay-region hydrogens, forming a diradical intermediate, and its rearrangements to 1-ethynyl, 2-ethynyl, and 4-ethynylacenaphthylene and pyracylene. This computational study investigates the structures and energies of these species and the proposed intermediates. Key mechanisms include the collapse of the diradical, hydrogen shift/benzene ring contraction rearrangements, 1,2-hydrogen shifts between vinylidene and ethynyl groups, and C-H vinylidene insertions. Relative Gibbs free energies of M06-2X/6-31G* and UM06-2X/6-31G* optimized geometries are compared in order to examine the barrier heights of the mechanistic pathway. The hydrogen shift/benzene ring contraction rearrangements are shown to be degenerate pathways. Additionally, computational evidence reveals the requirement for flexibility of the system in order to undergo these rearrangements, suggesting an increase in barrier heights for larger bay-region PAHs. Results on the diradical and vinylidene mechanisms will be presented. Elucidation of the mechanisms and barrier heights by which bay-region PAHs undergo rearrangements may supplement the synthesis of novel species.


CHED 1281

Antibacterial activity of cefotaxime and terpenes

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Essential oils are aromatic compounds that are found in an array of medicinal plants. Mixtures of these oils contain monoterpenes and sesquiterpenes that have been found to contain antimicrobial activities. It is thought that when placed in the actively releasing portion of an antibiotic, terpenes can increase the effectiveness of that compound. Cephalosporins are powerful antibiotics that have been found to be effective against both Gram-negative and Gram-positive bacteria. We are attempting to substitute
various terpenes for the methyl group of cefotaxime. The antibiotic was first worked up to produce a strong nucleophile. It was then formed into a tosylate before performing the attack on the specific terpenoid. The antimicrobial properties of this compound were tested against cefotaxime alone; the terpene alone; and a combination of both cefotaxime and terpene using Kirby-Bauer disk diffusion testing and minimal inhibitory concentration (MIC) testing. We predict that the newly synthesized compound will have the synergistic effect of both the cefotaxime and the terpene, therefore showing the greatest bacterial resistance.

CHED 1282

Analysis of porphyrin doped thiophene nanoparticles as potential water oxidizing catalysts

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A water soluble porphyrin (M-TPPS$_4$) was doped into conductive polythiophene nanoparticles (M = Mn$^{III}$, Co$^{II}$, or Cu$^{II}$). SEM images and EDS spectroscopy were used to characterize the morphology and success of doping. Cu$^{II}$-TPPS$_4$ doped polymers allow for metal to metal distances to be experimentally determined via electron paramagnetic resonance (EPR) spectroscopy. The Mn$^{III}$-TPPS$_4$ and Co$^{II}$-TPPS$_4$ were studied electrochemically to determine the water oxidizing capability of these polythiophene doped nanoparticles vs polythiophene doped thin films.

CHED 1283

Stabilized copper(I) N,S containing cryptands

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Electron transfer systems that drive photosynthetic respiration involve metalloproteins. Type 1 blue copper proteins are an important group of metalloproteins with redox potentials ranging from +372 mV to +680 mV.$^{1,2}$ The large redox potentials offer insight into the unusually stable Cu$^I$ center.$^2$ Organic macrocycles have been designed to increase the redox potentials with copper and are of current interest within our group. Cryptands L$_2$ and L$_3$ have been synthesized from 14[ane]N$_2$S$_2$ (L$_1$) in adequate yields. The cavity within the cryptand core encapsulates select metals and L$_3$ has been shown to stabilize Cu$^I$ from the initial Cu$^{II}$ oxidation state. Research has been focused on Cu$^{II}$/Cu$^I$ potentials and the rate at which the oxidation states interconvert with L$_3$. Use of X-ray Crystallography, Electron Paramagnetic Resonance (EPR), and Ultra-violet/Visible Spectroscopy will be crucial for the determination of copper potentials and binding modes. This presentation will emphasize the synthetic challenge of L$_2$, L$_3$, and metal-ligand binding.
Adapting a conventional synthesis of dihydrotetrazines to microwave conditions

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A recently acquired organic synthesis microwave instrument has made it possible to adapt several of our undergraduate organic chemistry laboratory experiments to microwave conditions. An experiment for synthesis of 3,6-bis(2-cyanopyridyl)dihydro-1,2,4,5-tetrazine has been a part of our lab curriculum for more than 15 years. Using conventional heating, the initial synthesis of the dihydrotetrazine requires a one hour reflux, followed by workup. In the interest of reducing reaction time as well as introducing state-of-the-art technology to our undergraduates, we have adapted this experiment to use microwave heating. Initial results reveal that the production of very pure dihydrotetrazine products can be obtained (albeit in low yields) with as little as 8 minutes of microwave irradiation. Our efforts to optimize conditions and increase yields and to include other starting materials (such as substituted benzonitriles) is ongoing. This experiment is part of a multi-step sequence illustrating the principles of inverse electron demand Diels-Alder reactions and is a valuable undergraduate learning experience incorporating heterocyclic chemistry and beautiful colors.

CHED 1285

Energy decomposition analysis to predict the explicit solvent shell in the keto-enol tautomerism of acetylacetone in water, acetone, and chloroform
The equilibrium concentration of the diketone and enol tautomer of acetylacetone as a function of solvent is investigated by computational calculations. The percentage of enol at equilibrium is experimentally determined by NMR in a protic polar solvent (water), non-protic polar solvent (acetone), non-protic apolar solvent (chloroform). An explicit solvent study was carried out combining an effective fragment potential with a polarized continuum. The general effective fragment potential (EFP2) method combined with a Monte-Carlo simulated annealing (MC/SA) is to identify minimum energy conformations of solvent-solute interactions. Full geometry optimizations and energy calculations with thermochemical corrections are done using a CPCM/M06-2X density functional with an extended basis. An energy decomposition method is used to predict the minimum number of explicit solvent molecules in this hybrid solvation method. The number of explicit solvent molecules necessary to accurately reproduce the experimental NMR results vary for each solvent.

CHED 1286

Synthesis, characterization, and analysis of diarylidenylpiperidone analogs of curcumin

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This project investigated the synthesis of a more bioactive analogue of the compound curcumin, which is naturally found in the spice turmeric. The challenge of this project was to address both the poor stability and the low solubility of the naturally occurring compound. Research has shown that diarylidenylpiperidone (DAP) compounds are viable analogues of curcumin. A diarylidenylpiperidone ring was used to replace the dicarbonyl moiety of curcumin to make the analogue stable at physiological pH. Attachment of poly(ethylene glycol) substituents to the phenolic hydroxyl groups of vanillin, used as a starting material in the synthesis of the DAP analogue, was attempted to increase aqueous solubility. The significance of this project is to enhance the many medicinal properties associated with curcumin, including uptake by cells to selectively induce apoptosis in cancerous cells. Future research might involve other methods of increasing the solubility of DAP compounds and assaying the efficacy of these compounds in cancerous cell lines.

CHED 1287

Effect of aromaticity on the stability of isonitriles prepared from the deprotonation/metalation of oxazolic species
Isonitriles, or isocyanides, are useful synthons in pharmaceutical synthesis through multicomponent reactions such as the Ugi and Passerini reactions because they provide a facile route to medicinal compounds such as lidocaine, bicyclomycin, and penicillin. Unfortunately, isonitriles have limited availability and stability, making them less attractive precursors. However, recent work on isonitriles has uncovered a new route to their synthesis through the deprotonation/metalation of oxazolic species at the C-2 position. This process produces an equilibrium between an open ring dianion (the isonitrile and a negatively charged oxygen atom) and a closed ring anion (where the negative charge is located at the C-2 position). The open ring dianion can be favored by running the reaction at -78°C. From there, the isonitrile product can be recovered by the coupling of an electrophile (i.e. benzoyl chloride, chlorotrimethylsilane, or iodomethane) to the negatively charged oxygen atom. The objective of this research is to further explore the relationship between the aromaticity of oxazolic species and isonitrile stability by comparing the isonitriles prepared from benzoxazole, oxazole, and 4,4-dimethyloxazoline. The effect of the electrophiles on the yields of the isonitrile compounds for each oxazolic specie will also be presented. The synthesized isonitriles will be purified by recrystallization and column chromatography and then characterized using FT-IR, NMR (1H and 13C), and MS. These techniques will confirm the success of the reactions by determining the isonitrile product yields and identities of any side products that may have formed by pathways competing with the isonitrile syntheses. It is anticipated that the more aromatic oxazolic species will produce higher isonitrile yields and have longer shelf-lives due to the general stability of aromatic over non-aromatic compounds.

CHED 1288

Synthesis of β-fluoroamines from alkenes

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Previously we have demonstrated that β-fluoroamides can successfully be synthesized from a variety of alkenes with the use of Selectfluor™ and anhydrous acetonitrile through an electrophilic fluorination process. A continuation of this project has been the reduction the β-fluoroamides to β-fluoroamines. A reduction process using trimethylsilyl chloride and LiAlH₄ has afforded the desired β-fluoroamines. Additional reduction protocols have also been explored. Spectroscopic data supports the formation of this class of compounds. In addition to being interesting building blocks, this class of compounds is of potential interest in the area of biomedical applications.

CHED 1289
Synthesis and characterization of potential polyol antifreeze coatings on glass substrates

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Petroleum companies have an invested interest in the prevention of gas hydrate formation within their pipelines, as gas hydrates cause significant problems in the production of natural gas and oil. Thermodynamic inhibitors of gas hydrates behave colligatively and are already used in large quantities, thus requiring the costly recycling of materials. A durable kinetic inhibitor acting non-colligatively and bonded to the surface would be a cost effective means of preventing gas hydrate formation. In nature the mealworm (Tenebrio molitor) produces a protein that is natural kinetic inhibitor of ice formation in order to protect the worm from frost damage. Using mealworm antifreeze protein as a model, we hypothesized that a designed polyol covalently attached to a glass surface could interfere with ice formation under freezing conditions in the same manner as the protein. The synthesis and characterization of the polyols, as well as their attachment to glass surfaces will be presented. A variation in the contact angles provided supporting evidence that the glass surfaces were indeed modified. We will also present our efforts to characterize the antifreeze behavior of the modified surfaces under frosting conditions in a designed experimental apparatus. This is a first step in designing polyol surfaces capable of gas hydrate inhibition in petroleum pipelines.

CHED 1290

Analogs for blue copper protein: Thio-pendant arm derivative of 9[ane]S$_2$N

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The mixed-donor ligand 9[ane]S$_2$N has been shown to dimerize upon coordination with Cu$^{II}$. Due to the ligand dimerization, it exhibits an irreversible Cu$^{II}$/Cu$^{I}$ reduction. Functionalization through use of a thiolate pendant arm L is currently being explored to prevent the dimerization and stabilize Cu$^{I}$. By increasing the redox potential, these ligands can now act as analogs to an important class of metalloproteins known as the Type I Blue Copper Proteins.

References
Role of acetic acid in kinetic isotope effects observed in Pd(iPr)(OAc)$_2$(H$_2$O) catalyzed oxidation of alcohols

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Oxidation reactions are one of the most commonly used reactions in organic synthesis. A palladium catalyst, Pd(iPr)(OAc)$_2$(H$_2$O), has been shown to be a successful catalyst in high yielding oxidations of alcohols, specifically primary and secondary benzylic, allylic and aliphatic substrates to aldehydes and ketones. A mechanism for this catalytic system has been proposed to include alcohol oxidation through the β-hydride elimination and the regeneration of the Pd catalyst through oxygenation by O$_2$ and protonation from acetic acid. During the course of these prior investigations, kinetic isotope effect (KIE) experiments showed that the KIE value increased with increased concentration of additive acetic acid without reaching an asymptote. The highest reported KIE for the oxidation of sec-phenethyl alcohol in this system is 5.4, whereas other palladium catalytic systems report KIE values below 2.0. The uncharacteristically high observed KIE values for the breaking of the C-H(D) bond in this Pd(NHC) system and the changing KIE values with increasing [HOAc] merit further experimental study into the role of additive acetic acid in Pd-(NHC)-catalyzed aerobic oxidation of alcohols.
Investigation of the role of Hagemann’s ester as a catalyst for natural product synthesis

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The Hagemann’s ester is a tool for natural product synthesis. The capability of synthesizing natural products with the use of a non-metal catalyst has been a cause to further research the ester. The reaction mechanism for synthesizing Hagemann’s ester has been investigated and the synthesis was found to depend on the amine used, along with the addition of a strong base. The ester was then investigated to determine successful use in the synthesis of a highly substituted analine with a non-metal catalyst, in a one-pot organocatalytic reaction. A high yield of C-3 alkylation onto the product was anticipated. The catalyst researched was pyrrolidine, and the primary reactant researched was nitrosobenzene.

CHED 1293

Synthesis of symmetric and asymmetric porphyrins

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Porphyrinic macrocycles are a class of red and purple pigments that consist of a substituted aromatic macrocyclic ring. Current investigations involve both the synthesis of symmetric and asymmetric porphyrins as well as their complexation to metals. While both have the ability to absorb visible light, the ability of asymmetric porphyrins with an incorporated tether to attach to TiO\textsubscript{2} nanoparticle films has made them attractive as potential dyes for dye-sensitized solar cells. The isolation and characterization of the symmetric and asymmetric porphyrins will be presented. The performance of the dye-sensitized solar cells with the asymmetric porphyrin products may also be discussed.

CHED 1294

Synthesis and properties of donor-pi-acceptor polyene dyes with azacycloalkane donors

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In this study, azacycloalkane donors in donor-pi-acceptor (D-pi-A) polyene dyes were used to determine structure-photophysical property relationships. Here we report the synthesis and properties of dyes 1a-d containing azacycloalkanes with a variety of
geometries at nitrogen. Microwave irradiation of dihaloalkanes and 4-bromoaniline resulted in 1-(4-bromophenyl)-azacycloalkanes. Lithium-halogen exchange of the bromides, followed by reaction with 5-(N,N-diethyl)pentadienal, gave 1-(4-azacycloalkylphenyl)-2,4-pentadienals. Knoevenagel condensation of the aldehydes with 1,3-diethyl thiobarbituric acid produced 1a-d. The UV and NMR solvatochromic properties of dyes 1a-d were compared to compounds with related aromatic amine donor groups.

CHED 1295

Synthesis of secondary amines

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The goal of this research was to synthesize secondary amines with other functional groups or steric bulk near the nitrogen atom. The relative rate of reaction with an isocyanate can then be measured and the effect of the nearby groups determined. The amines were made using two synthetic strategies, either a Michael addition or a reductive amination. When utilizing a reductive amination, the common reducing agent sodium triacetoxyborohydride was used and found to work well even in the presence of esters. In the compounds where esters were present after the amine was synthesized the esters were converted cleanly and efficiently to amides using a catalytic amount of triazabicyclodecene (TBD) in a microwave reactor. The relative rates of reaction of the amines with an isocyanate were then measured by competitive experiments using 1H NMR.

CHED 1296

Template-catalyzed polymerization of modified DNA nucleosides

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Template-directed polymerization is a unique mechanistic process that occurs during translation and transcription in biological systems. These reactions typically require physiological enzymes to produce reaction conditions that are favorable to polymerization. Investigations of alternative backbones and polymerization pathways to the traditional phosphodiester bond formation may make it possible to understand the origins of DNA and more efficient processes for creating biosynthetic polymers. Reductive amination has been suggested as a possible mechanistic alternative. In order to investigate this possibility the DNA monomers must first be modified to include a 5´-amine and a 3´-acetaldehyde. Our current research is focused on the modification of the adenosine monomer. This eleven-step synthetic process will be completed before the end of this academic year. Once completed, the modified adenosine monomer will be used in polymerization studies of homo-block polymers. The modified adenosine monomer will eventually be used in studies on hetero-block polymers after successful modification of the other three DNA monomers.

CHED 1297

Synthesis and experimental and computational analysis of curcumin derivatives and their difluoroboron complexes

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Curcumin, a derivative of the spice turmeric, is a fluorescent compound and therefore has the potential of being used for tumor imaging and photodynamic therapy. Alternative derivatives of curcumin are in high demand to obtain a compound with a long $\lambda_{\text{max}}$ absorbance value. A longer $\lambda_{\text{max}}$ (redshift) increases the effectiveness of skin penetration of the compound allowing for enhanced tumor imaging. Six compounds (CR2-7) with various substituents on the aromatic rings were synthesized along with their difluoroboron complexes (CR-BF2, CA2-7-BF2). All compounds were characterized by IR and NMR. Their photophysical properties were assessed using UV-Vis and fluorescence spectroscopy. Computational analysis was also done using the program Gaussian09 to obtain the optical properties. The derivative wavelengths ranged from 390-430 nm, while the BF2 analogs ranged from 400-500 nm. The high amount of conjugation and the strong electron donating groups located on the aromatic rings allowed the curcumin derivatives to experience a redshift of absorption. Continued analysis of these compounds can be done to determine if they are suitable compounds for tumor therapy uses.
Concerted nature of isocyanate reactions with alkenes

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Chlorosulfonyl isocyanate (CSI) is the most reactive isocyanate and it reacts with alkenes to give N-chlorosulfonyl-beta-lactams that are readily reduced to beta-lactams. Beta-Lactams are a class of antibiotics. CSI was found to react with alkenes via a Single Electron (SET) pathway. However, the mechanism changes to a concerted pathway for reaction of CSI with monofluoroalkenes that have ionization potential O=C=N-X CSI: X=-SO₂Cl Tosyl isocyanate: X= -SO₂-C₆H₄-CH₃ Trichloromethyl isocyanate: X= -CCl₃

values greater than 8.9 eV. Quantum chemical calculations show that the nature of the transition state becomes more concerted as the isocyanate substituent (X) becomes less electron-withdrawing. In this study we use the radical trap reagent TEMPO to probe the concerted nature of less reactive isocyanates like p-Toluenesulfonyl isocyanate (X = -SO₂-C₆H₄-CH₃) and Trichloromethyl isocyanate (X = -CCl₃).

Cu(I)-complexes as photoredox catalysts: An alternative to Ru(bpy)₃²⁺
The field of organic photochemistry has witnessed a recent expansion with the development of Ru(bpy)$_3^{2+}$-catalyzed photoredox reactions. This complex absorbs light and undergoes metal-to-ligand-charge-transfer (MLCT), generating a charge-separated excited state intermediate that can act as a single-electron transfer (SET) catalyst in redox reactions. Ru(bpy)$_3^{2+}$ and its analogs have been applied to a wide variety of redox reactions in organic syntheses. However, the Ru(bpy)$_3^{2+}$ complex is not without its drawbacks. Ruthenium and iridium, another metal commonly used in photoredox catalysts, are precious metals, which dramatically increases the price of the complexes and both have a level of toxicity, making them somewhat unsafe. This research project focuses on Cu(I)-complexes as cheaper, safer, and more environmentally friendly alternatives to Ru(bpy)$_3^{2+}$ in photoredox reactions. A library of homoleptic and heteroleptic Cu(I)-complexes using substituted-phenanthroline and phosphine ligands has been synthesized and screened in a model reaction, the reduction of 2-bromoacetophenone to acetophenone. The goal is to continue to expand this library in an attempt to find a photoredox catalyst that can compete with Ru(bpy)$_3^{2+}$.

CHED 1300

Synthesis and analysis of a series of N-acetyl D-glucosamine derivatives as organogelators

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Low molecular weight gelators are interesting small molecules with potential applications as advanced materials. Carbohydrate based small molecular gelators are especially useful since they can be obtained from renewable resources. We are interested in understanding the structure and gelation relationship for monosaccharide derivatives. Previously, various 4,6-benzylidene acetal protected alpha-methyl D-glucosamine derivatives have been found to be effective low molecular weight gelators. In order to study the effect of the 4,6-benzylidene acetal functional group and probe the requirement for gelation, we synthesized and analyzed a new series of analogs in which the phenyl group is replaced by a benzyl group. This can allow us to probe the effect of the aromatic group towards the self-assembling behavior and the presence of CH-pi interaction. In this presentation, the synthesis and characterization of the amide and urea derivatives of glucosamine modified with the new 4,6 acetal protecting group will be discussed.

CHED 1301

Synthesis and characterization of glucose triazole derivatives as organogelators
Low molecular weight gelators (LMWGs) have gained much attention over the last few decades. These small molecules can self-assemble in organic solvents or water and form reversible organogels or hydrogels. The gels have been studied for a variety of applications, including drug delivery and tissue engineering. Among the different classes of small molecular gelators, carbohydrate derivatives have certain advantages since they can be synthesized from naturally abundant renewable resources. Our lab has been working on the functionalization of readily available monosaccharide starting materials to obtain advanced functional materials. Several classes of glucose and glucosamine derivatives have been found to be effective LMWGs. In this research, we have studied the effect of introducing a triazole functional group to the monosaccharide derivatives. A series of glucose triazole derivatives have been synthesized and their gelation properties screened. Several new small molecule gelators are obtained. The synthesis and characterization of these glucose based LMWGs will be presented.

CHED 1302

Self-healing polymers: Studies of the Diels-Alder reaction between furan and N-4-fluorophenylmaleimide

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Stimuli-triggered self-healing polymers have the ability to repair a material. The most generally applicable external stimuli are light and heat. The Diels-Alder reaction has been used for many materials chemistry applications in which a thermo-reversible linkage is needed. By incorporating Diels-Alder cycloadducts within a polymer, sites for self-healing can be created throughout the material. While this approach is not new, there is still room for the development of new chemistries and for detailed fundamental exploration of the kinetics and thermodynamics of the reversible adduct-forming process. This paper will report a study of the reaction of N-4-fluorophenylmaleimide and furan using ¹⁹F NMR to follow reaction progress and various chromatographic techniques to separate the reaction products.

CHED 1303

Self-healing polymers: Synthesis of highly-fluorinated dienes and their model Diels-Alder reactions

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The Diels-Alder (DA) reaction has been the subject of renewed interest in the field of self-healing polymers because the DA reaction can be thermo-reversible within a moderate temperature window. This research focuses on the synthesis of highly-fluorinated dienes for use in the Diels-Alder reaction. Nucleophilic substitution reactions of furfuryl alcohol with decafluorobiphenyl under basic conditions afforded either 1-(furanmethoxy)nonafluorobiphenyl in a 62% yield or 4,4′-bis(furanmethoxy)octafluorobiphenyl in a 78% yield, depending on the reactant stoichiometry and reaction conditions. Diels-Alder reactions of these dienes with N-4-fluorophenylmaleimide were studied as models for the synthesis of linear DA polymers based on bis(maleimide) monomers. Reaction products were purified using chromatographic methods and characterized using $^1$H and $^{19}$F NMR spectroscopy.

CHED 1304

Synthesis of resveratrol

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A synthesis of the phytoalexin resveratrol was undertaken starting with 2 aldehydes, 4-hydroxybenzaldehyde and 3,5-dihydroxybenzaldehyde. The hydroxyl groups on each aldehyde were protected as methoxymethyl ether (MOM) protecting groups giving compounds 2 and 4. Titanium chloride mediated coupling was then used to produce fully protected resveratrol 5. The MOM protecting groups were removed using dilute acid to give resveratrol.

CHED 1305

Synthesis of 5- and 6-(4-fluorophenyl)-N-acetylgluoxylamides

Nickie Ngo¹, ngonn@hendrix.edu, Aline Umhire-Juru¹, Stephanie Hernandez¹, Linda Desrochers¹, Naresh Kumar², David Black², Thomas E. Goodwin¹. (1) Hendrix College, Conway, Arkansas, United States (2) Chemistry, University of New South Wales, Sydney, New South Wales, Australia
Cheah et al. have reported the synthesis of antibacterial peptidomimetics via ring opening of \( N \)-acylisatins with amino acid methyl esters (or methyl esters of di- and tri-peptides) to produce glyoxylamides (\textit{Tetrahedron Lett.} \textbf{2008}, 49, 2965-2968; \textit{Tetrahedron} \textbf{2011}, 67, 7603-7610). \( N \)-Acylisatins are more reactive in this manner than are the corresponding isatins themselves as the C2 carbonyl moiety of the former behaves as an imide carbonyl as opposed to the conventional amide carbonyl of the latter. We are using Suzuki-derived 5- and 6-(4-fluorophenyl)-\( N \)-acylisatins and a variety of amino acid methyl esters to prepare new mono-glyoxylamide peptidomimetics for antibacterial assays.

**CHED 1306**

**Synthesis of 5- and 6-(4-methoxyphenyl)-\( N \)-acetylglyoxylamides**

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Cheah et al. have reported the synthesis of antibacterial peptidomimetics via ring opening of \( N \)-acylisatins with amino acid methyl esters (or methyl esters of di- and tri-peptides) to produce glyoxylamides (\textit{Tetrahedron Lett.} \textbf{2008}, 49, 2965-2968; \textit{Tetrahedron} \textbf{2011}, 67, 7603-7610). \( N \)-Acylisatins are more reactive in this manner than are the corresponding isatins themselves as the C2 carbonyl moiety of the former behaves as an imide carbonyl as opposed to the conventional amide carbonyl of the latter. We are using Suzuki-derived 5- and 6-(4-methoxyphenyl)-\( N \)-acylisatins and a variety of amino acid methyl esters to prepare new mono-glyoxylamide peptidomimetics.

**CHED 1307**

**Synthesis of aspartame \( N \)-acetylglyoxylamides: A sweet reaction**

\textbf{Stephanie Hernandez}\textsuperscript{1}, \texttt{hernandezsv@hendrix.edu}, \textbf{Aline Umhire-Juru}\textsuperscript{1}, \textbf{Linda Desrochers}\textsuperscript{2}, \textbf{Naresh Kumar}\textsuperscript{3}, \textbf{David Black}\textsuperscript{4}, \textbf{Thomas E. Goodwin}\textsuperscript{1}. (1) Chemistry, Hendrix College, Conway, Arkansas, United States (3) Chemistry, University of New South Wales, Sydney, New South Wales, Australia (4) Chemistry, University of New South Wales, Sydney, New South Wales, Australia

Cheah et al. have reported the synthesis of antibacterial peptidomimetics via ring opening of \( N \)-acylisatins with amino acid methyl esters (or methyl esters of di- and tri-peptides) to produce glyoxylamides (\textit{Tetrahedron Lett.} \textbf{2008}, 49, 2965-2968; \textit{Tetrahedron} \textbf{2011}, 67, 7603-7610). \( N \)-Acylisatins are more reactive in this manner than are the corresponding isatins themselves as the C2 carbonyl moiety of the former behaves as an imide carbonyl as opposed to the conventional amide carbonyl of the
latter. We are reacting a variety of $N$-acetylisatins with aspartame to prepare a new set of glyoxylamide peptidomimetics for antibacterial assays.

CHED 1308

Green synthesis of spiropyrrrolizidines from isatin, proline, and $E$-4-phenylbut-3-en-2-ones

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We are developing an experiment for the organic chemistry laboratory by adapting a literature procedure (K. Revathy and A. Lalitha, RSC Adv. 2014, 4, 279-285) that involves the concerted, suprafacial, [4S + 2S] cycloaddition of an azomethine ylide with a chalcone. We replace the chalcone with an $E$-4-phenylbut-3-en-2-one to simplify the NMR spectra. An azomethine ylide is generated in situ via the decarboxylation of an iminium ion formed from the reaction of proline and isatin. The product of this three-component condensation is a spiropyrrrolizidine. We are exploring options for speeding up the reaction while still using green chemistry, for example using microwave energy. Spiropyrrrolizidines have been found to have anti-cancer and anti-bacterial properties.

CHED 1309

Enantioselective synthesis and characterization of phase 1 warfarin metabolites

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Coumadin (warfarin) is an anticoagulation drug for the treatment and/or prevention of thromboembolic events. Maintaining an optimal drug dose is challenging due to high inter-individual variability in patient response and a narrow therapeutic range. We use warfarin metabolite profiles from patients to improve understanding of the link between metabolism and treatment response. Phase 1 metabolism produces a variety of hydroxywarfarins which are converted to their glucuronide derivatives in Phase 2. We have prepared 6-, 7-, and 4'-hydroxywarfarins with ee >99% via an enantioselective, catalytic coupling. Borohydride reduction of the S-warfarin carbonyl produces two diastereomers, as does that of R-warfarin. These “warfarin alcohols” are also produced in vivo. We have separated the four enantiomers via TLC. Taken together, these efforts provide a simple and effective route to generate critical enantiomeric standards for identifying biomarkers to help predict patient Coumadin dose-responses.

CHED 1310

Synthesis of 5- and 6-(4-trifluoromethylphenyl)-$N$-acetylglyoxylamides
Cheah et al. have reported the synthesis of antibacterial peptidomimetics via ring opening of \( N \)-acylisatins with amino acid methyl esters (or methyl esters of di- and tri-peptides) to produce glyoxylamides (\textit{Tetrahedron Lett.} \textbf{2008}, \textit{49}, 2965-2968; \textit{Tetrahedron} \textbf{2011}, \textit{67}, 7603-7610). \( N \)-Acylisatins are more reactive in this manner than are the corresponding isatins themselves as the C2 carbonyl moiety of the former behaves as an imide carbonyl as opposed to the conventional amide carbonyl of the latter. We are using Suzuki-derived 5- and 6-(4-trifluoromethylphenyl)-\( N \)-acylisatins and a variety of amino acid methyl esters to prepare new mono-glyoxylamide peptidomimetics for antibacterial assays.

CHED 1311

Salt formation of potential acetylcholine esterase inhibitors

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Several compounds (in the free base form) with potential acetylcholine esterase inhibitory effects have been previously synthesized. These compounds were converted into salts in order to make them water-soluble and in an attempt to resolve enantiomers present in a racemic mixture of one of the compounds. Hydrochloride salts were prepared by dissolving the free base in sufficient volume of 0.5 M HCl in anhydrous isopropanol to contain 1.5-2 equivalents of HCl, chilling the solutions to maximize precipitation of the salt, and collecting the salt by pressure filtration under argon. Several of these compounds have more than one amine group that could be protonated. The number of equivalents of hydrochloric acid present in each compound was verified by potentiometric titration with sodium hydroxide. Attempts are currently being made to prepare salts of the chiral compounds with different stereoisomers of tartaric acid and dibenzoyl tartaric acid. Salts (and filtrates) were analyzed by \(^1\)H-NMR and HPLC.

CHED 1312

Design and synthesis of potential acetylcholine esterase inhibitors

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Acetylcholine esterase inhibitors currently have a number of medical applications, including symptomatic treatment of cognitive impairments. We report the preparation of a series of compounds (1-5) we hope will show promise as acetylcholine esterase inhibitors. Each compound was prepared starting with ethyl nipecotate or ethyl isonipecotate. Following N-benzylation with benzyl chloride, each ester was first hydrolyzed under basic conditions and then converted to the acid chloride using thionyl chloride. The acid chloride was then coupled with a variety of amines. Reduction of the resulting amide functional group produces an additional analog.

![Chemical structures](image)

**CHED 1313**

**Preliminary testing of N-benzyl isonipecotate derivatives as a potential acetylcholine esterase inhibitors**

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Neurodegenerative disorders such as Alzheimer’s disease are characterized by lower levels of acetylcholine in the brain. Acetylcholine esterase inhibitor drugs are used to mitigate cognitive decline by stabilizing acetylcholine levels. In this research, several new structurally similar compounds have been synthesized by the coupling of N-benzyl isonipecotate with a variety of amines. Analysis of the hydrochloride salts of these compounds is being conducted using the regenerating model system *Lumbriculus variegatus*. Acetylcholine esterase inhibition is being evaluated using the Ellman test, which measures the 5-thio-2-nitrobenzoate produced in the secondary reaction between thiocholine and dithiobis-nitrobenzoic acid.
Molecular docking of isoform-selective histone deacetylase 2 (HDAC2) inhibitors

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Histone deacetylase inhibitors triggers cell growth arrest, differentiation, and/or apoptosis in various cancers such as lung, prostate, breast and bladder. Molecular docking predicts the most likely conformation of ligands in a receptor binding site and thereby identifies key intermolecular interactions. They also provide a numerical measure for the binding affinity of a ligand, and can therefore predict the potency of a compound. In this study, a series of small molecules based on a marine natural product was designed and docked into histone deacetylase 2 (HDAC2) active site in order to identify potent inhibitors. These compounds were also docked into other histone deacetylase isomers to evaluate their selectivity. The docking results were used to guide the synthesis and optimization of these HDAC2 inhibitors.

Kinetic control mechanism: 1,2 vs. 1,4 addition in conjugated dienes

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Organic Chemistry textbooks have long used the addition of HBr to 1,3-butadiene as a classic example of kinetic vs. thermodynamic control. At high temperatures the thermodynamically favorable 1,4-addition product predominates. At low temperatures, the less stable 1,2-addition product predominates. The traditional explanation for this is that the activation energy of the 1,2-addition is lower, thus its rate is faster. Some texts, citing a 1979 experiment by Eric Nordlander, are stating that the real reason is what is being called a proximity effect. We are currently charting and will report on the movement towards this explanation in textbooks. In an attempt to better our understanding of this reaction, we are currently studying the addition of HBr to simple alkene systems, such as hexene, and 2,5-dimethyl-2,4-hexadiene. The hexene substrate studies are being conducted to help maximize product yield for the addition of HBr across a double bond. Coupled with this effort, the 2,5-dimethyl-2,4-hexadiene substrate moves the greater charge to carbon 4, allowing us to see if that charge plays a significant role in the determination of product ratios.

Use of dimethoxymethane in place of chloromethyl methyl ether to prepare methoxymethyl (MOM) esters
Chloromethyl methyl ether (CMME), a known carcinogen, is commonly used as a protecting group to produce the methoxymethyl (MOM) ester from a carboxylic acid. We investigated the use of dimethoxymethane (DMM) in place of CMME as a more green and cost effective way to produce the MOM ester. It is known that DMM may be used to make the MOM ethers, but we investigated it as a way to make the MOM ester instead. DMM and several catalytic Lewis acids were investigated to optimize the process.

Isonitriles have been investigated as ligands in the iron-catalyzed cross-coupling of N-aryl chlorides with secondary alkyl Grignard reagents. These reactions fail in the absence of ligands, but can be successful in the presence of isonitriles. The use of acyclic secondary alkyl Grignard reagents can result in the formation of some isomeric products in addition to the desired product. This is presumably due to the occurrence of reversible β-hydrogen elimination.

Role of dialkylmagnesium species in the cobalt-catalyzed Kumada coupling of aryl bromides

Research in our group has demonstrated that dialkylmagnesium species are responsible for the observed cross-coupling of aryl bromides with alkyl Grignard reagents catalyzed by cobalt N-heterocyclic carbene complexes. This knowledge has allowed us to find conditions in which reaction times can be shortened and yields improved over those in previous reports.
CHED 1319

Synthesis of NHC ligands for use in iron- and cobalt-catalyzed cross-coupling reactions

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A variety of N-heterocyclic carbene (NHC) ligands have been synthesized using modifications of known procedures. These ligands will be used to test the electronic effects of the NHC ligands in iron- and cobalt-catalyzed Kumada couplings. In addition, solid supported NHC ligands to be used in heterogeneous catalysis have also been synthesized.

CHED 1320

Synthesis of (-)-duryne and homologues

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(-)-Duryne and its homologues (B, C, D, E, and F) are cytotoxic acetylenes that are naturally occurring enynols isolated from the marine sponge *Petrosia* sp. These six linear terminal acetylenes' structures have been elucidated by NMR and FABMS analyses. These (-)-durynes were shown to have cytotoxic activity towards HeLa cells as well as inhibiting growth of several tumor line cells. Even though both (-) and (+)-duryne has been synthesized, we will present a new synthetic scheme that allows for a convergent synthesis of (-)-duryne and its five homologues.

CHED 1321

Microwave synthesis of *N*-phenyl succinimides and malenamides in undergraduate organic chemistry laboratory
Finding new and cleaner method to synthesize complex functional groups has become economically viable due to the increased environmental regulations and cost of research. N-Phenyl succinimide and malenamide derivatives have been shown to be significant anti-microbials and insecticides so they are vital to a sustainable society. This works to explore the steric and electronic variablities of the aniline while exploring the scope of the electrophile, succinic or maleic anhydride. Interestingly when maleic anhydride was used as the electrophile, hydration of the alkene provided hydroxysuccinimide product upon isolation. Isolation of the product from the water and ethanol provides cheap and environmentally friendly method of purification. All this work was done by microwave irradiation in 10 minutes versus traditional methods of heating 8-10 hours.

CHED 1322

Synthesis and characterization of furan-based ligands for use in lactide polymerization

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5-Methylfurfural, which can be synthesized from biomass-derived carbohydrates, was combined with 2,6-alkyl disubstituted anilines via reductive amination with NaBH₄ to make a series of small molecules for use as ligands. These ligands were added to tetrakisdimethylamidozirconium via a substitution reaction in toluene in an inert atmosphere. These zirconium complexes were then used to catalyze the polymerization of lactide. The ligands were produced in yields ranging from 50-90%, and the polymerization reactions provided polymers with yields ranging from 20-40% with molecular weights of approximately 5000 g/mol.

CHED 1323

Determination and use of diazonium ions for the presumptive testing of narcotics containing an activated aromatic ring

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Azo dyes, while commonly used commercially, are not often used in the field of forensic science. Azo dyes are produced through a chemical reaction where a diazonium ion is formed from an aromatic amine and then coupled with another activated aromatic compound. Narcotics typically contain rings in their structures with both activating and
deactivating groups attached and may be able to react with the diazonium ion to produce a colored azo dye. This reaction could prove to be useful in the presumptive identification of various narcotics. While there are a myriad of presumptive narcotic tests available, many of the reagents involved are only useful in detecting a small number of narcotics. It is the goal of this research to determine if diazonium ions can be used to presumptively identify multiple narcotics based on colorimetric properties of the dye produced. To produce the diazonium ions, a polymer bead support was used, resulting in low waste generation and a rapid diazonium formation. The produced solution was then reacted in small amounts with various narcotics to induce azo coupling. The reactions have so far produced similar yellow colors and precipitates of different intensities. It was determined that the uniform yellow color may be due to a reaction of the diazonium with the sodium hydroxide that is being used to deprotonate the narcotics during the coupling reaction. Further study is being completed to determine the effect that the solvents used in the reaction and the order of the reaction steps may have on the reaction.

CHED 1324

Caged phosphates in organic molecules

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Phosphates are an important functional group in organic molecules that have many biological and pharmaceutical applications, and thus methods to study this important functional group are needed. One method involves caging the phosphate, which places the phosphate in an inactive state by adding a particular group of atoms to the molecule. The active phosphate can then be released at a specific location and time, in test tubes or cellular studies, by excitation with light. In order to synthesize caged phosphates, caged phosphorylating reagents are needed. Our lab has previously demonstrated that pyrophosphates are effective phosphorylating agents under Lewis acid catalysis. Pyrophosphates can be synthesized from precursor alcohols in two steps via either a phosphate or phosphite. We are currently examining pyrophosphates based on 2-nitrophenyl and coumarin scaffolds. In the future, these caged phosphorylating reagents will then be tested in phosphorylations and uncaging experiments.

CHED 1325

Catalytic asymmetric monophosphorylation of diols

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Our project focuses on the chemical synthesis of phosphorylated molecules, such as FTY720-phosphate. The immunosuppressant drug FTY720 (Fingolimod) is a diol that is enzymatically phosphorylated in vivo to form (S)-FTY720-phosphate. We have
previously developed a method for the Lewis acid catalyzed mono-phosphorylation of diols, including a model compound for FTY720-phosphate. We are currently developing chiral Lewis acid catalysts for this phosphorylation reaction. Chiral catalysts, like enzymes, can provide the asymmetry necessary for phosphorylation of only the pro-(S) alcohol of FTY720. We are currently studying methods to attach chiral ligands to the Lewis acid and screening these catalysts for enantioselectivity.

CHED 1326

Synthesis of an amine-containing cyclooctyne via an intramolecular Nicholas reaction and subsequent dipolar cycloaddition with benzyl azide

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Cyclooctynes have been identified as imaging probes to perform bioorthogonal reactions with azides for in vivo imaging experiments. Bioorthogonal reactions refer to chemical reactions that occur selectively between abiotic functional groups in biological system without interacting with the chemistry of life. We have successfully prepared amine-containing cyclooctyne from commercially available 5-hexynol via an eight-step sequence, including acetylide addition to an aldehyde, Mitsunobu reaction and intramolecular Nicholas reaction. Our ongoing investigation is performing the azide-alkyne reaction between the amine-containing cyclooctyne and azide substrates.

CHED 1327

Evaluation of copper photocatalysts in the enantioselective α-alkylation of aldehydes

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Photoredox catalysis has recently emerged as an effective strategy for the synthesis of new compounds. In such reactions, a catalyst absorbs light to reach an excited state, and then initiates an electron transfer reaction. Most existing reports of this technique have used ruthenium or iridium catalysts; however, these metals are high in both price and toxicity, and thus we aim to develop more sustainable alternatives. We have
hypothesized that copper could be utilized as a replacement, as it is earth-abundant, safe, and relatively inexpensive. Furthermore, copper complexes are known with photophysical properties similar to the ruthenium photoredox catalyst Ru(bpy)$_3$Cl$_2$. This promise has led us to evaluate the use of copper complexes as catalysts in photoredox reactions. Specifically, we are focusing on the use of bis(phenanthroline) copper(I) derivatives as catalysts in the enantioselective $\alpha$-alkylation of aldehydes – a reaction that also uses a chiral catalyst to control facial selectivity. In the course of this investigation, we have tested a number of copper(I) complexes under a range of reaction conditions. Our results suggest that ligand substitution has a significant effect on reactant conversion and product yield. During this presentation, we will share data from specific trials, show how yield was affected by a variety of factors, and provide an analysis of these complexes in comparison to conventional photocatalysts.

CHED 1328

$\gamma$-Cyclodextrin mediated photoheterodimerization between cinnamic acids and coumarins

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Steering photochemistry of alkenes towards photodimerization over the facile isomerization pathway is pursued for its potential in applied chemistry. $\gamma$-Cyclodextrin (g-CD), a macrocyclic host composed of eight glucose units capable of simultaneously accommodating two aromatic alkenes, has been employed in the past to effect photodimerization of alkenes in the solid state and solution phases. This strategy has been employed to achieve high yields of photodimerization between identical alkenes (homodimerization); this has not been demonstrated for non-identical alkenes (heterodimerization). We have demonstrated that weak stabilizing interactions between non-identical alkenes could be utilized to direct photo-heterodimerization. The inclusion complex between g-CD and alkene pairs with complementary electronic and steric properties resulted in higher proportion of the 1:1:1 (hetero-) complex than the 1:2 (homo-) complex. Irradiation of the complexes yielded dimeric products whose selectivity was representative of the proportion of hetero- and homo-complexes. Our studies show correlations between strength of weak interaction and the proportion of the heterodimer, wherein alkene pairs with a higher electronic and steric complementarities yielded higher proportion of the hetero-dimer. Computational studies were performed to further understand the experimental findings, and predict the stereochemistry of major hetero-dimer.

CHED 1329

Probing the effects of conformation on concerted proton-electron transfer
Bidirectional concerted proton-electron transfer (CPET) involves the transfer of a proton and electron simultaneously to and from quantum mechanically different orbitals. We are investigating base-appended radical cations. These systems are designed to undergo bidirectional CPET, with the proton-accepting and electron-accepting sites spatially separated. Computational work revealed a kinetically unfavorable conformational shift in the reaction of 10-(2-pyridinyl)-10H-phenothiazine radical cation (PPT•+) with 2,4,6-tri-t-butylphenol. This shift is believed to be responsible for the higher experimental activation barrier for this reaction relative to that for a similar molecule, 10-methyl-3-(2-pyridinyl)-10H-phenothiazine radical cation, with the same donor. Hence, the conformational shift affects the intrinsic barrier for CPET, in parallel to the same effect in electron transfer. We hypothesize that altering the geometry of the central ring of the phenothiazine will further change the dynamics of this conformational shift. Current work is focused on 3,6-dimethoxy-10-(2-pyridinyl)-10H-carbazole radical cation, in which a five-membered ring replaces the central six-membered ring of the phenothiazine of PPT•+. Calculations indicate the molecule will remain planar throughout the reaction. Preliminary experimental work will also be presented.

Figure 1: 3,6-dimethoxy-10-(2-pyridinyl)-10H-carbazole radical cation

CHED 1330

Characterizing the excited states of multiple carbene and nitrene reactive intermediate precursors: A computational study

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Carbenes and nitrenes are highly reactive intermediates that have found numerous applications in several fields such as drug delivery, organic synthesis, photo-cross linking and photo-affinity labeling. While single carbene and nitrene precursors are
studied extensively, very few efforts have been made to investigate multiple carbene or nitrene precursors. Characterizing the spin-states of multiple nitrene and carbene intermediates will be far more complicated than conventional single carbenes and nitrenes due to the presence of several possible electronic arrangements yielding singlet, triplet as well as quintet states. Dicarbene and dinitrene intermediates would have significant applications in drug delivery, photo-cross linking, and non-conventional synthesis. In this work, a series of precursor molecules, ca. bis-azide, bis-diazo, and bis-diazirine compounds have been investigated by using chemical computations in order to characterize their ground and excited state properties. The reactive intermediate precursor units are separated by phenyl, pyridinyl, vinyl, and alkyl linkers. Vertical excitations and difference density plots are calculated to identify the location and the behavior of excited states, respectively. The location of excited states of multiple intermediate precursors do not differ substantially when compared to the single carbene/nitrene precursors. These calculations were intended to identify underlying parameters that govern the communication between the two reactive intermediate precursor groups in their ground and dissociative excited states.

CHED 1331

Complex decalin formation through the use of an asymmetric Rauhut-Currier reaction

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Carbon-carbon bond forming reactions play a central role in the creation of many natural products and biologically active molecules. Here, through utilization of the Rauhut-Currier reaction, carbon-carbon bond formation is possible with a simple and atom efficient method. In addition the Rauhut-Currier reaction yields a bicyclic structure common to many biologically active molecules from easily obtained substrates. Through our methods a bicyclic structure is reached through a highly efficient five step synthesis from the inexpensive, readily available benzoic acid. Employing a chiral catalyst in the fifth, and final, step of the synthesis will yield an enantioselective product.

CHED 1332

Development of π-stacking compounds for stationary phase modification

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In order to develop chromatographic methods to separate compounds based on their capacity to π-stack, we have synthesized highly conjugated compounds for stationary
phase modification via Functionalized Carboxylate Deposition (FCD). The compounds contain extended aromatic systems for π-stacking and carboxylate functional groups for adsorption onto the surface of silica. This presentation will focus on the synthesis and purification of the highly conjugated compounds, and discuss their application to chromatography.

CHED 1333

Synthesis of polymers for organic light emitting diodes

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Synthetic schemes to synthesize novel polymers to be used as organic light emitting diodes (OLEDs) are currently being explored. According to modeling, the target polyboronic acid and poly-amide imide compounds will exhibit a characteristic band gap width of 2.0 to 2.5 electron volts, which correlates to emission between 450 – 495 nanometers (blue region of the visible spectrum). A formyl group was substituted on to a pyrrole ring which was then brominated using N-bromosuccinamide producing 4-bromo-pyrrole-2-carboxaldehyde (BPC). Boc-glycine was cyclized using Meldrum’s acid to produce pyrrole-2,5-dihydro-4-hydroxy-2-oxo, 1, 1-dimethylethyl ester (boc-PHK). Boc-PHK was then brominated via Vilsmeier-Haak reaction using oxalyl bromide yielding boc-PBK. After removing the protecting group, the PBK and BPC rings will be coupled together, and PBK and a substituted phenylboronic acid will also be coupled. These monomers will be polymerized to form the target conductive polymers. Construction of the desired monomers are in still progress; final polymers will be tested for validation as candidates for OLED applications.

CHED 1334

Synthesis and recrystallization of diapocynin and its derivatives

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Current experimental evidence suggests that oxidative stress, or the overproduction of reactive oxygen species (ROS), plays a role in the appearance of numerous inflammatory diseases such as asthma, diabetic retinopathy, and atherosclerosis. The enzyme nicotinamide adenine disphosphonucleotide (NADPH) oxidase has been confirmed as the predominant source of ROS within endothelial cells, as well as in other cells that are affected by inflammatory processes. Previous studies have confirmed that apocynin and its analogs may be excellent inhibitors of NADPH oxidase, thus having
great pharmaceutical value. The three-dimensional structures of these molecules will be studied for their potential active sites with NADPH oxidase via x-ray diffraction. A variety of new synthesis reactions, including the reduction of apocynin and diapocynin, are underway as well to discover new methods of making these prospective pharmaceuticals. Experiments are in progress and results will be presented.

CHED 1335

Gold catalyzed cross-coupling using arenediazonium salt as the oxidant

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Discovery of the catalytic property of gold, supposedly an inert metal, has led to a “catalytic gold rush” among chemists. Homogeneous gold (I) and gold (III) catalysts are widely used due to their ability to activate alkynes and alkenes. However, the cross-coupling reactivity of gold is quite limited because of the high oxidation potential between gold (I) and gold (III) requiring a strong external oxidant such as SelectFluor or PIDA. This research will investigate the reaction of an arenediazonium salt, acting as a weaker internal oxidant, with a terminal alkyne catalyzed by gold (I) to form the cross-coupling product shown in Scheme 1. We hypothesize a proposed mechanism to yield the desired cross-coupling product. Starting with addition of the Au (I), the alkyne will react with it to form a gold acetylide, which is proved to be crucial for the oxidation of Au (I) to Au (III). The alkynyl group is a potential electron donor that makes gold more electron rich, which decreases its oxidation potential and makes it easier to be oxidized. After, the gold acetylide reacts with the diazonium salt, we believe there will be an appearance of a diazo-gold (III)-alkynyl complex. In order for the desired product to form, nitrogen extrusion must occur releasing nitrogen gas, followed by fast reductive elimination to yield the desired product. The DESI-MS spectrum is used to confirm the formation of the Au (III) intermediate. This research focuses to advance cross-coupling methodology with alkynes catalyzed by gold as well as study the mechanism to gain further insight in the redox gold catalysis.

CHED 1336

Exploration of long chain dialdehydes for use as linkers in catalytic metallodiporphyrins
Catalytic water oxidation has been a major goal of multiple groups world-wide for use in the hydrogen gas economy. Here we propose to synthesize diporphyrin molecules which can be used as water oxidation catalysts, linked by a chain of five or six carbon atoms. To begin, a Swern oxidation was performed on 1,5 pentanediol and 1,6 hexanediol to create their respective dialdehydes. However, due to minimal success the oxidative cleavage of trans-1,2-cyclohexanediol using diacetoxyiodo benzene was attempted as an alternative, producing 1,6 hexanedial (1). This dial was then reacted in a one pot synthesis with pyrrole and MgBr$_2$ to form 1,1,6,6-tetrakis(1H-pyrrol-2-yl)hexane (2).

Finally, 2 would then be reacted with benzaldehyde and pyrrole to form the linked diporphyrin complex. After the insertion of Mn or Co into the diporphyrin, forming the metallodiporphyrin, catalytic activity will be measured using electrochemical techniques.

Scheme 1: Reaction for the formation of 2.

CHED 1337

Structural changes induced by 8-Oxo-7,8-dihydroadenosine in RNA oligonucleotides may result in loss of function of RNA aptamers

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Aptamers are known to regulate various cellular metabolic and biochemical pathways. Reactions between reactive oxygen species and adenosine are known to produce the oxidative lesion, 8-oxo-adenosine (8-oxo-A). This modification is reported to form base-pair mismatches (8-oxo-A:G instead of A:U) that may inhibit formation of their intended (canonical) structure and/or induce changes in secondary structure. Thus, if present in aptamers of RNA, functional variations can be expected. This phenomenon was tested by conducting structural studies of RNA strands containing the modified lesion. We used sequences corresponding to aptamers with recognition for queuosine or aminoacridine. These aptamers were chosen based on their length (short, 15-34 nt long) and known behavior. The modified monomer was obtained via a 3-step reaction starting with bromination and acetylation of the C8-position followed by hydrolysis in the presence of ammonia to yield the desired lesion in ca. 53% yield. The oxidized
nucleotide was then protected at the N6- and C5'-positions by treatment with N,N-dimethylformamide dimethyl acetal followed by tritylation, respectively. Silylation of the C2' position was achieved using standard conditions in the presence of tert-butyldimethylsilyl chloride and silver nitrate. Phosphitylation of this material yielded the desired phosphoramidite in a ca. 41% yield (over 4 steps) of 8-oxo-A for its incorporation into oligonucleotides of RNA via solid phase synthesis. Each synthetic intermediate was characterized via NMR, IR, UV-Vis, and MS, while the identity of each oligonucleotide was confirmed via MALDI-TOF MS. Structural analysis were carried out using CD and PAGE. We found that the effects of 8-oxo-A were position dependent ranging from decreased activity to complete loss of functionality. In conclusion, oxidative modifications in adenosine may lead to deleterious effects in the function of RNA aptamers.

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<td><img src="image2.png" alt="Diagram" /></td>
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Structural changes on RNA aptamer, PreQ1, imposed by 8-oxo-A (One example)

**CHED 1338**

**Biological degradation of acetaldehyde in marine waters**

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Oxygenated hydrocarbons are ubiquitous in the atmosphere with levels ranging from low ppt (acetaldehyde) to low ppb (methanol). As an OH sink and an atmospheric HOx and ozone source, oxygenated hydrocarbons have a direct impact on the oxidative capacity of the atmosphere. The oceans are one of the largest sources of uncertainty in current atmospheric budget estimates of these species. A better understanding of the processes that produce and destroy these species in seawater would improve our understanding of the role of the oceans in cycling these species into or out of the atmosphere. We have measured the degradation rate of acetaldehyde in unfiltered and filtered southern California coastal waters. Rates were determined by following the concentrations of D-4 labelled acetaldehyde in spiked (nM levels) seawater in 100ml glass syringes as a function of time. Concentrations were determined by isotope dilution purge and trap gas chromatography mass spectrometry using C-13 labelled acetaldehyde as the internal standard. Degradation rates in 0.2um filtered seawater were not measurable. Degradation rates in unfiltered seawater were first order and ranged from 0.046 to 0.32 hr⁻¹. Bacteria levels were also measured in all samples. Acetaldehyde degradation rates scale with bacteria levels. Variability as a function of time, rainfall and other water quality parameters will be discussed.

CHED 1339

Reverse anomic effect-mediated synthesis of carbohydrate 1,2-orthoesters

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Carbohydrate 1,2-orthoesters have demonstrated great potential as an efficient intermediate product for glycosyl linkage formations of disaccharides, oligosaccharides and polysaccharides. The highly pH-responsive orthoester link, which decomposes fast even in a slightly acid environment, is also a latent candidate for drug conjugations for the application of tumor treatment. However, sugar orthoesters are usually produced as byproducts in carbohydrate chemistry. Herein, we report a reverse anomic effect (RAE)-mediated synthesis of carbohydrate 1,2-orthoester. When RAE-enabled promoters; including DMAP, TPP and imidazole were employed; 1,2-orthoesters with quantitative yield were achieved. The NMR analyses indicate that the synthesis is highly chemoselective with exclusive formation of orthoester linkages between a variety of donors and acceptors. This research should serve as a valuable tool for future syntheses of carbohydrate orthoesters.

CHED 1340

Solvent-free synthesis of biologically active stilbene derivatives

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Organic reactions, including the synthesis of pharmaceuticals, historically occur in the presence of a solvent. Recently, there are an increasing number of organic compounds reported to form in solvent-free conditions. Research to optimize conditions of the solvent-free Wittig reaction tested different bases, aldehydes with different melting points/reactivity, and influence of atmospheric moisture. It was found that reactions that afford high percent completion and short reaction time were performed in conditions using a low melting point aldehyde and hygroscopic bases while being open to atmospheric moisture. Therefore, in an attempt to connect these concepts, optimized solvent-free Wittig reaction conditions were applied in the synthesis of prospective chemopreventative stilbenoid compounds; (E) and (Z) resveratrol trimethyl ether (RTE). As a result the solvent-free synthetic pathway afforded high yield, short reaction time, and utilized a much more sustainable chemical pathway in comparison to traditional methods of synthesis.

CHED 1341

Synthesis of 2,5-disubstituted 3-fluorothiophenes from 2-thienyl carbamates via a directed fluorination/cross-coupling approach

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2,5-Disubstituted 3-fluorothiophene derivatives 1 are of interest as building blocks in liquid crystal materials synthesis. This poster details the development of 2-thienyl carbamates 2 and related compounds as flexible building blocks for the construction of 2,5-disubstituted 3-fluorothiophenes. Our approach involves oxidation of 5-substituted 2-thienyl trifluoroborates to the corresponding thienones 3 followed by O-trapping of the corresponding enolate as the 2-thienyl carbamate 2. Studies aimed at the elaboration of 2 to 2,5-disubstituted 3-fluorothiophenes 1 using a sequential directed orthometalation/fluorination/Ni-catalyzed cross-coupling approach will be presented.

CHED 1342

Au(I) catalyzed imine formation from α-diazooesters and azide

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Imines are well known, important functional groups with varying applications in both the material and biological science fields. The formation of the desired imine product is difficult to achieve through normal amine condensation reactions, requiring harsh conditions, this begs the question if the same result can be achieved through a more mild condition, more tolerant of sequential reactions and sensitive starting materials. Currently, the reaction of diazo compounds and azides is the preferred reaction pathway; this is due to the high energy of the two starting materials, leading to an increased reactivity. In a recent study, activation of the azide allowed for the formation of a reactive Rhodium-nitrene intermediate. While this route for the production of the imine product was sufficient, the proposed reaction path brought about questions for the difference in reactivity between the Rh(II) and Au(I) preferred pathways. Our groups recent work with α-diazoester Au(I) catalyzed reactions showed that Au(I) has the ability to form a “carbophilic cation”, this compound possesses the ability for ligand controlled chemoselectivity, preforming site selective Friedel- Craft like additions. This previous work leads to the thought process that the gold carbeneoid intermediate will be much the same, and that the increased reactivity would therefore allow for a more favorable condition through fine tuning, thus presenting the opportunity for a sequential reaction. The difference in the formation of the two transition species leads to the inquiry for the comprehensive investigation of the reactivity and selectivity differences in the gold carbeneoid and rhodium nitrene chemistry. The preliminary results from our comparative investigation, has shown gold to have a higher reactivity forming the desired imine product in >75% yields. With these results, we have begun to investigate the scope and screen possible sequential reactions.

CHED 1343

Expansion of electrophile scope in the transition metal-catalyzed coupling of Corey-Seebach umpolung reagents

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The transition metal-catalyzed cross-coupling of aryl electrophiles (i.e. –Br, –Cl, –OTf) with substituted Corey-Seebach umpolung reagents is described. Recently we disclosed the first examples of palladium-catalyzed cross-couplings of 2-aryl-1,3-dithianes with aryl bromides. Wanting to increase the utility of the transformation, we now report the first use of alternative electrophiles including aryl chlorides and triflates. Critical to expanding electrophile scope was the modification of our catalyst system. We found that the use of the third generation biphenyl Buchwald catalyst system engaged previously unreactive aryl triflates. Additionally we found aryl chlorides would react when moving to a nickel-based catalyst. The expanding reaction scope, our group’s current mechanistic understanding, and future goals are presented.

CHED 1344
Intramolecular halogen bonding of fluorinated haloarenes in solution

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Two compounds capable of intramolecular halogen bonding were studied by $^{15}$N, $^{13}$C, and $^{19}$F NMR spectroscopy. Fluorine atoms within the compounds were used to activate the iodine and bromine halogen bond donors and as spectroscopic handles. These two compounds were then compared to eight related control compounds. The $^{15}$N NMR showed the greatest effect of halogen bonding, with nitrogen atom halogen bond acceptors displaying chemical shift decreases of 6 ppm and 1 ppm in iodo- and bromo-functionalized systems, respectively. Similarly, $^{13}$C NMR spectra showed evidence of intramolecular halogen bonding in the alkynyl carbons of the 2-ethynylpyridine system, with chemical shifts up to 2.4 ppm different than related control compounds. The $^{19}$F nuclei provided a means to study the effects of solvents on halogen bonding by providing evidence of intramolecular halogen bonding in dilute samples. The magnitude of $^{19}$F chemical shift changes in different solvents was directly correlated to the strength of the halogen bond in solution. Halogen bond strengths were found to decrease in different solvents in the following order: cyclohexane > toluene > benzene > dichloromethane > acetone > pyridine.

CHED 1345

Manipulating the electronic properties of aryleneethynlenes with halogen bonding

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Aryleneethynlenes have been studied for years for both their electronic properties and their conformational flexibility. Control over the conformations of these conjugated systems allows access to molecules with desirable electronic properties. Previously, hydrogen bonding and transition metal coordination have been used as tools to alter the electronic properties of aryleneethynylene systems. In this study, halogen bonding is used to enforce planarity in molecules of this type. The result of this increased coplanarity is enhanced effective conjugation of the unsaturated backbone. Comparisons of electronic spectra of molecules with restricted rotation due to intramolecular halogen bonding and isomeric molecules that are not restricted by this intramolecular attraction demonstrate that a halogen bond can be used to bias the conformational preference of an aryleneethynylene structure. This type of control could potentially lead to the ability to tune the electronic properties of a variety unsaturated organic compounds.
Intramolecular halogen bonding of non-activated aryl halides in solution

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The purpose of this study is to investigate intramolecular halogen bonding in non-activated systems and to determine if these halogen bonds can be detected through $^{13}$C NMR in solution. The control molecules in this study possess a 3-ethynlpyridine unit (A) that is incapable of halogen bonding between the nitrogen and X atoms because of the location of the nitrogen on the pyridine ring. However, an isomeric 2-ethynlpyridine-based system (B) is capable of halogen bonding because of the proper alignment of the nitrogen and halogen atoms. Comparison of $^{13}$C NMR chemical shifts of these molecules in benzene-$d_6$ gives some indication of whether or not halogen bonding has occurred in the 2-ethynlpyridine systems. For example, the chemical shifts of the $C_\alpha$ and $C_\beta$ signals in A-I and A-Br are very similar. The chemical shifts of the $C_\alpha$ and $C_\beta$ signals of B-I and B-Br, on the other hand, vary due to differences in intramolecular halogen bonding in the benzene solution. Halogen bonding is indicated by a modest shielding of the $C_\alpha$ nucleus and a more significant deshielding of the $C_\beta$ nucleus. By utilizing intramolecular halogen bonding, this study probes the limits of halogen bonding in solution when entropic concerns are eliminated.

Metal binding and electronic properties of aryleneethynylene trapezoids

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Aryleneethynylene trapezoids have been synthesized in order to study their metal binding and electronic properties. The parent molecule contains a central benzene ring...
with rigid pyridine arms which are held in a trapezoid formation by coordination of the pyridine ligands to a transition metal center. The strength of metal cation binding and the electronic properties of the coordinated and uncoordinated ligand have been the major areas of study. Binding of the unsaturated ligand to Ag(I) and Pd(II) centers has been confirmed via x-ray crystallography and NMR spectroscopy. NMR studies reveal that binding of the Ag(I) cation is more dynamic than binding to the Pd(II) centers. Electronic spectra reveal that metal binding does little to inhibit the free rotation of the central benzene ring, making the UV-vis spectra of the complex very similar to the unbound ligand.

CHED 1348

Novel method of stereochemical management of Morita-Baylis-Hillman chemistry: Controlled acrylate ester synthesis

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The Morita-Baylis-Hillman (MBH) reaction is a tertiary amine catalyzed coupling of a conjugated, electron poor alkene (e. g. methyl acrylate or acrylonitrile) and an aldehyde giving allylic alcohol products. This reaction has enjoyed a great deal of attention in that it is capable of converting relatively simple compounds into those which contain multiple functional groups and new chirality centers. Manipulating the stereochemical outcome of this reaction typically employs asymmetric tertiary amine catalysis or substrate/chiral auxiliary control. We propose a new strategy for that combines both asymmetric catalysis and auxiliary control. This strategy involves the formation of an acrylate ester that features a chiral auxiliary that contains a tertiary amine that has been shown to be an effective catalyst for the MBH reaction. This method provides new options for green technologies in that the reaction is “one pot”, has a favorable atom economy, and allows for the possibility of catalyst recovery via methanolysis in a closing step.
Total synthesis of the cyclic depsipeptide natural product Aspergillicin A, and investigation of its cell permeability, pharmacokinetic property, and bioactivity

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Cyclic peptides are an important class of natural products that display a wide range of biological activities and are of interest in drug discovery. Many of these naturally derived compounds exhibit better than expected pharmacokinetic properties, and our goal is to understand why. In the Lokey Research group, we are interested specifically in understanding how cyclic peptides can achieve cell permeability, an important property of potential therapeutics. In addition to synthetic compounds, we also use naturally derived compounds as model systems. The Aspergillicins are natural product cyclic depsipeptides originally isolated from the marine fungus Aspergillus Carneus. The goal was to perform the first total synthesis of Aspergillicin A, and use further analogs as model systems to study the pharmacokinetic properties of cyclic peptides. Using Solid Phase Peptide Synthesis (SPPS), two different synthetic approaches were tried with the objective to compare the gathered data on our synthetic materials, which included HPLC and LCMS analysis as well as NMR results; to the literature. The final goal of this project is to run the compounds on a cytological profiling assay and test for bioactivity; and use them as a test case for the study of cell permeability. Testing for cell permeability will be achieved by running the compounds through parallel artificial membrane permeability assay (PAMPA). In addition, we hope to develop new synthetic methods for the synthesis of cyclic depsipeptides, which may be of use in the future synthesis of other natural products or drug-like compounds.
Multicomponent reaction to produce diversely substituted 2-imidazolines

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2-imidazolines are heterocyclic scaffolds that are recognized for their wide variety of biological properties. Substantial efforts have been made towards the synthesis of the
2-imidazoline core, yet single pot reactions to synthesize N-substituted 2-imidazolines from acyclic starting materials are scarce. Most commonly, syntheses of N-substituted 2-imidazolines involve 2 step procedures of 2-imidazoline core synthesis followed by either N-alkylation or metal-mediated N-arylation. The aim of our study was to develop a mild and efficient protocol by which N-alkyl and N-aryl substituted 2-imidazolines could both be prepared from similar acyclic starting materials. We developed a method that involved triflic anhydride-mediated dehydration of 2-(haloethyl)amides in the presence of amines, and explored this reaction for mechanistic insights. A significant use of the 2-imidazolines prepared in this study is to detect heterocycle-protein interactions in biological systems, a finding that will be further discussed.

\[ \text{CHED 1351} \]

**Click, click, xyclize: Amino wster-serived β-ketosultams via Dieckmann cyclization of the corresponding methylsulfonamides**

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The objective of this project is to synthesize monocyclic and bicyclic β-ketosultams through a strategy termed, "Click, Click, Cyclize." The starting materials, mesylated linear and cyclic aminoesters, undergoes a sequence of two click reactions (sulfonylation and benzylation) followed by cyclization (intra-molecular Dieckmann-like condensation) to yield the desired scaffolds. All products will be submitted to biological collaborators for screening various biological activities.

**CHED 1352**

**Synthesis of functionalized biscavitands**

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Cavitands are container molecules that have conformations that enable them to bind or entrap smaller compounds. The goal of our project is to develop a series of singly linked functionalized biscavitands that can self-assemble via hydrogen bonding. We utilize a resorcin [4] arene framework to create our molecules due to its easily modifiable structure. A synthetic route encompassing organometallic chemistry has been used to create and incorporate functionality on the biscavitands. Compounds with a similar framework to that of resorcin [4] arene have been reported to have biological applications due to their ability to mimic biological interactions. Characterization of all compounds will be made by NMR spectroscopy, high-resolution mass spectrometry, and infrared spectroscopy. We will explore how the linkers and functional groups will affect the self-assembling properties, shape, size, and guest complexation of these molecules.

CHED 1353

Structural studies of oligonucleotides of RNA containing 7,8-dihydro-8-hydroxyadenosine

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The relationship between oxidative damage to nucleic acids and the biogenesis of disease e.g., cancer and neurological disorders, gives relevance to the studies of oxidative damaged nucleotides on DNA and RNA. In this research we investigated changes imposed by oxidative lesion 7,8-dihydro-8-hydroxyadenosine (8-oxoA) on single and double strands of RNA and in short hairpins. Measurements carried out on RNA:RNA homoduplex and RNA:DNA heteroduplex structures showed depressed melting temperature ($T_m$) values of ca. 12-15. We found that increasing the number of lesions resulted in larger destabilization, as reflected in their $T_m$ value (ca. 10 increments per modification). The presence of the oxidative lesion in short RNA hairpins yielded different results that depended on its position: stem and/or loop. Incorporation of 8-oxoA at the stem lead to structure inhibition, destabilization, or formation of other structures, i.e., increased loop size (tetraloop hexaloop/octaloop). On the other hand, no effect was observed upon incorporation at the first base within the loop. Structural studies were carried out using Circular Dichroism, Mass Spectroscopy, and Gel Electrophoresis. Overall, this study shows that the effects of 8-oxoA on RNA structure are dependent on both the amount of damage and its position. While destabilization of the secondary structures may be beneficial, due to faster degradation of the strand, stabilization may result in survival of the oxidized species and altered functionality.
The RNA secondary structures containing 8-oxoA were studied via Circular Dichroism

CHED 1354

Investigating the use of copper photoredox catalysts in an enantioselective reaction

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Enantioselective photoredox reactions couple a photoredox catalyst with a chiral catalyst and have demonstrated significant synthetic potential. Our research is focused on the development of copper(I) photocatalysts for use in enantioselective photoredox reactions. Bis(phenanthroline) copper complexes have similar photophysical properties to known photocatalysts, such as Ru(bpy)$_3^{2+}$ and Ir(ppy)$_3$. However, copper has the benefit of being less expensive and less toxic. We are evaluating bis(phenanthroline) copper(I) complexes as catalysts in the α-benzyl alcohol of aldehydes, an enantioselective reaction that also requires a chiral catalyst. Cu(dap)$_2$Cl (where dap = 2,9-bis(p-anisyl)-1,10-phenanthroline) has been identified as the optimal catalyst. Optimization of reaction conditions and the evaluation of the reaction scope shall be discussed.

CHED 1355

Synthesis of conformationally constrained diarylether cyclophanes

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We report progress toward the synthesis of a series of chiral conformationally constrained diarylether cyclophanes with variation in the length of the bridging carbon chain. These cyclophanes are chiral by virtue of restricted bond rotation, not by the presence of stereocenters. Cyclophanes are a class of compounds that occur naturally and are conformationally constrained due to the presence of a carbon chain bridging the para positions of an aromatic ring. Many naturally occurring diarylether cyclophanes
have a seven-carbon bridge linking the diarylether component of the molecule. We report a method for the synthesis of diarylether cyclophanes with variation in the tether length. Experiments to determine the relationship between tether length and the barrier to racemization will be disclosed. Because of structural similarities to biologically active diarylether heptanoids, the synthesis of diarylether cyclophanes could lead to compounds with significant biological activity.

CHED 1356

Anion-responsive liquid crystals

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Previous efforts in the field of sensing have focused on developing materials that can respond to a stimulus (e.g. light or chemical) with a measurable output signal in the solid phase. The limited solubility of these materials in water is one of their biggest disadvantages, since water is the medium for most environmental-sensing applications. One approach to address this issue is to incorporate the small molecules into a larger assembly, which can respond to stimuli at the interface between water and a solid film. In order to employ this strategy, the present research focuses on studying the assembly of anion-responsive azo-benzenes in liquid crystalline (LC) phases. As a proof of the concept, azo-benzenes with long alkyl chain ureas were synthesized. The compound 1 showed evidence of LC thermal transitions in a differential scanning calorimetry analysis. Additionally, organic solutions of 1 exhibited a variety of color changes when exposed to tetrabutylammonium halide salts. As part of a structure-property study of the assembly of azo-benzenes, the compound 2 was synthesized and characterized with spectroscopic and thermal analysis. Future efforts will focus on characterizing both compounds with polarized optical microscopy as part of a larger structure-property study of their assembly.
Figure 1. Compound 1 in acetonitrile solution reacted to tetrabutylammonium halide salts. When the compound was exposed to a more basic halide salt, the color change was more intense and noticeable. Compound 1 in tetrabutylammonium fluoride solution created a green colored solution, while with other less basic halide salts, there was less of a color change.

CHED 1357

Synthesis and characterization of novel polyester polyols

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Succinic acid is a renewable feedstock that has been investigated to supplant petroleum-based adipic acid polyester polyols. Polyester polyols are used in the manufacture of many common materials such as foams, coatings, adhesives, and lubricants. A library of succinate and adipate polyesters were prepared using a Tin (IV) catalyst. Diols (3-methyl-1,5-pentanediol, 2,2-dimethyl-1,3-propanediol, 1,4-butanediol, 1,3-propanediol, and diethylene glycol) were varied to determine the influence of branching, chain length, and hydrophilicity, on the Tg, viscosity, crystallinity, density, and melting point of the polyesters. Molecular weight was quantified using ¹H-NMR endgroup analysis. Incorporating mixtures of diols into succinate polyesters was found to decrease crystallinity, lowering the melting point. Succinates and adipates were found to possess comparable viscosities. The structure-property relationships between mixed diol succinates and adipates were evaluated.

CHED 1358

Asymptotic behavior of travelling wave solutions to reaction-diffusion equations
We will discuss travelling wave solutions to reaction-diffusion equations of the form:

\[ u_t = u_{xx} + u^p (1-u^q) \]

which can be used as a mathematical model for various biological phenomena, as well as to model problems in combustion theory. We identify conditions on the wave speed so that travelling wave solutions exist for the case \( p \geq 1 \) and \( q \geq 1 \). Moreover, we estimate the rate of decay of the travelling wave solutions. When \( p > 1 \) and \( q \geq 1 \), this estimate requires center manifold theory because the typical linear methods fail to work. Through the mathematical analysis of reaction diffusion equations, the results of this research create further studies and application in physical and industrial chemistry.

**CHED 1359**

**Interfacial interactions and adhesion properties of selected monomer and polymers probed by SFG spectroscopy and atomic force microscopy**

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This study entails to utilize sum frequency generation spectroscopy (SFG) as an interface specific technique to identify chemical structures and elucidate the molecular conformation at the air-liquid, air-solid and solid-liquid interfacial boundaries. This study will generate a model system based on the 2-hydroxyethyl-2-methylprop-2-enoate (HEMA) and poly (HEMA) scaffolds. The monomer will be functionalized to study the impact of inductive and steric effects to the organization of interfacial molecules. Solvent effects to monomer and polymerization will also be studied at the interface. HEMA was chosen for its ease of modifying the –OH functional group to emphasize its selection as the starting material. At the polymeric state, SFG spectroscopic/microscopic techniques will be utilized to chemically identify the domain formations at the surface of homogeneous or heterogeneous polymer; and atomic force microscopy (AFM) will be used to assess adhesion properties. The correlation of both the chemical structure and adhesion results will contribute to the prediction of the effectiveness of polymers as coating materials. The project should also provide SFG orientation and distribution data from the in situ polymerization of HEMA and functionalized-HEMA, as well as obtain information on the organization of surface molecules and polymer formation with respect to time, temperature and concentration of polymer initiator. Overall, this new fundamental approach to obtain and understand the chemical structure and adhesion correlation results as surface properties will aid us and other scientists to fabricate new and better coating materials for corrosion inhibition/biofilm prevention.

**CHED 1360**
Why is there order in the purple membrane? A biological application of ultrafast Raman imaging

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Bacteriorhodopsin is a photoactivated proton pump found in the purple membrane of halobacteria and forms the basis of a simple photosynthetic system. Upon photon activation, the retinal chromophore in bacteriorhodopsin isomerizes, allowing a proton to be transported across the membrane. Relief of the resulting electrochemical gradient is coupled to ATP synthesis. Bacteriorhodopsin forms two-dimensional crystalline patches in the purple membrane, organizing in tessellating hexagonal units of three proteins surrounded by few lipids. It is not currently known why such an ordered structure exists. Using a femtosecond stimulated Raman spectroscopy imaging technique, changes in the local membrane environment upon activation of bacteriorhodopsin can be tracked to assess the effect of activation of one protein on the quantum efficiency of its neighbors. Thus far the purple membrane has been isolated using the method published by D. Oesterhelt and W. Stoeckenius (1974) and characterized by Raman spectroscopy. Initial Raman images have been taken with diffraction limited resolution. An understanding of the mechanism by which halobacteria maximize energy yield will inform current efforts to design synthetic light-harvesting systems.

CHED 1361

Structures and CH...O interactions of fluorinated ethylene...carbon dioxide complexes as determined by microwave spectroscopy

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The purpose of this investigation was to study weak interactions between fluorinated ethylenes and carbon dioxide. Gas-phase complexes of fluoroethylene (FE)...CO2, 1,1-difluoroethylene (DFE)...CO2, and 1,1,2-trifluoroethylene (TFE)...CO2 were studied using chirped-pulse Fourier-transform microwave spectroscopy. Precise orientations of each complex were determined by analysis of spectra of several isotopologues for each dimer. All of the complexes form CH...O contacts between a CH group of the ethylene and an oxygen atom of CO2. In the FE and TFE complexes, CO2 may align either on the FCCH side or FCH end of the ethylene molecule, giving a planar overall structure. Both orientations were observed for FE...CO2 while only the end configuration was seen for TFE...CO2 and a side configuration was observed for DFE...CO2. To assign the rotational spectra of these complexes, experimental data was compared to ab initio predictions. Although ab initio calculations indicated lowest energy orientations of the FE and DFE complexes that were nonplanar with CO2 molecules positioned above the ethylene molecules, they did predict a planar minimum energy structure for TFE...CO2.
that agreed with the experimental result. Experimental procedures, comparisons between orientations of all complexes, as well as differences between ab initio and experimental results will be discussed.

CHED 1362

Electronic spectroscopy of gold sulfide (AuS)

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Band systems for four different ground state electronic transitions in the visible region were recorded for gold sulfide (AuS). The molecules were generated in a hollow cathode sputtering source and probed by laser excitation spectroscopy with a pulsed dye laser. The ground state is an inverted $^2\Pi$ state, and the assignments for the four transitions were determined to be $A^2\Sigma$–$X^2\Pi\ _{3/2}$, $B^2\Sigma$–$X^2\Pi\ _{3/2}$, $C^2\Delta$–$X^2\Pi\ _{3/2}$, and $C^2\Delta$–$X^2\Pi\ _{3/2}$. In addition, transitions from the upper $^2\Pi$ spin orbit component of the ground state were also seen to both $^2\Sigma$ states as well as to the $C^2\Delta\ _{3/2}$ state. We have fitted the vibrational band origins to determine the term energies and vibrational constants of each state. We also determined the $X^2\Pi$ spin-orbit splitting to be 1304 cm$^{-1}$. Finally, the $C^2\Delta\ _{3/2}$–$X^2\Pi\ _{1/2}$ (0,0) band was recorded at high resolution using a single-mode ring laser in order to resolve the rotational structure, enabling us to determine the rotational and centrifugal distortion constants of these two states.

CHED 1363

Investigation of the spectroscopic properties of newly synthesized pyrimidines

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A class of newly synthesizable pyrazolopyrimidine organic dyes observe fluorescence behavior due in part to a combination of excited state intramolecular proton transfer (ESIPT) and electron transfer (ET). Stoke’s shift of dyes range anywhere from 4800 to 8800 cm$^{-1}$ and lifetime measurements of ESIPT yield anywhere from 1.0-2.9 ns. Some varieties of these molecules observe solvatochromism properties. Steady-state absorption, steady-state emission, and emission lifetime spectra reinforce these conclusions. These molecules could have applications in cutting-edge technology which includes use in molecular electronics and fluorescence sensing.

CHED 1364

Gas-phase reactions of Cu$^+$ ($^1S$, $^3D$) with CF$_3$CH$_2$Cl, CF$_3$CH$_2$CH$_2$Cl, and CF$_3$CH$_2$CH$_2$Br: Proximity effects in substrates with competitive reactive sites
Effects of chain length were explored in the gas-phase reactions of Cu⁺(1S, 3D) with halogenated short chain organic compounds. Reactions of CF₃(CH₂)ₙ-X (X = Cl, Br; n = 1, 2) with Cu⁺ ions formed in a sputtering glow discharge were carried out under near-thermal conditions using a selected ion drift cell. In this work, we sought to study the effects of separating the preferred association site (the more electronegative –CF₃ end) with the preferred reaction site (the –X end). State-specific product formation was characterized using ion-mobility spectrometry. These results show that association products are formed primarily via Cu⁺(1S), whereas Cu⁺(3D) initiates a number of bimolecular processes. These include halogen abstraction, HX abstraction, and several products indicating that the metal induces other, more complicated rearrangements of the substrate. State-specific kinetic data were obtained for all three neutrals, which reveal that the overall reactions are very efficient, with rate constants for both copper states on the order of 10⁻⁹ cm³·molec⁻¹·s⁻¹. Preliminary findings indicate that product branching ratios remain the same for processes exhibited by more than one reactant neutral. This implies that changes in proximity of the preferred association site to the preferred reaction site do not influence efficiency of the reaction or branching ratios.

CHED 1365

Photodecomposition of phenylalanine on the surface of titanium dioxide

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Organic compounds have yet to be detected on the Martian surface despite strong arguments for their existence. This study focuses on a possible explanation for this observation. One mechanism that has not been investigated thoroughly is the photodecomposition of organics on the surface of TiO₂, which has an abundance of 0.65% in Martian soil. A method was developed to deposit phenylalanine onto the surface of the anatase and rutile forms of TiO₂. The deposited phenylalanine was then irradiated with UV light to induce a photocatalytic reaction with the TiO₂. The products of this reaction were analyzed via fluorescence and NMR spectroscopies to determine whether reaction had occurred and to identify the products. This information was then used to develop a reaction mechanism that explains the lack of organic compounds on Mars.

CHED 1366

State-specific reactions of Cu⁺(1S,3D) with SF₆ and SF₅Cl: Thermochemical control over product formation

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Reactions of the gases SF$_6$ and SF$_5$Cl with the $^1$S ground state and $^3$D excited states of Cu$^+$ were carried out in order to examine parameters influencing S-X (X=F,Cl) bond activation. Experiments were conducted using a selected ion drift cell apparatus. Both Cu$^+$ states were prepared in a glow discharge utilizing Ne as the working gas. Ion mobility spectrometry (IMS) revealed state-specific product formation for both gases. Cu$^+$(1S) reacts with both SF$_6$ and SF$_5$Cl to yield association products and is not observed to induce any bimolecular chemistry. Conversely, Cu$^+$(3D) reacts with both compounds to yield SF$_3^+$, and with SF$_5$Cl to form CuCl$^+$. SF$_3^+$ does not appear to react further with either neutral reactant, whereas CuCl$^+$ reacts in an efficient secondary process with SF$_5$Cl to yield SF$_5^+$. Additional higher-order fragmentation products were observed to occur in trace amounts with both substrate molecules. Thermochemical requirements for fragmentation products in both reactions indicate that the neutral byproducts must involve some degree of bond formation to proceed exothermically. Candidates for possible product channels were evaluated on the basis of energetics and conservation of electron spin. State-specific kinetic measurements show that both Cu$^+$ states are consumed efficiently by SF$_5$Cl, whereas SF$_6$ reacts with Cu$^+$(1S,3D) slowly. This suggests that the rate-determining step in the SF$_5$Cl reaction involves activation of the weaker S-Cl bond.

CHED 1367

Thiol based adsorbate detection using Surface Enhanced Raman Spectroscopy

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Detection of low concentrations of harmful species in aqueous solution has traditionally been difficult due to interference from other impurities in the solution. We are working on the development of a reusable chemical sensor that takes advantage of the low detection limit inherent in Surface Enhanced Raman (SER) Spectroscopy. Quartz slides are coated with a layer of silver nanoparticles embedded in a boron nitride nanosheet using the protocol developed by Lin et al. To these, thiol based organic amines are attached. SERS is used to detect the success of this reaction. The terminal amine is used to couple the acetic acid derivative of p-tert-butyl calix-4-arene (PBCA) to the surface. PBCA has been shown to selectively trap four ring polyaromatic hydrocarbons. Reactions are done in a flow cell that remains in the Raman instrument to avoid signal variation due to non-uniform surface morphology. Determination of a calibration curve for the detection of pyrene shows proof of concept.

CHED 1368

Electron stimulated desorption and post-Irradiation analysis in a single ultrahigh vacuum chamber

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Previous ultrahigh vacuum (UHV) studies, which involved the state-resolved detection of products desorbing during electron irradiation of multilayer films deposited on metallic substrates, have provided valuable insight into radiation-induced chemical events. Analysis of products desorbing during electron irradiation, however, may not provide a complete understanding of condensed-phase radiolysis. For example, dissociative electron attachment may produce large charged fragments that remain trapped in the film because these high-mass species do not possess sufficient kinetic energy to overcome the polarization energy of the film. Therefore, analysis of the chemical products remaining in the multilayer thin films after irradiation is also necessary.

Following our initial post-irradiation study, research groups at Bremen (Germany), Sherbrooke (Canada), and Georgia (USA) have demonstrated that temperature programmed desorption analysis of the chemical products in the multilayer thin films following low-energy electron irradiation can provide additional information of importance with regard to understanding condensed-phase radiolysis. Following the successful implementation of two post-irradiation techniques (temperature programmed desorption and infrared reflection absorption spectroscopy), we have recently installed a new high intensity electron gun to perform electron stimulated desorption (ESD) experiments. Performing electron stimulated desorption and post-irradiation studies in a single UHV chamber using the same electron gun will be important in further exploring the dynamics of condensed phase radiolysis.

CHED 1369

Metastable fragmentation and photofragmentation of photoionized thiophene clusters

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Clusters of thiophene molecules undergo photoionization by 248 nm excimer laser radiation and mass analysis in a time-of-flight mass spectrometer. Ions of the formula \((\text{C}_4\text{H}_4\text{S})_n^+\) are observed from \(n = 1\) to \(n > 20\). Selected cluster ions are isolated with a time-based double-pulse mass gate and metastable fragmentation products are measured. The same ions are further probed by photofragmentation (1064, 532, 355 nm). The fragmentation patterns are analyzed for information about parent cluster ion structures. Selected ions are modeled computationally with HF and DFT methods to aid in the interpretation of experimental data.

CHED 1370

Computational study of nitrogen oxide decomposition by copper exchange ZSM-5 zeolites

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Anthropogenic nitrogen oxide production has increased significantly in recent years. Experimentally, copper-catalyzed ZSM-5 zeolites have been proposed as efficient decomposers of nitrogen oxide gases, but theoretically, the mechanisms behind nitrogen oxide decomposition are largely unknown. A computational study of the Cu-ZSM-5 zeolite using the ONIOM (B3LYP/6-31+G(d):UFF) model drew very different results in comparison to the results gathered by using the all-quantum (B3LYP/6-31+G(d)) cluster model approach. We propose the ONIOM model as a more accurate model for analyzing the intermolecular interactions between zeolites and gases. In both models the nitrogen oxide molecule adsorbed by forming an O—Cu covalent bond. But the cluster model shows a stronger interaction (1.758 Å) and a smaller N-O-Cu angle when compared to the ONIOM method (1.988 Å). Furthermore, a natural bond orbital analysis indicates a larger π-back bonding interaction with the metal center in the cluster model compared to that in the ONIOM model.

CHED 1371

**Determination and prediction of infinite dilution equivalent conductivities for ions in water at high temperatures and pressures**

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The equivalent conductance at infinite dilution, \( \Lambda^\circ \), is a fundamental property of an aqueous electrolyte that is directly proportional to diffusion coefficients. Previous work on determination of \( \Lambda^\circ \) over a wide range of temperature and pressure, from room temperature and 0.101 MPa to 800°C and about 500 MPa, has shown that \( \Lambda^\circ \) is well described by a simple function of viscosity and density. Using a new extrapolation of transference number data of NaCl and KCl, fits for the equivalent conductance of ions were found, using the additive property of \( \Lambda^\circ \) for salts, where \( \Lambda^\circ = \lambda^+ + \lambda^- \). The resulting ionic \( \lambda^\circ \) were then regressed to the equation:

\[
\lambda^\circ = b \eta^{(a+c/\rho)}
\]

where \( \eta \) is the solvent viscosity, \( \rho \) is the solvent density, and \( a, b, \) and \( c \) are fitting parameters for each ion for which there was available data. An attempt was then made to correlate the parameters to room temperature physical properties of the ions, such as partial molar entropy, partial molar volume, and \( \lambda^\circ \) itself. It was found that the best correlating quantity was \( \lambda^\circ \). Using linear fits of the parameters along with known \( \lambda^\circ \) at 25°C and 0.1 MPa for ions for which there is no high temperature data, the three parameters required to predict \( \lambda^\circ \) at high temperatures and pressures were calculated. It is believed that these parameter estimates will yield \( \lambda^\circ \) accurate to 20 percent to temperatures up to 873 K and solvent densities between than 0.5 and 1.0 g/cm\(^3\).

CHED 1372

**Characterization of novel cyano-based room temperature ionic liquid electrolyte for lithium-ion batteries**
Because of their potentially superior thermal stability and safety compared to conventional organic electrolytes, room temperature ionic liquids (RTILs) have been studied by many research groups. A novel RTIL composed of 5-cyanotetrazolide anion and N-butyl-N-methyl-pyrrolidinium cation with lithium bis(oxalato)borate conduction salt is tested in lithium metal electrochemical cells. Plating-stripping results in symmetric cells affirm the electrolyte’s ability to reversibly transport lithium ions from one electrode to the other. Overpotentials calculated from the plating-stripping tests suggest an optimal salt concentration of 1 mol kg⁻¹. Simplified symmetrical cell tests give lithium ion transference number (tᵢₗᵩ) estimates. The highest is attributed to the 0.1 mol kg⁻¹ electrolyte, and the results suggest the formation of a solid electrolyte interphase (SEI) from the decomposition products of the electrolyte. Based on these results, the RTIL exhibits interesting characteristics for lithium-ion batteries.

CHED 1373

Revisiting water radiolysis

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The goal of our research is to obtain a fundamental understanding of water radiolysis, an important topic that has been studied extensively since the discovery of natural radioactivity in 1896. Water radiolysis has applications for treatment of wastewater, radiation treatment of cancer, preservation of food, and cooling in nuclear reactors. Radiolysis of “dirty” water ice in the interstellar medium could have led to the synthesis of "complex" organic molecules which could be precursors for prebiotic molecules. To study the radiolysis of water, nanoscale-thin films of solid amorphous water are deposited on a Mo(110) single crystal substrate at 90 K in an ultrahigh vacuum (UHV) chamber with pressure as low as 5×10⁻¹⁰ Torr. An electron gun is used to irradiate the thin films with low- and high-energy electrons ranging from ~5 to 1000 eV. Post-irradiation analysis of the species left behind in the film is done with temperature-programmed desorption (TPD) and infrared reflection absorption spectroscopy (IRAS). Because copious amounts of low-energy (< 20 eV) secondary electrons are produced when high-energy radiation interacts with condensed matter, we wish to verify the hypothesis that it is these low-energy electrons that mediate high-energy condensed-phase water radiolysis.

CHED 1374

Silica sol-gels containing calcein blue as surface-enhanced Raman spectroscopy (SERS) sensors for metal ions
Surface-enhanced Raman spectroscopy (SERS) is a spectroscopic technique which is of increasing interest due to its specificity, sensitivity and limited background interference from aqueous media. Despite these various advantages, SERS is limited by the requirement that a suitable surface be present to obtain strong signals. As a result, the development of new surfaces for SERS is an area of great research interest. In this study, silver doped silica sol gels were investigated as possible substrates for SERS measurements. Gels were prepared via the base catalyzed hydrolysis of tetramethyl orthosilicate in the presence of colloidal silver nanoparticles. The organic dye calcein blue was chosen as a target molecule for detection due to its ability to bind dissolved metal ions and thus act as a sensor; target molecules were introduced to the gel matrix via inclusion in the reaction mixture or by diffusion following gel synthesis. Spectra obtained from synthesized sol-gels indicate that they are viable substrates for the SERS of calcein blue.

CHED 1375

Xenon-129 NMR and surface tension of aqueous micelle solutions

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Xe-129 nuclear magnetic resonance spectroscopy (NMR) was used to study the environment inside of various surfactant systems. The surface tension was measured through the drop weight method to determine the concentration at which surfactants congregate and form micelles, the critical micelle concentration (CMC). This study attempts to create a database of the forces within different micelle systems to understand the various conditions that affect the properties of micellar solutions. Systems that were previously studied include the addition of salts, alkanes, hydrotropes, and charged surfactants to ionic surfactants. The additives affected both the CMC and the micelle structure. The addition of salt caused the salting out effect, the addition of alkanes had no affect on the micelle properties, and hydrotrope additions decreased the surface tension. Current research focuses on the mixing of ionic surfactants with nonionic surfactant. We hope to gather information about the effect that anionic surfactants have on nonionic surfactants since nonionic surfactants lack the repulsive head groups and we can focus on the repulsive forces within a micelle. This information will be useful when predicting hydrophobic drug solubility in micellar solutions for drug delivery targeting.

CHED 1376

Ammonia radiolysis of astrochemical interest
The experiments in our laboratory simulate the thin films of extraterrestrial (e.g., interstellar, planetary, and cometary) ices, where ammonia is the most abundant nitrogen-containing compound. These icy grains are exposed to many forms of high-energy radiation (e.g., cosmic rays and γ-rays), which create copious amounts of low-energy (< 20 eV) secondary electrons. From post-irradiation temperature-programmed desorption (TPD) experiments, we have found evidence for the formation of hydrazine (N$_2$H$_4$) and diazene (N$_2$H$_2$) after irradiation of condensed ammonia with 1 keV electrons. The hydrazine yield as a function of incident fluence (electron dose) is reasonably well fit by a pure quadratic function, consistent with two independent dissociation events leading to the formation of hydrazine. While hydrazine formation was observed in films as thin as 15 monolayers (ML), diazene synthesis was detected only in films exceeding 25 monolayers in thickness. The cross-section for the destruction (reaction plus desorption) of condensed ammonia was determined to be 9×10$^{-18}$ cm$^2$. These experimental results provide a basis from which we can begin to understand the mechanisms by which ammonia is radiolytically processed in interstellar ices.

**CHED 1377**

**Kinetic modeling of catalytically active aerogels**

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A three-way catalytic converter is capable of converting toxic emissions such as carbon monoxide, unburned hydrocarbons and nitrogen oxides to less hazardous waste such as carbon dioxide, water, and nitrogen. Catalytically active aerogels such as cobalt-alumina, copper-alumina and vanadia-alumina aerogels are potential alternatives to the traditionally used platinum group metal catalysts. These aerogels have been tested on a catalytic test bed, which simulates the conditions experienced by a conventional three-way catalyst in automobiles, and have shown promising catalytic activities. In the work presented here, MATLAB is used to construct global models for the reactions to aid in understanding of the reaction mechanisms and reaction rates. Initial calculations are performed assuming a dual-site mechanism for CO and unburned hydrocarbons. The surface reactions of chemical species inside the catalytic converter will be further studied using the Reaction Mechanism Generator software package. Results of the theoretical models will be compared to experimental data.

**CHED 1378**

**Kinetics of aminopropyl-triethoxy silane on porous silicon and subsequent reaction with 4-(methylthio) benzoyl chloride studied using FTIR**
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The kinetics of the surface reaction between Porous Silicon and aminopropyl-triethoxy silane (APTES) was studied using FTIR to determine the rate law and optimum attachment conditions. Results suggest that once a monolayer is established, the APTES undergoes a zero order polymerization to form multilayers. Further surface architecture was explored in which the reaction between 4-(methylthio) benzoyl chloride with the amino silanized porous silicon plates was studied to determine the rate law for attachment using FTIR. The reaction was carried out under pseudo first order conditions and confirmed a second order overall rate law.

CHED 1379

Colloid particle motion and aggregation in silica aerogels: Experiment and simulation

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Silica aerogels are materials of interest due to their high porosity and surface area in addition to their low thermal conductivity. Silica microparticles will be incorporated into the aerogel network before gelation, and by controlling the arrangement of microparticles in the aerogel matrix, the material composites can also be tailored to exhibit desired electrical properties. An electric field will be applied to the aerogel-particle solution, and as the silica networks form, the particles will flow in response to the electric field. This field can be adjusted to create patterns with the microparticles. The motion of the microparticles will be monitored over time with a microscope with a built-in camera as the gel network polymerizes and becomes fixed. An existing Monte Carlo model with the code written in Fortran will be used to simulate the motion of the nanoparticles.

CHED 1380

Determination of the hydrogen bond effect on nitrile vibrational frequency through solvatochromic models

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Nitrile group is often used as a indicator for its solvent environment. Earlier researches discovered the linear relationship between nitrile vibrational frequency (IR) and solvent property parameters based on solvatochromic models. Same approach is used to build the models for the benzonitrile and 2,4,6 - trimethyl benzonitrile in varies solvents. For
the low frequency bands of large solvents and formamide, the obtained models do not apply due to different hydrogen bond network. Gaussian calculations suggest the high angle hydrogen bonded environments cause blueshift for the nitrile frequency and the low angle ones cause redshift. The rearrangement of solvent molecules due to solvent-solute interactions also alters the nitrile frequency.

CHED 1381

Computational analysis of conformational tunneling of glyoxylic acid

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Quantum mechanical tunneling allows a chemical system to convert to a lower-energy state despite having insufficient energy to pass over an intervening energy barrier. Recent matrix-isolation experiments have indicated that anti-Z-glyoxylic acid can convert to anti-E-glyoxylic acid via tunneling even at temperatures near 0 K. We have applied a variety of high-level ab initio quantum chemical wave function methods to analyze the tunneling behavior of glyoxylic acid and to estimate its conformational tunneling rates. Second-order Møller-Plesset perturbation theory and high-order coupled cluster theory were used in conjunction with correlation-consistent basis sets to optimize geometries, determine an intrinsic reaction path, and compute tunneling rates. Our computational results reveal that tunneling is indeed operative in glyoxylic acid isomerizations. Such studies of quantum mechanical tunneling reveal the surprising facility with which molecules of biochemical significance can undergo conformational changes.

CHED 1382

Surface IR spectroscopy and computational study of MHDA on GaAs(100) surface

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In the past 20 years alkanethiols have drawn attention due to their ability to bind to metal surfaces. Most notably, their potential use as linkages for biosensors and their ability to form metal organic frameworks (MOF) for medical applications has shown promise. We investigated the adsorption of MHDA on a GaAs(100) surface using surface IR spectroscopy and computational chemistry. All computations were performed using the cluster model approach at the B3LYP/SDD level of theory. Results from frequency computations for MHDA showed a C—H stretching of 3021 cm⁻¹ and 3108 cm⁻¹. These results are comparable to our experimental data of 2975 cm⁻¹ and 3016 cm⁻¹. Computations showed covalent interaction between S and As with a bonding distance of 2.34 Å.
CHED 1383

Diffusion of alkylbenzenes in \( n \)-alkanes

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Capillary flow techniques have been used to measure the translational diffusion constant, \( D \), of benzene and a series of alkylbenzenes in \( n \)-dodecane and \( n \)-pentadecane at room temperature. The alkylbenzenes are toluene and those with chains of 2, 3, 5, 6, 8, 11, 14, and 17 carbon atoms. The results in both solvents are in approximate agreement with the predictions of theories that model the benzene ring as the head of a diffusing lollipop and the alkyl chain as its handle. Our data also are compared with the predictions of cylinder diffusion models, as are the diffusion constants for \( n \)-alkanes diffusing in benzene, carbon tetrachloride, and \( n \)-alkanes. The dependence of the alkylbenzenes’ diffusion on their sizes relative to those of the \( n \)-alkane solvents are consistent with a similar correlation for the diffusion of \( n \)-alkanes.

CHED 1384

Characterization of an ethanol-benzene complex using matrix isolation infrared spectroscopy

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A 1:1 complex of ethanol (\( \text{C}_2\text{H}_5\text{OH} \)) and benzene (\( \text{C}_6\text{H}_6 \)) was characterized by matrix isolation infrared spectroscopy. Co-deposition experiments of these two molecules were performed in both argon and nitrogen (\( \text{N}_2 \)) matrices at 20 K and yielded new peaks for the O-H group stretching within the ethanol and the out-of-plane bending vibration within the benzene. Identification of the new peaks assigned to the 1:1 \( \text{C}_2\text{H}_5\text{OH}:\text{C}_6\text{H}_6 \) complex was partly determined by comparing the co-deposition spectra to the separate monomer spectra of ethanol and benzene in an argon and nitrogen matrix. Theoretical calculations using the Gaussian 03W computational chemistry program at the B3LYP level with the aug-cc-pvdz basis set were performed for the \( \text{C}_2\text{H}_5\text{OH}:\text{C}_6\text{H}_6 \) complex. The theoretical infrared spectra were compared to the experimental spectra to help assign the peaks of the 1:1 \( \text{C}_2\text{H}_5\text{OH}:\text{C}_6\text{H}_6 \) complex.

CHED 1385

Conformational elucidation of diphenylureas in varying solvent environments

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Elucidating properties of biomolecules is developing interest due to their materials and catalytic applications. Modeling these biomolecules using supramolecular mimics to generate artificial enzymes are advantageous as it can perform in non-aqueous environments, and can be selective for production of generally unfavorable pathways. One class of compounds that fold into secondary structures in solution and mimic enzyme structure is synthetic oligoureas. In particular, diphenylureas, specifically \(N,N'-\text{dimethyl-}N,N'-\text{diphenylurea (DMPU)}\) and \(N,N'-\text{diphenylurea (DPU)}\), has gained interest due to their ability to conform in solvent environments with different polarities. In this work, the thermodynamics, conformational and dynamic preferences of these monomeric units will be investigated using temperature-dependence NMR spectroscopy and computational chemistry. Current results of DMPU in \(d_6\)-DMSO (\(\varepsilon = 46.7\)) and CDCl\(_3\) (\(\varepsilon = 4.81\)) show temperature-dependence (296 K to 350 K for \(d_6\)-DMSO studies, and 223 K to 323 K for CDCl\(_3\)) peak shifts of the \(^1\text{H}\) and \(^{13}\text{C}\) resonances. For example, the \(^1\text{H}\) methyl resonance peak of DMPU in DMSO becomes more defined and shifts upfield by \(\sim 0.05\) ppm with temperature decrease, while in CDCl\(_3\), the peak becomes broader as it displays a shoulder, and shifts \(\sim 0.15\) ppm downfield at lower temperature. The \(^1\text{H}\) phenyl resonances, as well as the \(^{13}\text{C}\) methyl and phenyl resonances follow similar trend. In CDCl\(_3\) at 323 K, the \(\text{cis-cis}\) isomer is dominant, while the shoulder emerging at lower temperature may be due to the presence of the \(\text{cis-trans}\) isomer. Preliminary results on DPU in DMSO demonstrate that the nitrogen \(^1\text{H}\) peak becomes deshielded by \(\sim 0.20\) ppm on going from 350 K to 296 K, and more defined at lower temperature. Similar trends are observed for the \(^1\text{H}\) phenyl resonances. MD simulations of DMPU in both solvents demonstrate that \(\text{cis-cis}\) and \(\text{cis-trans}\) isomers are populated at RT, while \(\text{trans-trans}\) is dominant in DPU under similar conditions.

CHED 1386

Synthesis and extraction of metallocarbohydrynes

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Synthesis and isolation of metallocarbohedrynes was attempted using the arc-discharge technique followed by soxhlet extraction. Parameters such as electrode composition, discharge pressure, and discharge current were varied during the investigations. Optimization of these parameters will be discussed.

CHED 1387

Reaction mechanism for the conversion of creatine to N-formyl-N-methylglycine by hypochlorous acid in aqueous solution

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The reaction of creatine with hypochlorous acid is of biological interest. The absorbance of the reaction mixtures as a function of time has been measured at pH 4, 7, and 10. The rate of the reaction and the observed spectral changes differ significantly over this range. A unified mechanism leading to the known product, N-formyl-N-methylglycine, has been proposed. These experimental spectral have been fit using rate constants for the important steps of the mechanism and molar absorptivities of the various proposed intermediates. Insight into this very complex mechanism are gleaned from the analysis and are the subject of this presentation.

CHED 1388

Energetic, structural, and spectral data for noble gas hydride cations in the interstellar medium

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Due to the recent discovery of ArH⁺ in the Crab Nebula, questions of the existence of other noble gas hydride cations, like ArH₂⁺, NeH₂⁺, ArH₃⁺, and NeH₃⁺, have arisen. As part of our exploration of this area, we show that ArH₂⁺ is an intermediate in the proposed reaction that leads to the molecule detected in the Crab Nebula ArH⁺: Ar⁺ + H₂ -> ArH⁺ + H. Additionally, Ar + H₂⁺ -> ArH⁺ + H is also shown to be another potential reaction leading to ArH⁺. Ne are H₂⁺ are found as the products of the equivalent reaction rather than NeH⁺ + H. This gives a possible explanation as to the absence of NeH⁺ in the Interstellar Medium (ISM). Following from this, high-level quantum chemical computations also provide the necessary rovibrational spectroscopic data for NeH₂⁺, ArH₂⁺, ArH₃⁺, and NeH₃⁺ through the use of quartic and cubic force fields. The most common isotopologues have also been included in this study: ²⁰Ne, ²²Ne, ³⁶Ar, ³⁸Ar, ⁴⁰Ar, ¹H, and D. The dipole moments for the dihydride cations are relatively large at 5.61 D for NeH₂⁺ and 4.37 D for ArH₂⁺. The spectroscopic constants, structural data, and energetics provided will assist in the potential detection of these open-shell noble gas hydride cations in the laboratory as well as, potentially, in the ISM.
The rotational spectrum of the ground and excited vibrational states of ArH$_2^+$ in THz at 40 K with the shorter lines corresponding to $^{38}$ArH$_2^+$ and the taller lines to $^{36}$ArH$_2^+$ based on the relative natural abundances of the argon isotopes.

CHED 1389

Spectroscopic and microscopic analysis of aggregation effects in N-alkylated perylene diimides

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Perylene diimides (PDIs) are conjugated organic molecular compounds that can potentially be used in thin film material devices, such as solar cells and field effect transistors. One of the main factors affecting the viability of making PDI devices is the control of the morphology of these films. Here we report a spectroscopic and microscopic analysis of the thin film formation of geometrically altered PDI molecules. This study, through a survey of several linear and branched N-alkylated PDIs, aims to advance what is known on aggregation effects on PDI electronic properties. The
spectroscopic signatures of the thin film aggregates were analyzed using a global fitting procedure. The results show that although the solution phase spectra are nearly identical for all compounds, the electronic states associated with charge transfer in the films can shift from 530 to 580 nm, depending on the side chain attached to the central PDI moiety. The neutral states do not exhibit as much of a pronounced shift. The films having a larger degree of charge transfer also show enhanced crystallization properties. Finally, the orientation dependence of aggregates was examined via polarization absorption microscopy. The charge transfer states exhibit a larger degree of molecular alignment compared to the neutral aggregation states.

CHED 1390

Role of low-energy (< 20 eV) electrons in astrochemistry

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In the interstellar medium, UV photolysis of ice mantles surrounding dust grains is thought to be the mechanism that drives the formation of “complex” molecules. The source of this reaction-initiating UV light is assumed to be local because externally sourced UV radiation cannot penetrate the ice-containing dark, dense molecular clouds. Specifically, exceedingly penetrative high-energy cosmic rays generate secondary electrons within the clouds through molecular ionizations. Hydrogen molecules, present within these dense molecular clouds, are excited in collisions with these secondary electrons. It is the UV light, emitted by these electronically excited hydrogen molecules, that is generally thought to photoprocess interstellar icy grain mantles to generate “complex” molecules. In addition to producing UV light, the large numbers of low-energy (< 20 eV) secondary electrons, produced by cosmic rays, can also directly initiate radiolysis reactions in the condensed phase. The goal of our studies is to understand the low-energy, electron-induced processes that occur when high-energy cosmic rays interact with interstellar ices. Using post-irradiation temperature-programmed desorption (TPD) and infrared reflection absorption spectroscopy (IRAS), we have investigated the radiolysis initiated by low-energy (5 – 20 eV) electrons in condensed methanol, ammonia, and water at ~ 90 K under ultrahigh vacuum (1×10^{-9} Torr) conditions. Our experimental results suggest that low-energy, electron-induced condensed phase reactions may contribute to the interstellar synthesis of “complex” molecules previously thought to form exclusively via UV photons.

CHED 1391

Calculating the J=0 vibrational states of noble gas trimers using an energy selected basis

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Small noble gas clusters are useful benchmark systems for studying the properties of van der Waal clusters. Here we present an efficient quantum method for calculating the \( J = 0 \) vibrational energy levels of noble gas trimers using an energy selected basis (ESB) representation. In the ESB approach, for each coordinate \( (q_i) \) a one-dimensional effective Hamiltonian \( (H_{qi}) \) is defined in which the effective potential \( (V_{qi}) \) is the result of minimizing the true three-dimensional potential with respect to the other coordinates. The eigenstates \( (\Phi_{n,q_i}) \) and eigenenergies \( (\epsilon_{n,q_i}) \) of each marginal Hamiltonian are calculated using a discrete variable representation (DVR). The ESB then is composed of direct product basis functions \( (\Theta_{nlm} = \Phi_{n,q_1}\Phi_{n,q_2}\Phi_{n,q_3}) \), but only those functions for which \( \langle H \rangle_{nlm} < E_{cut} \) are used. Iterative diagonalization is used to calculate the eigenvalues and eigenfunctions of the resulting matrix. Our results are compared with previous calculations in literature with respect to accuracy and efficiency.

CHED 1392

Analysis of the metal sulfate-sodium silicate “reverse chemical garden” reaction

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Injecting sodium silicate solution into less dense metal sulfate solution causes precipitation of metal silicates in downward-growing structures—the reverse of the well-known “chemical garden” phenomenon. The reaction produces qualitatively different structures depending on the reaction conditions (injection rate of aqueous sodium silicate and concentration of copper(II) sulfate). We report a new quantitative methodology for analyzing the growth of these structures, fostering an improved understanding of the reaction.

CHED 1393

Matrix isolation studies of tetrakis(dimethylamino)titanium IV & ozone

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Matrix isolation studies are important in understanding and improving the design of semiconducting thin films. Semiconducting thin films have a wide range of applications in electronic devices. Tetrakis(dimethylamino)titanium is an important metalorganic precursor used in chemical vapor deposition and a good candidate for studies of semiconductor thin film formation. The purpose of the study described herein was to investigate the mechanism of thermal and photochemical reactions of tetrakis (dimethylamino) titanium (IV) with ozone using matrix isolation techniques and
theoretical calculations. Ozone is used as an oxidizer because it has significant advantages such as high oxidation potential, cleanliness, volatility and it leads to rapid and effective metal oxide thin film formation. The matrix isolation technique was used to isolate and characterize reactive intermediates at a low cryogenic temperature of 14 degrees Kelvin and under high vacuum. The chemical species was trapped in an argon matrix and infrared spectroscopic techniques were used to characterize the intermediate. Those data are presented and discussed as is the method development.

CHED 1394

Investigating the influence of lithium intercalation on dispersive electron mobility kinetics in dye-sensitized solar cells

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Dye-sensitized solar cells provide an inexpensive technology to harvest solar energy. However the multiple kinetic processes and the influence of various parameters, such as lithium intercalation, on these kinetics are still not fully understood. This study uses accessible instrumentation and materials to examine the electron mobility kinetics within the TiO$_2$ nanoparticle film. Lithium intercalation into these films and how it affects the dispersive electron transport kinetics are of particular interest.

CHED 1395

Thermodynamics contribution to the stability of PrP$^C$ in model plasma membranes

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Prion diseases are a type of transmissible spongiform encephalopathies, a group of fatal neurodegenerative diseases in humans and other mammals. The prion protein is the main component of prions. Prion proteins propagate biological information by conversion of the cellular conformer of the prion protein, PrP$^c$, to the infectious misfolded scrapie conformation, PrP$^{Sc}$, in the absence of nucleic acid. Prion diseases can be present as sporadic, inherited, iatrogenic, or acquired disorders. Much knowledge has been contributed to the possible cofactors inducing the conversion of PrP$^c$ to PrP$^{Sc}$. However, we are far from understanding the role of plasma membrane surfaces as a possible cofactor in the induction of conformational changes in PrP molecules. To fill this gap, we employ molecular modeling techniques to monitor the thermodynamic stability of the well-studied Syrian hamster PrP$^c$ protein inserted in plasma membranes. Preliminary results suggest that the stability of PrP$^c$ is modulated by the relative orientation and the hydrophobic mismatch of the PrP$^c$ protein when embedded into the model membrane.
CHED 1396

Computational and crossed molecular beam study in the synthesis of boronylallene

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The gas phase reaction of boron monoxide radical and allene was investigated computationally through \textit{ab initio} electronic structure calculations and experimentally using the crossed molecular beam technique. The reaction proceeds through the formation of a van der Waals complex isomerized by the addition of the boron monoxide radical to the terminal carbon atom of allene. The chemically active intermediate decomposes via Hydrogen elimination at the boronyl carbon to synthesize boronylallene in an exothermic reaction. RRKM statistical calculations suggest minor reaction pathways leading to a 1-propynyloxoborane and 3-propynyloxoborane product. The boronylallene reaction was compared with the cyanoallene and boronyl–methylacetylene reactions to probe differences and similarities of the isoelectronic systems. We present a novel gas phase synthesis of the elusive boronylallene, which has proven difficult to isolate in the condensed phase, and demonstrate that the crossed molecular beams technique is useful method for synthesis of highly reactive organyloxoboranes.

CHED 1397

Characterization and the effect of pH and temperature on the degradation of creatine ascorbate, di-creatine ascorbate and creatine di-ascorbate

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The purpose of this research is to use proton NMR to characterize three newly synthesized creatine salts; creatine ascorbate, di-creatine ascorbate, and creatine di-ascorbate. Additionally, data from the stability study to determine the kinetic degradation and shelf life of the three compounds will be reported. The effect of different temperatures, solvents, and pH will be observed for the three creatine salts over a 45 day time range to explore the effect on kinetic degradation. Comparison of these results to previous studies on the degradation of other creatine salts performed within our research group will be presented.

CHED 1398

Investigating the neutron inelastic scattering cross sections for $^{54}$Fe through γ-ray spectroscopy
As Generation IV nuclear reactors are developed, advanced data on the behavior of structural materials, especially the naturally occurring isotopes of Iron, are needed. This research investigates the excitation of $^{54}$Fe levels resulting from inelastic neutron scattering. Due to the need for high resolution information, γ-ray measurements were made using the 7 MV Van de Graaff accelerator at the University of Kentucky Accelerator Laboratory and its neutron production and γ-ray detection facilities. A highly enriched sample of $^{54}$Fe, a 5.8% naturally occurring isotope, was bombarded with an almost mono-energetic neutron beam ranging in energies from 1.5 to 4.7 MeV in 200 keV steps. The resulting γ-ray emissions were collected using HPGe detectors and analyzed to reconstruct the excited level structure of the $^{54}$Fe nucleus and its decays; γ-ray production cross sections were deduced and used to determine neutron inelastic cross sections. Standards of Al, Ti, and V were analyzed in the same manner and compared with ENDF cross sections to establish an absolute normalization factor for the neutron inelastic cross sections measurements on $^{54}$Fe. Results from our studies and comparisons to ENDF evaluated cross sections for $^{54}$Fe will be presented.

CHED 1399

Compositional characterization of cobalt lithium phosphate thin films using atomic absorption spectroscopy

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Cobalt phosphate, lithium phosphate, and cobalt lithium phosphate thin films were prepared by spin casting aqueous precursor solutions onto silicon substrates. In cobalt lithium phosphate films two methods were used to control the cation ratio present in the films. One series of samples was prepared by spin casting alternating layers of cobalt phosphate and lithium phosphate solutions. The ratio of cobalt phosphate to lithium phosphate layers was varied in order to control the cation ratio. In the second series, the two precursor solutions were mixed in varying ratios before spin casting. In each case, the final film compositions were examined by etching the films with nitric acid and using atomic absorption spectroscopy to measure the concentration of the cobalt and lithium metals. In the cobalt phosphate and lithium phosphate films, x-ray reflectivity data were collected to determine the absolute thickness of the films. Following this, films were etched with a known volume of nitric acid, and the concentration determined using
atomic absorption spectroscopy. The concentrations were then correlated to film thickness, allowing film thickness to be approximated using atomic absorption spectroscopy.

CHED 1400

Driving forces of the stability of Alzheimer’s Aβ aggregates in model membranes

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Alzheimer’s disease is a common form of dementia that affects about 5 million people in the United States of America. A wealth of data links the disease to the misfolding and clumping of the Aβ peptide. The precise mode by which the aggregates induce toxicity, however, is unknown. Recent findings suggest that cell membrane disruption induced by Aβ aggregates triggers cytotoxicity. The goal of our research project is to gain insight into the mechanism by which Aβ aggregates perturb the local environment of model plasma membranes. We use coarse grain molecular dynamics simulations to monitor the interactions of the aggregate at different levels of insertion in model membranes. Our preliminary results suggest that the aggregate’s motion is modulated by the relative orientation and surface electrostatics of the protofilament. These observations shed light on the stability of the aggregate’s insertion mode and the mechanism of membrane disruption.

CHED 1401

Vacuum ultraviolet photolysis matrix isolation infrared spectroscopy of GeH\textsubscript{4} in argon and nitrogen atrices

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Germane (GeH\textsubscript{4}) was deposited in matrices of argon and nitrogen (N\textsubscript{2}) at 12 K with simultaneous vacuum ultraviolet (VUV) photolysis, producing transient species (unstable molecules) studied using infrared spectroscopy. Based on previous literature research, VUV photolysis of germane in an argon matrix produced fragments of the formula GeH\textsubscript{x} (x = 1, 2, 3). Based on previous work with silane (SiH\textsubscript{4}) from our group, VUV photolysis of germane in a nitrogen matrix was expected to produce fragments of the formula GeH\textsubscript{x}N\textsubscript{2} (x = 1, 2, 3), but instead produced fragments of the formula GeH\textsubscript{x} in a nitrogen matrix. Theoretical calculations were performed using the Gaussian 03W computational chemistry program for each observed fragment, using density functional theory with the B3LYP functional and the aug-cc-pVDZ basis set. The theoretical calculations elucidated probable structures of the observed fragments, as well as simulated infrared spectra of each fragment. These simulated infrared spectra were
compared with the experimental spectra to help assign observed infrared peaks to specific fragments.

CHED 1402

Sum frequency generation at the DMSO/air interface: Theory meets experiment

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With the recent development of High Resolution Broadband Sum Frequency Generation (HRBBSFG) it is possible to obtain true SFG spectra with negligible instrumental line broadening. This allows quantitative analysis of the spectrum using complex Lorentzian fitting, and through the polarization null angle (PNA) method the molecular orientation can be determined. Using the polarizability tensor and dipole moment of individual vibrational modes to construct the full hyperpolarizability tensor allows for orientational averaging of the third rank tensor without use of generalities. For both symmetric and asymmetric vibrational modes of DMSO the results of the PNA method can be recreated computationally and various experimental configurations can be tested, such as changing incident angles for both IR and visible wavelengths. The results confirm the validity of the PNA method and the polarization selection rules of SFG, as well as create a standard procedure to be used with calculated polarizability tensors and dipole moments for vibrational modes of other molecules.

CHED 1403

Determination of the limiting equivalent conductivity and thermodynamic equilibrium constant for the formation of LaCl²⁺ Ion-pairs in water

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A flow conductance cell was used to determine the equivalent conductivities for aqueous solutions of lanthanum chloride and lanthanum chloride/hydrochloric acid mixtures at 25.00 °C with ionic strengths between 0.00003 and 0.263 mol kg⁻¹ solvent. Non-linear regression was performed on the data using the Turq-Blum-Bernard-Kunz (TBBK) conductivity equation, which has been shown to adequately model unsymmetrical electrolyte mixtures. Preliminary calculations yield a statistically significant thermodynamic equilibrium constant Kₐ for the LaCl²⁺ ion-pair of 95 ± 29. The λ˚ of the ion-pair was found to be 101.2 ± 3.7 S cm² equiv⁻¹, which is believed to be the first accurately reported λ˚ for an ion-pair. This value is larger than λ˚ for the La³⁺ ion (69.35 S cm² equiv⁻¹), which indicates a larger mobility for the ion-pair than for the metal ion.
CHED 1404

Accurate quantum models of methylphosphonate adsorption onto a stable rutile surface

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Modification and functionalization of TiO$_2$ surfaces by adsorption of phosphonic acids is of great interest in view of its applications in biomaterials and corrosion protection. Experimental studies indicate strong and stable P-O-Ti bond formation during adsorption of phosphonic acid on TiO$_2$ surfaces. However, the mode and strength of adsorption continues to be debated. We have investigated the adsorption modes and bonding strength between the rutile (110) surface and methylphosphonate using quantum chemistry with periodic boundary conditions. The Crystal09 quantum software package was used with the Perdew-Wang ‘91 functional and various basis sets. The surface free energy, structure, ligand binding energy, and vibrational spectrum were computed. The computations indicate tridentate bonding between the rutile (110) surface and methylphosphonate, which is consistent with experimental data from FTIR spectroscopy. Understanding the mode and strength of adsorption can lead to a new generation of biomaterials that could withstand corrosion and prevent biological rejection.

CHED 1405

Synthesis and characterization of indium phosphide quantum dots for use in laser diodes

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The study of quantum dots consisting of colloidal nanocrystal semiconductor particles in strong quantum confinement have become a very important topic of interest due to their applications in medical imaging, quantum computing, solar cells, and diode lasers. Indium phosphide quantum dots in particular have been used in laser diodes. The goal of this study is to synthesize indium phosphide quantum dots and characterize through: Tunneling Electron Microscopy, Ultraviolet-Visible Spectroscopy, and Fluorescence spectroscopy. These quantum dots will then be used to prepare a diode. Lastly, the diode will be prepared for use in a custom built laser.

CHED 1406

Rovibrational analysis of SiOH$^+$, HSiO$^+$, and other third row atom hydroxides
The ionosphere is an important layer in the Earth’s atmosphere that allows radio communication to distant locations due to electrically charged atoms and molecules that are constantly bombarded by ultraviolet radiation from the sun. Most importantly for our study, SiOH$^+$ and its other isomeric partner, HSiO$^+$, are likely among the molecular species responsible for radio proliferation. Studies have been made to provide the existence of these molecules in the gas phase by the use of neutralization-reionization mass spectrometry (NRMS). It has also been proposed that due to distribution of the ground state, Si$^+$ reacts with H$_2$O in the ionosphere to create SiOH$^+$. Our computations of SiOH$^+$ make use of quartic force fields and high-level coupled-cluster theory to derive the rovibrational spectroscopic constants for SiOH$^+$ and HSiO$^+$. These computations provide data in order to examine the possibility that these two cations may exist in the ionosphere or even in the larger interstellar medium (ISM), the region between stars. Astronomical observations and laboratory experiments of SiOH$^+$ and HSiO$^+$ may further advance our understanding of the ISM and ionosphere but only if reference data is available. This work serves to provide this data for comparison. Additionally, other third row atom-including (Si, P, S) hydroxide anions, cations, and neutrals data are also reported.

CHED 1407

Impact of tetrazine location in benzobisaxozole possessing cruciforms

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A series of molecules possessing benzobisaxozole cores and various aryl ring substituents (i.e. phenyl and thiophenyl) coupled with tetrazine were examined using TD-DFT B3LYP/6-31G*. The HOMO, LUMO, and optical band gaps were generated and compared. In addition, the electrostatic potential maps and the frontier orbitals were examined. The results of these studies is presented here.

CHED 1408

Proposal for a more efficient acoustic array design to determine flow through a cylindrical conduit

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A new design is proposed for the existing acoustic array, a device used to measure the flow rate through a cylindrical conduit via a series of transducers. The original acoustic array consists of a 2.000 inch diameter steel pipe with 128 transducers located along
the top, spaced 2.000 inches apart along the length of the pipe. The total length of the original acoustic array in this configuration is over 21 feet long (254 inches). The analog acoustic information obtained from the array is sent through an amplifier, an analog digital converter, and then to a computer to be analyzed in order to determine rate of flow. The new design proposes a 3.000 inch diameter steel pipe with 128 transducers located along the equatorial axis of the pipe, spaced 0.287 inches apart. This new design leads to a more manageable apparatus, as the pipe length needed will be decreased from over 21 feet to less than 3.5 feet in length.

CHED 1409

Kinetics and dynamics of the photorearrangement reactions of aryl-substituted thiophenes

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Conjugated polymers provide an excellent material for applications in molecular electronics and organic photovoltaic devices due to their low cost and flexibility compared with traditional inorganic conductors. These new organic-based materials are often constructed from oligomeric backbones consisting of thiophene-based subunits. However, aryl-substituted compounds sometimes undergo unwanted photorearrangement reactions under irradiation, which potentially degrades the material over prolonged exposure and therefore limits the efficiency of devices. Therefore, these reactions need to be studied and understood in order to intelligently design new materials for optimal performance. This contribution reports new quantum yield measurements for the solution-phase rearrangement reactions of several aryl-substituted thiophene compounds, as well as complementary transient absorption spectroscopy measurements that reveal the excited-state lifetimes and intersystem crossing rates. The target compounds are two- and three-ring systems that provide simple models for probing the electronic and nuclear dynamics of conjugated molecules in response to optical excitation. Quantum yields for the very low-yield decomposition reactions were measured by following the change of the static absorption spectrum as a function of irradiation time. The transient absorption spectra of the thiophene-based molecular building block compounds were measured using ultrafast pump-probe spectroscopy.

CHED 1410

Characterization of a methanol-hexafluorobenzene complex using matrix isolation infrared spectroscopy

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Matrix isolation infrared spectroscopy was used to characterize a 1:1 complex of methanol (CH$_3$OH) with hexafluorobenzene (C$_6$F$_6$). Co-deposition experiments with CH$_3$OH and C$_6$F$_6$ were performed at 20 K using argon as the matrix gas. New infrared peaks attributed to the CH$_3$OH-C$_6$F$_6$ complex were observed near the O-H stretching vibrations of CH$_3$OH and near the out-of-plane bending vibration of C$_6$F$_6$. Identification of the new infrared bands to those of the complex were established by comparing the co-deposition spectra with the spectra of the individual monomers and by performing density functional theory calculations for the CH$_3$OH-C$_6$F$_6$ complex at the B3LYP/aug-cc-pVDZ level. The calculations predict a stable minimum for the complex, termed a lone pair-π structure. Comparing the calculated shifts of the vibrational frequencies to the experimental shifts, it is concluded that the lone pair-π structure is consistent with the experimental frequencies and is most likely the observed geometry of the complex in the matrix isolation experiments. Co-deposition experiments were also performed using deuterated methanol (CD$_3$OD) and hexafluorobenzene at 20 K in an argon matrix and the analogous peaks of the CD$_3$OD-C$_6$F$_6$ complex were observed.

CHED 1411

**Microparticle transport across ionic liquid based interfaces**

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The self-assembly process of microparticles and liquid-liquid interfaces is driven by strong adhesive forces up to the order of 10$^6$ kT. Microparticles can transport across a liquid-liquid interface, but they first must overcome the capillary forces that exist between the surface of the particles and the liquid interface. This usually requires the application of a shear force, or even the use of surfactant functionalization. However, with some ionic liquids (ILs), the spontaneous transport of microparticles without any external agitation is possible because of the ionic liquid's exceptional extraction capabilities. The systems investigated included IL/water and IL/oil interfaces. In these systems, single particles as well as clusters of particles were able to adsorb to, then cross, and detach from the liquid-liquid interface into the ionic liquid droplet. This phenomena occurred because the dissolved ions in the non-ionic liquid bulk phase covered the surface of the particles, causing hydrophobization and leading to more desirable interactions with the ionic liquid. Thus, the particles were able to overcome the adhesive forces and cross the liquid-liquid interface. Fluorescence intensity of particles in the continuous water phase in the presence of ionic liquid droplets was measured to quantify the degree of absorption with respect to each ionic liquid.

CHED 1412

**Location of deuterated ammonia in Sagittarius B2**
Multiple transitions of singly-deuterated ammonia was detected in Sagittarius B2 using the Karl G. Jansky Very Large Array (VLA) with a resolution of 3" and the Australia Telescope Compact Array (ATCA) with a resolution of 10". Deuterated ammonia was detected in two sources in the Northern core of Sgr B2. The most commonly known source, the Large Molecule Heimat, had a velocity of ~61 km/s. The other source we designate as h had a velocity of ~73 km/s. Multiple transitions of ammonia and the isotopologue $\text{^{15}NH}_3$ were detected as well. $\text{NH}_3$ is a useful tracer of temperature, but in Sgr B2 the transitions were too optically thick to measure accurately. Instead $\text{^{15}NH}_3$ was utilized to find a rotation temperature and thus kinetic temperature. The temperature of h was higher than that of LMH, which is unexpected, because LMH is more chemically complex and contains an embedded ultra-compact HII region, suggesting it is the more evolved source, and should have a warmer temperature. The column densities of $\text{^{15}NH}_3$ and $\text{NH}_2D$ were used to find the deuterated fractions in each source. The ratio of $^{14}\text{N}$ to $^{15}\text{N}$ previously measured in Sgr B2 was used to approximate the amount of ammonia. The deuteration fraction was found to be ~40x higher in h than LMH, which is surprising given h is the hotter source and fractionation reactions that lead to higher deuteration of molecules are favored in cooler temperatures. We will discuss possible explanations for these discrepancies.

CHED 1413

**Synthesis of chloromethylsilyl isocynate**

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$\text{SiH}_3\text{CH}_2\text{Cl}$ when reacted with Ag-NCO was expected to produce $\text{SiH}_3\text{CH}_2\text{NCO}$, however $\text{CH}_2\text{ClSiH}_2\text{NCO}$ was obtained. As apparent metathesis between Ag-N and Si-H bonds occurs to form the observed product and Ag-H which rapidly decomposes to evolve hydrogen gas. We confirmed this finding by reacting $\text{SiH}_2\text{BrCH}_2\text{Cl}$ ($\text{BBr}_3$ to $\text{SiH}_3\text{CH}_2\text{Cl}$) and $\text{SiH}_2\text{ClCH}_2\text{Cl}$ (SnCl4 to $\text{SiH}_3\text{CH}_2\text{Cl}$) with Ag-NCO, and $\text{CH}_2\text{ClSiH}_2\text{NCO}$ was obtained. The infrared spectra of three products obtained from the three reactions were identical and have been identified by CNMR, HNMR, infrared, and microwave spectroscopy. The molecular orbital _ab initio_ calculations of this compound indicate that the _trans_ conformer is 0.5 kcal more stable than the gauche form.

CHED 1414

**Sustained photocurrent in CdS/$\alpha$-Fe$_2$O$_3$ stacked thin films on titania-coated transparent conductive substrates**
The viability of water-splitting catalysts as commercial sources of renewable energy is strongly dependent on the ability of these materials to utilize the visible portion of the solar spectrum, though most narrow band gap materials ($E_g < 3\text{eV}$) are capable of efficiently driving only one half of the water splitting reaction (i.e hydrogen evolution reaction or the oxygen evolution reaction), not both. In the absence of sacrificial reagents, these materials are subject to deactivation or decomposition. Stacked thin films of CdS ($E_g 2.4\text{eV}$) and $\alpha$-$\text{Fe}_2\text{O}_3$ ($E_g 2.2\text{eV}$) have been fabricated by sequential electrodeposition on titania-coated transparent conductive oxide substrates to photocatalytically drive the full water splitting reaction. Under visible irradiation, $\alpha$-$\text{Fe}_2\text{O}_3$ is known to drive the oxygen evolution reaction, leaving behind an accumulation of conduction band electrons. These electrons act to suppress the decomposition of the hydrogen evolution catalyst, CdS, which would otherwise proceed due to oxidation of sulfide by trapped valence band holes. Stabilization of the composite is confirmed by a two-electrode photocurrent decay experiment. Further research is underway to optimize the relative film thicknesses.

CHED 1415

Gel properties of polyisoprene and stearic acid shape memory composite

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Shape memory polymer blends consist of a permanent cross-linked network and a temporary network. The former generates large entropic forces upon deformation that drive shape recovery while the latter inhibits the entropy-driven recovery of the system and is designed to be easily modulated. A previous study by Weiss et. al. indicated that shape memory behavior is consequential of dipolar interactions between an ionomeric permanent network and crystalline zinc stearate temporary network. However, Brostowitz et. al. demonstrated shape memory behavior by swelling natural rubber (NR) with stearic acid (SA), a composite devoid of an ionomeric phase. It is believed that SA crystals inhibit the entropic movement of the cross-linked network back to its unstrained state until the system is brought to its switching temperature ($T_s$)—the melting point of stearic acid ($T_m = 70^\circ\text{C}$). Above this temperature, shape memory is observed as the system is entropically driven to recovery.

In this study, we aim to test the validity of the above statement by better characterizing the interactions of the permanent (NR) and temporary (SA) networks. Differential scanning calorimetry (DSC) showed one-phase mixing at all SA concentrations. Optical microscopy also demonstrated one-phase mixing at all concentrations and revealed cooling rate dependent crystal formation. Using plate-plate oscillatory shear rheology,
the viscoelastic properties of the SA/NR composites were investigated and found to have a SA concentration dependence. Each of these findings suggest tunable shape memory can be achieved with these composite materials.

CHED 1416

Smart hydrogel thin films for organophosphorus nerve agent detection

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Since the development and use of organophosphorus compounds as nerve agents and pesticides, methods of dealing with their toxicity to humans have been intensely researched. Smart hydrogels are defined as hydrogels that undergo relatively large and abrupt changes in their architecture or physical properties in response to environmental changes. Specific molecular recognition is a remarkable feature of the smart hydrogels that will allow them to be used to fabricate amazing sensing devices. This research project focused on the design, synthesis, and characterization of smart hydrogel thin films created on gold coated microscope slides. The thin hydrogel layers functionalized with fluorescent coumarin markers will potentially have fast quenching rates when exposed to nerve agent mimics. Fluorescence quenching of the thin films could easily be observed under UV light, enabling the naked eye detection of organophosphorus nerve agents which will allow for real world applications.
Synthesis and characterization of polyaniline-TiO$_2$ nanocomposites

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Polyaniline-TiO$_2$ nanocomposites were synthesized by oxidative polymerization at the presence of ammonium peroxydisulfate at 273.15 K. TiO$_2$ nanoparticles in the range of 10-60 nm were synthesized by sol gel method using titanium isopropoxide. The polymerization and doping of polyaniline were accomplished simultaneously at the presence of TiO$_2$ nanoparticles in an aqueous solution of 1.0 M HCl. TiO$_2$-polyaniline nanocomposites were characterized by SEM, XRD, FTIR, and Raman spectroscopy. The four-probe method was used to measure the electrical conductivity of composite films prepared by the spin-coating method on ITO glass. The nanocomposite samples were found to be partially crystalline with conductivities of $1.0 \times 10^{-2}$-$8.0 \times 10^{-2}$ S/cm. XRD studies confirm a TiO$_2$ particle size between 10-60 nm. The experimental work conducted, the characterization results, and the interpretation of these results are presented in this poster presentation.

Ring-opening metathesis polymers (ROMP) with organic radical groups for treatment of traumatic brain injuries (TBI)

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Hypotension and the resulting hypoxia resulting from hemorrhagic stress have the potential to threaten internal organs through oxygen deprivation, resulting in cellular death, especially in the brain. Traumatic brain injuries (TBI) occurring in conjunction with severe hemorrhagic stress can cause irreversible damage to neurons due to this oxygen starvation, resulting in damage in the form of reduction of cognitive function. A proposed treatment using isotonic solutions containing hemoglobin-based oxygen carriers (HBOC’s) which were intended to provide oxygen, similar to red blood cells, was developed. However, HBOC’s were found to have excessive oxidative potential, causing damage to the injured cells from the superoxide radical released by the protein. To address this, HBOC’s have been modified to incorporate polyethylene glycol (PEG) and (2,2,6,6-tetramethylpiperidin-1-yl)oxidanyl (TEMPO) covalently bonded to the protein. These polynitroxyl PEGylated hemoglobin (PNPH) derivatives combine antioxidant activity with a larger molecular size which significantly reduces the toxicity of HBOC’s. These PNPH’s are limited by strict ratios between the two functional groups as well as a demanding synthesis. In our research, we plan to incorporate TEMPO functional groups into organic polymers with controlled molecular weights to bind to the hemoglobin protein. For this purpose, we have developed syntheses for 7-
oxanorbornene derivatives containing TEMPO functionalities for use as monomers in ROMP. We will present preliminary results in the monomer and homopolymer syntheses, as well as the characterization of the products.

CHED 1419

Synthesis and characterization of 3-trifluoromethylstyrene copolymers

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Fluorinated polymers are of great interest due to their unique combination of properties such as chemical inertness to acids and bases, low dissipation factors, and excellent weather resistance. Similarly, copolymers exhibit interesting properties due to different characteristics that each individual monomer contributes to the whole. The 3-trifluoromethylstyrene monomer was synthesized in two steps. 3-bromobenzotrifluoride was converted into a Grignard reagent and reacted with acetaldehyde to make the 1-phenylethanol derivative. This was then dehydrated to make 3-trifluoromethylstyrene. The purified the styrene monomer has been made and polymerization with methyl methacrylate is forthcoming. From here characterization of the resulting materials and comparison to other similar copolymers will be presented.

CHED 1420

Novel polymeric redox mediator for use in biofuel cells

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The promise of in vivo powering of implanted medical devices provides impetus for research on glucose/O₂ biofuel cells¹. Linear poly(ethylenimine) (LPEI) modified with ferrocene redox mediators has been successfully used in the past to fabricate bioanodes for use as glucose sensors and in biofuel cell systems². While very useful and effective, the redox potentials available to the ferrocene moiety and it’s derivatives limit the electrochemical potentials (voltages) that can be generated in such biofuel cells. This project aims to decrease the redox potentials of the bioanodes through the use of the nitrophenoxo moiety as a mediator. Reaction of 4-nitrophenol with an excess of a dibromoalkane generates an Ω-bromoalkynitrophenyl ether, which can be attached to an LPEI backbone by a substitution reaction³. The mole ratio of the two reactants is used to control the substitution of the mediator on the polymer and was found to effect the solubility of the polymer in water. This polymer shows a reversible, one electron reduction potential at -0.20 volts versus SCE in a PBS buffer, significantly lower than for most ferrocene redox couples. The polymer was used to fabricate glucose oxidase-based glucose sensors with varying degrees of crosslinking. High degrees of crosslinking result in poorer current responses, and interaction of the mediator with the
glucose oxidase seems to be different from its interaction with ferrocene moieties. Amperometric data taken at -0.058 volts versus SCE shows an initial glucose response at 10-20 nM, with a slow, continuous increase in current, rather than the expected Michaelis-Menton behavior. Effects of changing the length of the alkane chain and redox moiety will be discussed.

CHED 1421

Phase-selective studies of polyisobutylene-bound dyes using antileaching agents

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The recovery and recyclability of catalysts is an objective of green chemistry that can achieved by attaching polymeric supports to such catalysts. For example, polymer supported catalysts, ligands, sequestrants or reagents and liquid/liquid biphasic systems have been used to facilitate organic synthesis by recovering and recycling of catalysts using a polymer’s phase selective solubility. Thermomorphic biphasic systems consist of two or more immiscible solvent phases at room temperature, where the polymer supported catalyst is phase-selective to one of the phases and exemplify this green chemistry strategy. However, while these strategies allow for single phase reactions, small amounts of leaching of the polymer-bound catalyst still occurs. This project describes a new inexpensive way to further minimize this loss of a ligand or precious metal catalyst. Polyisobutylene (PIB), a hydrophobic polymer, was used as the polymer support. Polyisobutylene-bound dyes were first prepared and then used as surrogates of the polymer-bound catalyst to test how polymeric cosolvets affect the separation efficiency of these catalyst/ligand analogs. Studies with hydrophobic alkane phase-selectively soluble polyisobutylene-bound dyes in different polar/non-polar solvent mixtures showed that the leaching of the polymer-supported dye into the polar phase could be significantly decreased by the use of polymer cosolvents. UV-Visible spectroscopy studies showed that both polymeric additives and changes in the nature of the alkane cosolvent contribute to the desired anti-leaching effects in these biphasic systems.
**CHED 1422**

**Synthesis of hierarchically porous polymer network for carbon dioxide capture**

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Due to the increasingly negative impact of carbon dioxide gas emissions on the environment, carbon dioxide capture has been considered a potential, low-cost solution for the reduction of emissions. While previous studies have proved that hierarchical structure improves the efficiency of adsorption, the preparation process lead to several disadvantages including large weight loss of precursor materials and unpredictable side-reactions at high temperatures. In this experiment, a hierarchically porous polymer network (HPPN) was synthesized using a novel method to allow for more accurate control of the porosity distribution and also systematic study of the structure-property relationship to discover the effect of hierarchically porous structure on CO$_2$ adsorption/desorption. Silica nanoparticles were activated with 4-bromo-phenyl(trimethyl) silane to act as a sacrificial template in the synthesis of HPPN. Tetrakis(4-bromophenyl)methane was polymerized in the presence of activated silica and resulted in a porous polymer network (PPN) surrounding the nanoparticle template. The removal of silica templates resulted in materials with hierarchical pore dimensions, 2-5 nm originated from the intrinsic molecular porosity and 15-30 nm from sacrificial silica nanoparticles. Due to the silica aggregates present in the commercial starting materials, the weight ratio of silica particles to monomers was critical to the structures and properties of the HPPN. With an optimized feeding ratio, the HPPN proved to maintain the high porosity of the PPN network while also introducing the hierarchical structure for more efficient CO$_2$ adsorption and desorption.

**CHED 1423**

**Synthesis of four-armed calixarene-core polylactide/polyethylene glycol star block copolymers using click chemistry**

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The chemical synthesis of polymer building blocks that have varied molecular architectures and are rationally designed to self-organize or assemble into higher-order structures is critical to the design of multifaceted materials. Recently, our research has focused on the synthesis of four-armed calixarene-core polylactide (PLA)/polyethylene glycol (PEG) star block copolymers. These polymers have the potential to form aqueous micelles for use in drug-delivery applications. To prepare the new star block copolymers, a four-armed PLA star homopolymer was made by lactide ring-opening polymerization using a tetrafunctional calixarene initiator. In order to synthesize the star block copolymers, the PLA end groups were functionalized with alkynes and then coupled with an azide-functionalized PEG via a copper(I) catalyzed Huisgen dipolar
cycloaddition reaction (a click reaction). Initial attempts at the coupling reaction on a NMR scale have been successful and suggest that the reaction proceeds to completion. No-deuterium (No-D) NMR spectroscopy is currently being used to optimize the quantity of PEG and catalyst needed to allow for complete coupling, while also allowing the resulting products to be easily purified. In this presentation, the synthesis of four-armed calixarene-core PLA/PEG star block copolymers will be described in detail.

CHED 1424

Investigating the polymerization mechanism of cyanoacrylate with fingerprint constituents

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Cyanoacrylate is a widely used compound for a variety of applications, but the mechanistic details of the polymerization reaction during the development of latent prints are still unknown. The polymerization of cyanoacrylate with individual components is investigated by fuming amino acids and oils with cyanoacrylate then analyzing the extent of polymerization by mass. Serine, the most abundant amino acid in secretions that form fingerprints, is used as the model amino acid due to the amino, carboxylic acid and alcohol functional groups. The individual functional groups are analyzed using isopropanol, acetic acid, and propylamine. From the data obtained in this experiment, the combination of the amino and carboxylic acid functional groups are responsible for polymerization, while the alcohol functional group generates very little polymerization. The results also suggest that a very basic pH leads to optimal polymerization, while an acidic pH hinders polymerization. Results are further compared to glycine, another amino acid present in fingerprint secretions. The effect of oils on the polymerization reaction of the amino acids is also presented.

CHED 1425

Synthesis of a macroinitiator and its use in the preparation of poly(styrene-b-methacrylonitrile): An advanced undergraduate laboratory project in polymer chemistry

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Here we report a new experiment involving the synthesis of a macroinitiator and its use in the living synthesis of the diblock copolymer poly(styrene-b-methacrylonitrile). Initially, 1-(1-phenylvinyl)pyrene is prepared from a multi-step synthesis requiring the use of various methodologies, including: proper solvent and reagent preparation, organolithium
and organomagnesium chemistry, oxidation, dehydration, and product purification and characterization. It is then used in the synthesis of a terminally functionalized polystyrene oligomer for use as an anionic macroinitiator for the subsequent preparation of poly(styrene-b-methacrylonitrile).

This experiment is appropriate for a senior level lab course in advanced organic or polymer chemistry. Students will gain experience in multi-step organic synthesis, product separation and purification, living polymerization, polymer modification, and advanced characterization techniques. In particular, students will learn first-hand how important interactions are across the boundaries between several different disciplines of chemistry.

CHED 1426

Synthesis of asolectin-containing latexes by emulsion polymerization

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100% bio-based vesicles, for use in drug delivery or nanocatalyst stabilizer, have been prepared by the emulsion copolymerization of tung oil and asolectin, a natural phospholipid from soybeans, in a xylene/water emulsion. The free radical polymerization was initiated by azobisisobutyronitrile (AiBN) at 60°C in a convection oven. After the reaction, the emulsion was salted out, and the precipitates were filtered and dried for further analysis. MALDI-TOF results indicate a significant increase in molecular weight, which implies successful polymerization of the comonomers used. Changes in the Raman spectrum of the components before and after the reaction, along with differential scanning calorimetry (DSC) analysis have been used to verify completion of the reaction.

CHED 1427

Synthesis and applications of ionic liquid monomers in free radical polymerizations

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This presentation seeks to analyze how ionic liquids can be synthesized for use in free-radical polymerizations. This includes a summary of primary research methods and techniques for acid-base neutralizations involved in creating such monomers. This presentation also explores various applications of ionic liquid monomers and the polymerization of several different cross-linked polymers. Several of these polymers were successfully synthesized. The polymers were tested for adhesive properties and toxicity at varying initiator concentrations. Results from these tests will be used to ascertain practicality of these cross-linked polymers in real-world applications.
Synthesis of high molecular weight poly(ε-caprolactone) star polymers and their degradation properties

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Organic polymers seem to be excellent materials to use as bone scaffolds because they have tremendous strength, flexibility, biocompatibility, and degradation properties. In this study, mPEG-dendritic lysine moieties were synthesized to generation zero, generation 0.5, and generation 1.5 cores, and then the cores were hyperbranched utilizing a lysine AB₂ monomer. The hyperbranched polymers were then utilized in a bulk ring opening polymerization of ε-caprolactone to yield star co-polymers of about 600,000 g/mol average molecular weight. Physical blends were made with varying percentages of hydroxyapatite (HA) in order to determine the flexibility and strength of the composite materials. Due to the heterogeneous films that resulted, new films were made by synthesizing the HA in the presence of the polymer. These in-situ composites were then tested to compare the flexibility and strength of the composites and explore their viability as bone substitutes. Compared to an mPEG/PCL co-polymer film, the in-situ composites revealed significant improvements in flexibility and strength, showing the need for the hyperbranched portion of the molecule. In previous studies utilizing the dendritic star polymer little to no enzymatic degradation of the polymers was seen. Therefore, the degradation properties of the hyperbranched polymer were studied over the same eight-week time frame to explore the impact of the change in polymer structure on its degradation characteristics. Both elastase and trypsin were utilized and the results were compared to the previous degradation of the mPEG-dendritic polylysine structures.

Synthesis and polymerization of (E,E)-[6.2]-(2,5)furanophane-1,5-diene

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This work describes the synthesis of (E,E)-[6.2]-(2,5)furanophane-1,5-diene via a 1,8-Hoffmann elimination of an ammonium hydroxide intermediate. In addition the polymerization of this diene to give a [3.2]furanophane containing polymer will be discussed as well as it's characterization.

Biocompatible material used for drug delivery
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Methacrylate hydrogels synthesized with copper paddlewheel filler material will be assayed for applications in controlled drug release. Hydrogels are polymeric materials which can absorb large amounts of water, and coupled with their porosity make them quite similar to human tissue. The filler material along with EGDMA will serve to crosslink the polymer chains and is proposed to modulate the diffusive properties of the material. The paddlewheels contain two coppers that coordinate with four carboxylate ligands at near 90 degree angles. The paddlewheel material can form hydrogen bonds via their ligand’s hydroxyl groups, serving as crosslinkers between the methacrylate pendant groups of the polymer. The aim of this project is to ultimately provide a biocompatible material that intrinsically delivers drugs over prolonged periods of time. Differential Scanning Calorimetry, UV-Vis and FT-IR spectrophotometery are techniques used to characterize these hydrogel materials and their diffusive properties.

CHED 1431

Poly(ionic) liquids: Imidazoles with ester linkages

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It is well known that polymers can be created through condensation of a carboxylic acid and an alcohol giving an ester linked polymer and water. Starting with substituted imidazoles, we have designed a variety of N,N-substituted imidazolium diesters and dialcohols to become monomers in the synthesis of polyesters. These polyesters with imidazolium backbones are expected to be effectively odorless ionic liquid monomers that will lead to odorless polymers. A plastic of this nature would be useful for enclosed chambers in which air quality is extremely important.

CHED 1432

Synthesis of metal-organic frameworks for adsorption of disease-relevant peptides

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Amyloid-beta (Aβ) plays an important role in the pathogenesis of Alzheimer’s disease. As Aβ accumulates, misfolded monomers arise promoting the recruitment of additional peptides to this unique, misfolded conformation. These misfolded monomers are far more prone to aggregation than the native Aβ species, inducing the formation of
oligomers, and eventually larger species of Aβ called fibrils and plaques. The intermediates of this process are thought to be more deleterious than their larger plaque counterparts, due to their solubility and potential to block neuronal synapses and disrupt cellular signaling. Ample research has been conducted to examine the deleterious properties of Aβ; however, too little is known concerning the transition of Aβ to its misfolded conformer. As an intrinsically unstructured protein, Aβ(42) does not have a specific tertiary form. Rather, the peptide sequence adapts a series of conformations depending on what is thermodynamically favorable. There is evidence to suggest that the misfolded conformation of Aβ(42) has a far more defined structure than native Aβ(42). The problem arises in the misfolded form’s ability to aggregate quickly, before the structure of the misfolded monomer can be studied in detail. This renders quantitative characterization techniques such as X-ray crystallography somewhat useless unless a procedure is developed to strategically immobilize the Aβ for analysis. We propose the use of metal-organic frameworks (MOFs) as mechanisms to adsorb and sequester Aβ(42). As a class of highly porous materials comprised of metal clusters and organic ligands, MOFs have numerous characteristics that make them suitable for peptide adsorption. The propensity of MOFs to adsorb a diverse array of small organic molecules by means of tailoring them to possess the desired structural characteristics and functionality affirms their viability.

CHED 1433

CdSe quantum dot band edge tuning through photooxidation on nanopatterned polymers for applications in hybrid cell photovoltaics

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Solar energy is on its way to becoming a major contributor to the global energy demand. Currently, Silicon solar cells dominate the market, but Si cells are thick, heavy, and rigid and increases in efficiency are beginning to plateau as they get closer to the Schokley-Queisser theoretical limit of 33.7%. Hybrid cells, consisting of an organic polymer and an inorganic semiconductor, are typically thin, light, and flexible and can be made easily using roll-to-roll printing. Unfortunately, hybrid cell efficiencies cannot yet compete with Si cells on the market. This study aims to increase cell efficiencies using surface patterning and quantum dot band edge tuning. Poly(3-hexylthiophene-2,5-diyl) (P3HT) and CdSe quantum dots (QD) were used. It has been shown that P3HT can be mixed with high density polyethylene (HDPE) without significantly decreasing the P3HT’s photoactive properties. Channels were embossed into the P3HT:HDPE mixtures using Polydimethylsiloxane (PDMS) stamp patterning. These channels drastically increase surface area and contact with the CdSe QDs which were deposited using drop casting. The films were characterized with fluorescence, uv/vis, dektak, and SEM. Once on the patterned films, the QDs’ effective size can be tuned through photooxidation without significantly damaging the P3HT film. This shift in effective size of the dots creates a
gradient and allows for a broaden in range of absorption as shown through UV/vis measurements.

CHED 1434

Synthesis of sustainable monomers for a polyurethane

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The aim of this project was to develop a renewable polyurethane from a dihydrocarvide- and menthide-based polyamine. Synthesis of dihydrocarvide presented difficulties due to unwanted side products. Previously published procedures for the Baeyer-Villiger oxidation of dihydrocarvone to dihydrocarvide produced a mixture: 60% desired lactone and 40% epoxide. Optimal synthesis of dihydrocarvide was studied through the addition of various salts, Lewis acids, and oxidants. Superior results were ultimately obtained through the use of catalytic amounts of oxidants including sodium molybdate, potassium permanganate, and Dess-Martin periodinane. These conditions led to lactone in 96-98% purity by 1H NMR and an isolated yield of 85%. Subsequent copolymerization of menthide and dihydrocarvide was successful with good control of polymer molar masses determined from 1H NMR spectra. Polyamine synthesis studies are ongoing.

CHED 1435

NMR study of the active form of the polymerization catalyst formed between Tp*Rh(cod) and 4-ethynyltoluene

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Tp*Rh(cod) is a catalyst that can be used to polymerize phenylacetylene derivatives. It contains a rhodium ion and a boron centered scorpionate ligand in which three dimethylpyrazole rings are attached to the boron atom. We are interested in determining the effect of scorpionate ligand structure on the efficacy of the catalyst. The purpose of this study is to use 13C NMR spectroscopy to determine the active form of the catalyst that forms between Tp*Rh(cod) and 4-ethynyltoluene. These studies show that only a small fraction of the catalyst complexes in the reaction mixture participate in the reaction. Most are inactive. In the catalyst complexes that do react, cyclooctadiene is detached from the rhodium ion.

CHED 1436

Titanium and tantalum complexes bearing optically active tartrates as catalysts for the polymerization of D,L-lactide
The physical properties of polylactide (PLA), especially its rates of chemical and biological degradation, are determined by the three-dimensional orientation of the substituents along the polymer chain (i.e., its microstructure). Considerable effort has been devoted to controlling PLA microstructure, and numerous catalysts have been developed towards this end; notably, many of these catalysts possess optically active ligands. Recently, attention has been paid to the development of titanium- and tantalum-based lactide polymerization catalysts due to their potential for both high activity and biocompatibility. Herein we report the preparation and ability of titanium and tantalum complexes bearing optically active tartrate ligands to catalyze the polymerization of D,L-lactide. Specifically, we discuss the effect of ligand architecture upon the rate of the polymerization reactions, as well as on the microstructure of the resultant polymers.

CHED 1437

Lactones derived from fatty acids: New monomers for the production of bioplastics

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Biodegradable plastics derived from renewable, agricultural resources (e.g., corn and soybeans) have the potential to provide a foundation for sustainable commercial products that alleviate the environmental problems associated with their petroleum-based analogs. Recently, rapid advances have been made in the development of biodegradable polymers. For example, polylactides (PLA) are polyesters with the potential for commercialization in the fiber, film, and packaging industries.
Despite its promise, PLA currently only displaces a limited range of petroleum-based plastics. One reason is that commercially available PLA deforms at relatively low temperatures, thus making it unsuitable for applications such as microwave-safe containers. Herein we report the synthesis of different analogs of D,L-lactide (1-4) prepared from palmitic and stearic acids. These monomers contain a 14-16 carbon chain, and upon polymerization are expected to yield comb polymers with different physical properties than PLA. Consequently, the potential commercial viability of these polyesters will hopefully promote further development of other related bio-plastics.

CHED 1438

Ion conducting polymer electrolytes as electroactive polymers

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Electroactive polymers (EAPs) are polymers that change either shape or size when an external voltage is passed through them and regain their original composition upon reversing the polarity of the voltage. EAPs have drawn attention due to their biomedical and human affinity applications because they have the ability to mimic muscle movements. There are several types of EAPs: electric, ionic, and molecular. The polymer electrolyte poly(ethylene oxide), -(CH₂-CH₂-O)ₙ- was investigated for its use as an electroactive polymer. Lithium salts were dissolved in the polymer making the ion-conducting polymer. When a potential was applied, the ions moved to the contact electrodes which caused local swelling at the surfaces. This swelling caused the polymers to bend proving their electroactive nature. Techniques such as atomic force microscopy, ATR-FTIR and XRD. will be used to study this phenomenon. A discussion of the mechanism for ion conduction will be given.

CHED 1439

Synthesis and characterization of sol-gel based AlFPO₄ glasses

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Much research has recently been done on the production of durable, low $T_g$ glasses for optical applications as well as spectrum band conversion to increase solar cell efficiency. One of the methods of production that contains interesting capabilities is the sol-gel method. This low $T_g$ method of glass production proves advantageous over melt glass methods in terms of cost, preparation, and in the production of thin films while still providing durability and doping capabilities. The goal of this research is to prepare various composition aluminum phosphate based xerogels through a sol-gel route and then convert the gels into glasses through heat treatment. Characterization data will be obtained using RAMAN spectroscopy and fluorometry methods to obtain structure and functionality of the glass. This data will then be compared with traditional melt-quench glasses to determine if this route provides a viable route while producing a comparable glass environment.

CHED 1440

Polycation-DNA interaction thermodynamics: tailoring gene delivery systems

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Innovations in gene therapy have brought researchers closer to finding treatments for genetic disorders through the regulation of gene expression. For such treatments, one must transfec

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Study in the polymer crystallization kinetics and the birefringence of polyethylene glycol

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The crystallization rates of polyethylene glycol were studied to determine the effects of molecular weight on spherulite formation and polymer crystallization. In addition, the birefringence of the PEG crystals was explored to gain a better understanding of polarized light and birefringence. It was shown that increasing molecular weight affects spherulite nucleation and increases crystallization time.

CHED 1442

Diarylethene containing π-conjugated polymers: The effects of binding site on photochromic and electrochemical behavior

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Photochromic molecules have been studied for use as molecular switches and in variable transmission optics, sensors, and optical data storage media. Most of the diarylethene class of photochromes show highly desirable thermally irreversible photochromism and some of these molecules have been examined in polymeric systems. The molecular subunit involved in the cyclization and cycloreversion processes is usually part of the polymer main chain leading to a loss of photochromic activity. This work centers on a newly developed phenanthrene based diarylethene (1) and its incorporation in a meta-linked conjugated polymer (P2) where the photochromic component is removed from the polymer main chain. The effects of the photochrome in the ring-opened and ring-closed forms on the polymer optical and electrochemical processes will be examined. For comparison, a control polymer (P1) and a polymer where the thiophene groups are part of the main chain (P3) will also be synthesized and studied.
Energy demands across the globe are rising every year, and the cost of extracting the fossil fuels needed to power those needs are growing as well. Developing more sophisticated means to collect solar energy is an important part of reducing the global need for fossil fuels. Plastic solar cells offer a less expensive alternative to silicon, although they currently do not have the efficiencies needed to be competitive. Our strategy to overcome the inefficiencies of plastic solar cells is to incorporate lead sulfide nanoparticles into the polymer. This will take advantage of lead sulfides ability to generate two excitons from one photon in some situations. \(7\text{-bicyclo[2.2.1]hept-5-en-2-yl}\text{-7-oxoheptanoic acid} (1)\) contains a functional group that can coordinate with lead sulfide nanoparticles and a polymerisable norbornene moiety. The synthesis and characterization of the nanoparticle coordinated monomer will be presented.
Temperature effects on the impact properties of polymer coatings used in armor protection

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Protection against improvised explosive devices (IEDs) and small-arms fire continues to be a priority for military and security forces. A fundamental understanding of how polymer coatings improve armor protection can lead to new materials and advances in the field. The goal of this project is to study the effects of temperature on the impact resistance of polymers, specifically how the impact resistance of a polymer changes around its glass transition temperature (Tg). Below Tg, amorphous polymers are glassy and stiff. At Tg, the polymers transition to rubbery behavior and significant changes in mechanical properties are observed. In this project, poly(methacrylate)-based polymers with Tg values close to room temperature were injection molded into thin films and coated onto metal substrates. High-speed ballistic impact tests were conducted to determine the impact resistance (V50) of these films. Elevated temperatures were studied to understand the temperature effects on impact properties. In addition, differential scanning calorimetry (DSC) and mechanical property testing were used to characterize these materials. These data will be presented to understand how the thermal state of a polymer influences its impact resistance and ability to dissipate energy in high-energy impacts.

Synthesis of polymer capable of underwater adhesion

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The purpose of this experiment is to find a new polymer capable of underwater adhesion. The criteria for underwater adhesion is that it is capable of hardening and sticking two surface together after being applied to them while underwater. This specific polymer accomplishes this by mimicking a protein found in sea mussels. The mussels use this protein to stick onto rocks underwater and keep from drifting away.
Researchers have already made close mimics of the protein, but nature can be sloppy at times and there might be some derivatives of the polymer to give some advantageous properties.

In this research the biomimetic polymer has been altered. The monomer responsible for attaching to other surfaces has been brought further away from the carbon chain. The monomer responsible for attaching the polymer to itself and hardening has been brought closer to the carbon chain. This should result in some interesting outcomes in the performance of the polymer. As well as altering the monomers themselves, the amount of the cross-linking monomer will be altered while the surface binding monomer is kept constant. This is done to find the best ratio in maximizing adhesive strength. The polymer will be characterized by NMR to ensure it was made before testing the adhesive strength. Adhesion will be tested on aluminum substrates with a cross-link initiating ionic solution.

![Diagram of polymer structures](image)

**CHED 1446**

**Spatially specified natural fiber welding via inkjet printing**

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Ionic liquids make excellent biopolymer solvents due to their unique chemical and physical properties that allow them to disrupt the hydrogen bonding network that makes biopolymers so difficult to process. Natural fiber welding (NFW) is the full or partial dissolution and subsequent regeneration of a biopolymer substrate through the use of ionic liquids (IL). This process allows for the integration of functional materials into the three dimensional structure of the biopolymer materials. The application of ionic liquid solutions via inkjet printing allows for the quick and high-resolution spatial control of NFW; specifically, the speed, reproducibility, and resolution of modern inkjet printers allows for three-dimensional surface modification of the biopolymer substrate to be carried out. Printing these IL solutions is challenging due to their physical properties.
Consequently, the rheology of the IL solutions used for NFW plays a large role in determining the printability of the solution and the degree to which NFW and substrate modification occur. The physical properties of the ink solutions can be controlled via changes in temperature, the addition of co-solvent, and polymer loading. In the present work we will relate how changes in the aforementioned ink parameters affect the printability of the ink solutions, as well as present the current progress on building functional surface structures using inkjet printing.

CHED 1447

Synthesis and utilization of ionic microgel dispersions for uptake and release of active species

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In this presentation we synthesize monodisperse ionic microgel particles which undergo large volume phase transitions in response to environmental stimuli such as pH and temperature. These aqueous particles have tunable size-change qualities with respect to the adjustable volume phase transition temperature (VPTT). As a response to environmental stimuli, the prepared microgel particles demonstrate the ability to uptake and release various active species such as surfactants and rheology modifiers which alter the bulk viscosity of a surrounding fluid. In addition, this study elucidates the effective adsorption of iron oxide nanoparticles (Fe₃O₄-NPs) upon pH variation. The loading of the Fe₃O₄-NPs within the colloidal particles and morphology can be manipulated by tunable interactions between the Fe₃O₄-NPs and ionic microgel particles. The extent of active species loading and the ensuing relative swelling/deswelling behaviors within the colloidal polymer networks are explained in terms of their various fundamental binding interactions.

CHED 1448

Radiopaque shape memory polymers

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Shape memory polymers are a category of smart materials that can be programmed into a temporary shape when an external stimulus and a mechanical force are applied. When activated by a second external stimulus, the temporary shape can controllably switch back to the original shape. The use of these stimuli-sensitive polymers can reduce the invasiveness of many medical procedures. In addition to allowing minimally invasive surgery, replacing traditional metal-based implants with polymeric materials has advantages like tunable biodegradability and mechanical properties. However, these advantages sacrifice the ability to monitor an implant by x-ray computed
tomography due to a deficiency of electron dense atoms. This research explores inherently radiopaque, shape memory polymers through the synthesis of a unique copolymer containing an aliphatic, iodinated monomer. By investigating different monomer ratios, polymer properties could be modified to form a variety of radiopaque polyesters capable of being imaged using computed tomography and performing triggered conformational shape change.

CHED 1449

Carbon fiber precursors derived from lignin and acrylonitrile vinylimidazole blends

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Lignin is a byproduct of wood pulping in the papermaking industry, since it is one of three major components of wood along with cellulose and hemicellulose. As a byproduct of papermaking, this carbon rich macromolecule is cheap and abundant, making it a good candidate for incorporation of it in carbon fiber precursors. Very little is known about the biosynthesis of lignin or the methods behind the sporadic branching of its three components; sinapil alcohol, coniferil alcohol, and p-cumaril alcohol. Because of this, not much has been determined about the chemical and mechanical properties of this ever varying macromolecule. Studies have been done of lignin blends with polyethylene oxide (PEO) for carbon fiber precursors with promising results. So, in this project lignin blends with acrylonitrile vinylimidazole (ANVIM) will be analyzed to see the mechanical properties of the blends and how well suited they are for the production of carbon fibers.

CHED 1450

Visualizing chemistry: From idea to research to practice
What makes a successful revolution in teaching? It starts with a fundamental idea that many acknowledge as true. Next, the idea has to be researched to better understand how it affects teaching and learning. Finally, the idea has to be incorporated into the everyday process of teaching and learning. This is how the revolution of the particulate nature of matter started. Alex Johnstone presented the idea that chemists present chemistry on the symbolic level with equations and symbols and work with it on the macroscopic level in lab and demonstrations but understand it on the particulate level of particle interaction. Researchers, including Vickie Williamson, demonstrated just how important particulate knowledge is in student learning. My own research on this topic demonstrated how useful the particulate approach was in helping students, especially women, increase their achievement in chemistry. This presentation will trace Vickie’s contribution to the particulate nature of matter revolution and show how her work influenced many of us.

CHED 1451

Limitations of engagement as a goal for design: Visualizations and beyond

Student engagement is often promoted as a goal for design interventions in textbooks, supplementary materials, and activities or demonstrations. While a worthy goal in general, research indicates that interventions or design features intended to engage students do not necessarily encourage effective processing or learning gains.

This symposium presentation will begin by reviewing collaborative work on chemistry visualizations with the honoree, Dr. Vickie Williamson. In one study, we found that static visualizations were often presented in textbooks as decorative images without instructional support. This was true despite a demonstrated need for practice and representational competence when students use these visualizations. In another study we found that engaging, concrete, dynamic visualizations can sometimes distract learners from more relevant particulate-level animations.

Next, related text-based research from outside the chemistry domain will be presented. In one set of studies, we found that including interesting, but irrelevant, details in a text about lightning and tornadoes distracted readers from the relevant content. And this distraction was maintained even when effective interventions (i.e. retrieval practice) were added. In a more recent set of studies, we compared memory for psychological concepts after reading interesting anecdotes vs. more “boring” descriptions of experiments. While students enjoyed the anecdotes, and believed they learned well from them, students remembered information from the experimental texts better.
In sum, visualizations and other interventions that create concrete, engaging, or interesting materials are not necessarily effective, and are sometimes counter-productive. Research from Dr. Williamson and others has demonstrated that these interventions are useful when they facilitate conceptual thinking about ideas that might otherwise be inaccessible. Finally, cognitive frameworks that may account for these effects will be discussed.

CHED 1452

Providing opportunities for students to increase their understanding of chemistry: Guided inquiry, computer simulations and animations, and active learning

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The following quote from a well-known chemistry educator, “The structure of the traditional general chemistry course does not appear to be effective for promoting deep conceptual understanding or an interest and pleasure in learning chemistry,” sets the stage for this presentation. General chemistry textbooks, traditional lectures, traditional general chemistry laboratories, course examinations and algorithmic end-of-chapter problems, on-line homework problems all contribute toward students’ lack of conceptual understanding and lack of problem-solving abilities. Active learning instructional activities have been implemented in general chemistry courses at Iowa State University, Oklahoma State University, the University of Oklahoma, and the University of Oregon. These activities are a blend of POGIL (Process-Oriented Guided Inquiry Learning) and SWH (the Science Writing Heuristic). In large lecture settings, we are piloting web-based instructional materials through the use of before, during and after class activities. Students use a series of computer simulations to collect and analyze data. During class, students work in small groups, using the data generated to complete guided-inquiry tutorials. Features from two of the computer simulations along with the tutorials designed by Gelder, Abraham, and Greenbowe will be discussed. Preliminary analysis of data on the performance of students on ACS exam questions and instructor-generated questions will be presented.
Lines, labels, and arrows: The role of graphical devices in visualizations

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Some of the earliest evidence that molecular-level animations can help students understand chemical processes was produced by Vickie Williamson. Her work inspired many to produce and use visualizations in the classroom and has led to additional research projects. Most of these projects have been concerned with the accuracy or clarity of molecular representations and how they can support learning. However, some also examine features of visualizations that can make them successful or that may lead to new misconceptions. We have investigated the role of graphical devices in visualizations and have found that communication tools such as lines, arrows, and labels can help learners identify the important aspects of a visualization. However, graphical devices such as arrows can cause confusion when their meaning is not clear. Our research has also shown that novices use graphical devices to communicate mental images of atoms and molecules in different ways than experts and that those differences need to be taken into account when analyzing student representations.
Research into practice: Visualization of the molecular world using animations and simulations

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The chemical education research literature demonstrates that many student misconceptions are due to an inability to visualize the structures and processes at the molecular level, as represented by chemical formulas and equations. We need to assist students to develop useful mental models of the molecular world to make the conventional symbolism meaningful. Early seminal work by Vickie Williamson and Michael Abraham was instructive on the potential of animations for this purpose. However, we know that students do not change their mental model by simply showing them complex visualizations.

The challenge is to develop sequences of learning activities (learning designs), informed by an evidence-based cognitive model for how we learn from multimedia visualizations[1]. I will demonstrate one learning design with VisChem animations[2] and Odyssey simulation software, and show how both animations and simulations are required to visualize structures and processes at this level satisfactorily. The focus will be on the challenge of directing student attention to specific features in these visualizations to understand concepts as diverse as molecular reactivity, dynamic equilibrium, reaction mechanisms, hydrophobicity, and chemical speciation.


Effects of e-homework systems on male and female students' understanding of the particulate nature of matter

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Understanding the particulate nature of matter is important to understanding many aspects of general chemistry and for future success in chemistry. Students evaluated in this study were not only exposed to static drawings in lecture regarding the particulate nature of matter, but in addition used various online e-homework systems (e.g., SmartWork, ALEKS, Sapling, and OWL) that at times presented animations reflecting how we perceive actions of atoms and molecules. The purpose of this study was to investigate how male and female groups of students interpret summative assessment questions designed to elicit their understanding of the particulate nature of matter. The eight concepts assessed were gathered from students' responses from over 9,000 first-semester general chemistry final exam questions on density, isotopic nuclear symbols, chemical reactions, Lewis structures, formal charges, gas laws, states of matter, and acid/base concepts. In the majority of the cases evaluated on the average males outperformed females. One of the major stumbling blocks to successful performance (scores of greater than 70 percent) is the understanding of basic vocabulary reflective of accepted particulate terminology. As expected, overall successful students exhibited fewer misconceptions than unsuccessful students, but common "distractors" still hold appeal as possible answers. Also, discussed will be student performance under each of the various e-homework systems used.
Award Address (ACS Award for Achievement in Research for the Teaching and Learning of Chemistry sponsored by Pearson Education). Quest for student understanding of the particulate nature of matter

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The goal of chemistry education research (CER) is to improve student understanding. CER investigates the theoretical issues surrounding the teaching and learning of chemistry and the assessment of various teaching techniques or strategies in light of these issues. One line of CER focuses on the difficulties students have with the particulate nature of matter. These difficulties result in students’ inability to visualize particle behavior, and thus, students’ inability to fully understand chemistry concepts. The quest to improve student understanding of the particulate nature of matter has been the long-term focus of many researchers, resulting in a growing body of knowledge in the area. The quest has been the focus of my own research, which is built on that of others and hopefully has added to our knowledge base. This talk will focus on the use of particulate animations in the classroom, including what data eye-tracking can give and the investigation of student characteristics which impact how a visualization will be received. Further, new areas for visualization research will be outlined.

CHED 1457

Using three types of instructional videos to assist students’ laboratory preparedness in a physical chemistry lab

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Having students perform laboratories in a “round-robin” fashion is a common solution to having many students perform laboratory experiments using limited equipment. This is particularly true in upper level laboratories such as physical chemistry where more sophisticated instrumentation is used. This approach creates a challenge for how to present pre-laboratory instruction to prepare students to conduct and analyze the experiments. We have developed a series of instructional videos for an upper-division physical chemistry laboratory course to address this challenge. Each experiment in the course has three videos associated with it: a pre-lab mini-lecture video, which goes over some of the theoretical considerations of the experiment; a professionally filmed experimental procedures video; and a video detailing the use of features in spreadsheet programs (e.g. curve fitting, peak picking etc.) and other necessary resources for students to analyze their data. A practical aim of the videos is to increase students’ preparedness when they approach all aspects of the laboratory experiments. Students are required to view each of the videos before the laboratory period, and must complete online quizzes based on the content of the videos in order to be admitted to lab. Preliminary results based on observations of students in lab indicate that they often refer to the videos as a source of information when carrying out experimental
procedures. Production and implementation of such videos is relatively low-cost and could benefit students, lab staff, and instructors alike by increasing students’ preparedness.

CHED 1458

Assessing a problem-based learning NMR & MRI laboratory experiment

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In problem-based learning (PBL) student learning centers on a complex problem that does not have a single correct answer. Instead, students work together to identify what they need to learn in order to solve the problem. In this novel PBL lab, students work together to develop content and process knowledge on a “need-to-know” basis. The project culminates with the students deciding if a company should purchase a NMR/MRI spectrometer to use in quality control for their citrus fruit. The Terranova NMR/MRI spectrometer, which uses the Earth’s magnetic field as the static field and current through a coiled wire as the oscillating magnetic field, is used. The simplicity and inexpensiveness of the system allowed for a lab design that permits students to experiment with parameters and to visualize subsequent effects in the FID and frequency spectrum. In the first three-hour lab block, students learn about the instrument and 1-D NMR spectra, including the quantum principles that make the technique possible and how parameters affect spectra. In the second week, students apply their knowledge to take 3-D MRI imaging that helps them address the project’s original problem. The lab, student generated data, and qualitative data on learning outcomes will be presented. The findings from this research have implications for implementation into chemistry programs and reform of future physical chemistry experiments.

CHED 1459

What factors affect the escapability of a molecule from a liquid? A molecular dynamics experiment for the physical chemistry laboratory

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Given the significance of molecular dynamics (MD) in chemistry research, experiments that allow students to explore these techniques are underrepresented in the physical chemistry laboratory curriculum. We describe an experiment in the POGIL-PCL (POGIL in the physical chemistry laboratory) framework in which students perform MD simulations on pentane isomers in the condensed and gas phase. The experiment consists of two learning cycles: 1) calculation of the enthalpy of vaporization of each isomer and decomposition of the cohesive energy; 2) exploration of the liquid-vapor
phase transition of neopentane. We describe student reaction to this experiment and the effect on their understanding of intermolecular forces. This experiment has been designed to be available with readily available molecular dynamics packages. We discuss the supporting information provided to instructors who implement these experiments, the barriers they have found to that implementation, and strategies for overcoming those barriers.

CHED 1460

3D printing to create computationally derived models in the physical chemistry laboratory

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3D printing has been combined with computational chemistry exercises in the undergraduate curriculum, empowering students to create accurate, physical models of pedagogically interesting systems. The costs, low maintenance, and reliability of 3D printers have trended favorably in recent years to an extent that it is now possible to implement this technology within an academic setting. Several student lab projects are presented, including the 3D printing of simple geometry-optimized, ball-and-stick models of common chemical structures, as well as the fabrication of more realistic, space-filling models of proteins and molecular complexes. The conversion of Protein Data Bank (PDB) structures into 3D printed models and the use of quantum computational software to generate accurate structural representations of chemical complexes for 3D printing is described. Together, these activities represent a highly motivational means of getting physical chemistry students to further engage in chemistry. Several web and software resources that can be utilized by chemists in support of 3D printing activities are reviewed.

CHED 1461

Computational exercise to explore the nature of hydrogen bonding

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We designed a computational exercise to explore if the nature of the hydrogen bond is due to electrostatic, i.e., dipole-dipole interaction or rather strong form of n-σ* donor-acceptor interaction exhibiting the expected strong cooperative effects associated with intermolecular charge transfer. We selected classic textbook examples to study, such as (HF)\(_2\), (H\(_2\)O)\(_2\), (NH\(_3\))\(_2\), HF...H\(_3\)N, H\(_2\)O...H\(_3\)N, where both molecules exhibit dipole, to test whether there is any correlation between dipole strength and hydrogen bond energy (ΔE\(_{H..B}\)). In addition, we selected another class of dimers, which includes HF...F-F, H\(_2\)O......HC=CH\(_2\) and others, where one monomer is nonpolar. In both classes, we obtain all experimental descriptors associated with hydrogen bonding such as
CHED 1462

Can we make stew with these beans? An introduction to experimental inquiry for the physical chemistry laboratory

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We describe an experiment to introduce students to physical chemistry experimental inquiry through exploration of a standard problem in food science: water uptake by a dried bean or fruit. The experiment has been developed in the POGIL-PCL (POGIL in the physical chemistry laboratory) framework with a focus on experimental design and data analysis and modeling. Three learning cycles are present: 1) qualitative experiments on chickpea hydration that introduces students to decision-making; 2) refinement of the procedure to explore the system quantitatively in the context of standard models; 3) exploration of additional systems using the developed techniques and analysis. We discuss student response to the experiment and their success in meeting the experiment's learning objectives.

CHED 1463

Kinetics of the carbon dioxide hydration reaction: Quantitative experiment for the undergraduate physical chemistry laboratory

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The reversible hydration reaction of carbon dioxide plays a key role in metabolism and photosynthesis.

\[
\text{CO}_2 \text{(aq)} + \text{H}_2\text{O} \text{(l)} \rightleftharpoons \text{H}_2\text{CO}_3 \text{(aq)} \text{ Slow step}
\]

\[
\text{H}_2\text{CO}_3 \text{(aq)} \rightleftharpoons \text{H}^+ \text{(aq)} + \text{HCO}_3^- \text{(aq)} \text{ Fast Step}
\]

Carbonic acid (\(\text{H}_2\text{CO}_3\)), a product of respiration, is transported from cells to lungs by the blood stream where it is converted to dissolved \(\text{CO}_2 \text{(aq)}\) by dehydration. The inter-conversion of carbon dioxide to carbonic acid proceeds very slowly at physiological pH which leads to a buildup of carbonic acid in the blood stream. Carbonic acid, once
formed, ionizes instantaneously producing hydrogen ions that would be lethal to life. To counter the unfavorable kinetics of this reaction all animals have a zinc containing enzymatic catalyst, carbonic anhydrase, that provides an active site so that a water molecule can be quickly stripped from carbonic acid to produce dissolved CO$_2$, which is subsequently converted to exhalable CO$_2$ gas, averting a lethal build up of hydrogen ions in the blood stream. Carbonic anhydrases, essential to sustain life, are found in all kingdoms of life.

We will describe a kinetics experiment for physical chemistry students to determine the rate constant ($k_1$) for the uncatalyzed hydration of carbon dioxide that can be conducted with readily available lab equipment. We will share experimental methods, data and analysis, and compare our results with those of other researchers.

pH versus time when a solution containing seltzer water was injected with aliquots of NH$_4$OH under catalyzed and uncatalyzed conditions at 0 °C.

CHED 1464

How to make the most appealing fruit salad: An inquiry-based enzyme kinetics physical chemistry laboratory

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Engaging students in more authentic science practice is a goal for many laboratory programs. Inquiry-based laboratory experiences provide students the opportunity for more independence in designing experiments and interpreting the results in a meaningful way. An experiment to explore the enzyme kinetics associated with the browning of apples (and similar fruits) was developed for the physical chemistry on-line (PCOL) project and revised for the POGIL physical chemistry laboratory project. In this experiment students describe the Michaelis-Menten mechanism for enzyme catalysis, including explaining the meaning of the parameters. The experiment requires students to use a number of skills, including analyzing and manipulating equations and graphical representations to appropriately model experimental results. The experiment can be extended to have students study the inhibition of the reaction, including determining the type of inhibition. An overview of the experiment will be presented along with strategies for implementation in environments where students perform the experiment simultaneously and using a "round-robin" approach.

CHED 1465

Scholarship of teaching: Online courses as means of publishing innovations

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The National Science Board wrote in 1996 that "Great teaching is a form of synthesis and scholarship." Though this truth has been increasingly recognized in the past two decades, teaching as a form of scholarship differs from other forms of scholarship in that it is much more difficult to publish. We publish lessons plans, we publish innovative ideas, and we publish research on teaching. But publishing the teaching itself requires non-traditional means. The rise in availability of on-line courses creates exciting possibilities for demonstrating how lessons plans, innovative ideas, and creative approaches are actually implemented. At Rice, we have developed a novel General Chemistry curriculum based on the development of concepts through inductive reasoning. Teaching using the Concept Development Study approach has been published via our Coursera course, "Chemistry Concept Development and Application." We will discuss our observations and results.

CHED 1466

Analysis of peer-to-peer interactions in introductory online courses

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Interactive learning with small group discussions can be facilitated in a myriad of ways in a traditional classroom setting at a brick and mortar institution. In asynchronous online learning classes in which students reside in wildly different time zones, on the other hand, peer-to-peer interaction often occurs via writing on discussion forums or peer-review assignments. This study aimed to evaluate how peer-to-peer interactions
through writing impact student learning in introductory-level online courses. This was accomplished via qualitative coding analysis of peer-to-peer interactions in writing through the forums and through peer assessment assignments. Student generated writing in these venues was found to enhance learner understanding, link to course learning objectives, and generally contribute positively to the learning environment. This highlights the importance of writing-to-learn as a significant pedagogical practice that should be encouraged in online coursework.

CHED 1467

Toward the development of academic social networks: A new paradigm for online STEM eLearning

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Toward the development of Academic Social Networks: a new paradigm for online STEM eLearning

CHED 1468

Generalized organic chemistry for a global student population: Organic chemistry on Coursera

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Sophomore organic chemistry courses typically cover a wide variety of structures and reactions with the aim of helping the student develop a broad appreciation for the behavior of organic molecules. They embrace what could be described as a "bottom-up" approach based on the behavior of functional groups in a very limited laboratory context. This kind of organization obscures connections between functional groups and does not lend itself to lifelong learning. For our intermediate organic chemistry MOOC, we embraced a "top-down" approach beginning with generalized building blocks of organic structures and elementary steps of organic reaction mechanisms. These and other foundational concepts were used to develop a course designed for lifelong learning and broad applicability—goals consistent with our highly educated, professionally diverse student body.

CHED 1469

Design of an independent student laboratory for a survey of organic chemistry distance learning course

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An independent laboratory course that includes student experiments performed in a kitchen environment has been developed to accompany the Survey of Organic Chemistry course offered at Mississippi State University. The one semester, introductory organic chemistry course has been converted to a distance learning format and our university has struggled to find an acceptable laboratory experience that can accompany the lecture course. This new independent laboratory course combines both kitchen-based experiments and online exercises to reinforce important concepts in organic chemistry. A unique feature of this independent laboratory offering is the inclusion of student cell phone photos as documentation for the lab reports. Students performed 8 experiments in their kitchen that reinforced structural characteristics and behaviors of organic compounds (acidity and pH of organic compounds, polymerization, saponification reactions), used reactions to identify and analyze the reactivity of alkenes (KMnO₄ addition, I₂ addition, aldol condensation) and taught students important laboratory techniques (recrystallization, extraction, chromatography). Online exercises utilized ChemSketch to explore stereochemistry and conformational changes related to reactions. Student responses and learning outcomes will be explored as a result of this unique laboratory offering.

CHED 1470

Intro to solid state chemistry: A mastery-based learning and assessment model

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abstract text not available

CHED 1471

Development of an online hypermedia environment as a complement to the traditional textbook and its impact on the on-campus classroom

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In the 1990s the author of this presentation had his first opportunity to develop a distance learning chemistry course with broadcast cable television as the means of delivering lectures to students. For his traditional on-campus sections he found himself merely repeating that which was recorded in the studio. This led him to require his on-campus students to watch the pre-recorded lectures before coming to class. This enabled class to be used primarily as a time of interactive study and hands-on/mind-on activities. This gave the on-campus students a tremendous learning advantage. It also made clear the distinction between “content delivery” and “content facilitation”. Through content delivery the student passively receives information, which is done well-enough outside of the classroom. Content facilitation is where students attempt to articulate what they think they have learned from the delivered content. This is a more difficult
phase of learning best accomplished within the classroom with classmates under the expert guidance of the course instructor. Since embracing this mode of teaching, the presenter has specialized in the creation of chemistry content in multiple formats, including textbooks and video tutorials now embedded within a structured hypermedia-learning environment located at ConceptualAcademy.com. The textbook is where students can read. Conceptual Academy is where they can watch and listen. When tightly integrated, these two complementary formats provide a robust means for delivering content to a broad range of student learning styles. When held accountable, students thus come to class fully prepared to learn. In this session, the presenter will showcase the online resources available through Conceptual Academy. In addition to hundreds of video tutorials, quizzes, and other online study supplements, this includes a library of student-centered learning activities that the instructor might use for on-campus classes to complement to a lighter emphasis on lecture presentations. Many of these on-campus activities, including team-based learning, are now being ported into Conceptual Academy for the benefit of the purely online student. So, while online courses have inspired innovations for the traditional on-campus classroom, the reverse is also true: on-campus innovations can impact the online environment as well. These two seemingly different avenues of teaching are fertile ground when blended together.

CHED 1472

Online-on campus dialogue: Lessons from Harvard’s Science and Cooking course

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When creating an online course, instructors tend to draw on their experience in on-campus courses. Online courses, in turn, can inspire changes to on-campus teaching. As further iterations of a course are developed, this creates an ongoing process of give and take where online and on-campus courses continue to motivate instructors to break new ground and optimize their methodology in both forums. This talk discusses the give and take that occurred over two iterations of the online and on-campus versions of the general education course Science and Cooking at Harvard. Science and Cooking aims to teach basic chemistry and physics through food and cooking. It annually draws several hundred on-campus students and was recently converted to an online course on the edx platform with more than 100,000 registrants. The talk will be an exploration of the different iterations of the course development process, including practical examples, successes, challenges, and research findings from both the on-campus and online courses – as well as a few, sometimes, surprising outcomes.

CHED 1473

Potential use of phenazine derivatives in the inhibition of the La Crosse virus
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Phenazine compounds are found as natural products that are predominately synthesized by pseudomonas bacteria. Preliminary assays have shown that exposure to the supernatant of pseudomonas bacteria causes an inhibitory effect on the La Crosse Virus (LCV). We aim to synthesize phenazine derivatives, both naturally occurring and purely synthetic, that will then be assayed against LCV in order to ascertain whether these phenazines are directly responsible for the observed inhibition. Using phenazine-1-carboxylic acid, a compound produced by pseudomonas, as a starting material, we plan to synthetically modify this compound to provide an array of compounds that will be tested against LCV.

CHED 1474

Posttranslational modification of nitrogenase in Rhodobacter sphaeroides

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Nitrogen is an essential element for life. In nature nitrogen is found primarily in two forms: N\textsubscript{2} and NH\textsubscript{3}. Highly specialized organisms are capable of reducing gaseous N\textsubscript{2} to NH\textsubscript{3}, a form available to living organisms, by the nitrogenase enzyme. In many of these specialized nitrogen fixing bacteria the nitrogenase enzyme is regulated by a post-translational modification known as ADP ribosylation. This, however, is not the only regulatory pathway. In Rhodobacter sphaeroides a different mechanism is believed to take place. It is hypothesized that it instead goes through a post-translational covalent modification by a small organic group, possibly a methyl or acetyl group. This was tested by anaerobic purification of the active and inactive forms of enzyme, followed by mass spectrometry analysis. A mass difference corresponding to a methyl or acetyl group between the active and inactive forms would indicate a post-translational modification.

CHED 1475

Assignment of the HN-HSQC NMR spectrum of heat stable protein kinase inhibitor (PKI)

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Protein kinase inhibitor (PKI) is a 75 residue protein responsible for the inhibition and nuclear export of protein kinase A (PKA). The exportin CRM1 binds the nuclear export signal of PKI and transports the PKI:PKA cargo through a nuclear pore complex. We are interested in investigating the mechanism by which PKI, an intrinsically disordered
protein, is involved in the binding and recognition of PKA for inhibition and nuclear export. Our goal is to use NMR to characterize the binding of PKI to PKA, as well as the binding of CRM1 to their complex. To initiate these studies, we optimized the expression and purification of recombinant PKI. We then conducted multi dimensional NMR experiments in order to assign each of the resonances in the HN-HSQC spectrum of PKI. The assignment will be presented. With the assignment we can begin characterizing PKI in complex with the other components of the nuclear export system.

CHED 1476

Chalcones and analogs of caffeic acid phenethyl ester with xanthine oxidase inhibiting and radical scavenging properties: Tools capable of suppressing oxidative stress in cells

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Xanthine Oxidase (XO) is an enzyme responsible for the conversion of hypoxanthine to xanthine to uric acid and for the generation of Reactive Oxygen Species (ROS) found within the blood and lungs. These ROS are the cause of reperfusion injuries that follow the reintroduction of oxygen after an ischemic event, such as a myocardial infarction or stroke. Two classes of compounds were investigated for their ability to inhibit xanthine oxidase and scavenge ROS. The first class of compounds is known as chalcones, with the second being analogues of caffeic acid phenethyl ester (CAPE). The ability of these compounds to inhibit xanthine oxidase was determined by measuring the rate of uric acid production using spectroscopic methods. Computational docking was used to identify crucial inhibitor/receptor interactions and to visualize inhibitor binding at the molecular level. Additional assays with the stable free radical 2,2-diphenyl-1-picrylhydrazyl were carried out to measure the radical scavenging capacity of the chalcone and CAPE derivatives. Many of the tested compounds possessed at least one of the two desirable properties, with some being able to fulfill both objectives. In addition to the two in vitro methods, in vivo cell viability assays were performed to assess a compound’s ability to reduce oxidative stress in neuro-2a cells exposed to Beta-amyloid peptide.

CHED 1477

Bioconjugating biotinylated gold nanoparticles (Au-NPs) to fluorescent streptavidin: Study of Au-NPs interaction with and photothermal effects on cells
Gold nanoparticles (Au-NPs) have a wealth of pharmaceutical and biomedical uses. Notably, the ability of metallic nanoparticles to absorb light and turn this light into heat has put them at the core of on-going studies exploring their effectiveness in destroying cancerous cells. In order to gain a better understanding of how NPs cause cell death, Au-NPs have been crosslinked to a fluorescent protein to specifically target cultured cancer cells. We are presenting the results of linking 5 nm and 10 nm Au-NPs to fluorescent streptavidin, introducing the bioconjugated NPs to 1299 cells and observing photothermal effects on the cells due to the NPs. We analyzed the nanoparticle-protein system with high performance liquid chromatography diode array (HPLC), dynamic light scattering (DLS) and UV-Vis spectroscopy. The photothermal effects in the Au-NP protein solutions were investigated using a MGL III-532nm-300 mW laser.

CHED 1478

Determining junctional tension in skin cells using Ecad-TSMod

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Mechanical forces can alter the shape and growth of cells and tissues, and are thought to be important for organ morphogenesis. However, our ability to measure the mechanical forces imposed on a tissue is limited. Here we propose to measure the mechanical tension across a sheet of epithelial cells by generating a cadherin-based tension sensor. E-Cadherin (Ecad) is a protein responsible for cell-to-cell adhesion. In this experiment we are modifying the E-Cad gene and adding a Tension Sensor Modification (TSMod) in the cytoplasmic domain of the protein. The EcadTSMod has two fluorescent domains (CFP & TFP) that will be used to determine junctional tension. What we want to know is if membrane domains containing PCP proteins are under more or less tension than the other membrane domains that do not contain PCP proteins. After transfecting skin cells with the fluorescent domains genes, it was found that the intensity of the FRET is directly proportional to the tension between cells. During the process it was also found that in order to have an in vitro grown polarized tissue, the cells must be grown on an air-liquid interface.

CHED 1479

Direct amidation of carboxylic acids via microwave-assisted synthesis: Greener organic laboratory options
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The traditional synthesis of amides from carboxylic acids is wasteful and involves the use of hazardous reagents. Some textbooks suggest that direct amidation is not a viable option. An alternative approach involves the use of a microwave reactor to convert the acid salt to an amide using urea and benzimidazole. This synthesis is considered greener because it is single-step, solvent-free and uses safer reagents than the typical synthesis. This simple green chemistry procedure is appropriate for the undergraduate organic chemistry laboratory equipped with a microwave reactor.

CHED 1480

Undergraduate laboratory experience on kinetics: Using the FeIII-TAML system with common food dyes

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This study focuses on formulating an undergraduate laboratory experience on catalyzed decay kinetics of common Food, Drug & Cosmetic (FD&C) dyes. The catalyst, FeIII-TAML (Tetra-Amido Macrocyclic Ligand), activates hydrogen peroxide and has shown effectiveness in the degradation of a variety of pollutants. This provides an excellent teaching model for undergraduate laboratories that can be beneficial in the study of fundamental chemical concepts. The experimental parameters are designed to allow students to study kinetics and determine rate laws under various reaction conditions. By adjusting the peroxide concentration, students can be also introduced to the Michaelis-Menten mechanism. In addition to serving as a didactic kinetics experiment, this lab also introduces concepts of green chemistry and allows for further discussion. The concepts of catalysis and degradation are themes that can be directly connected to principles of green chemistry.

CHED 1481

Preventing general chemistry students from sinking into the chemical ocean

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General chemistry provides a critical foundation for students interested in advancing in the sciences. Due to the vast amount of material introduced in general chemistry, it is vital that students get across the “chemical ocean.” The chemical ocean is a term that encourages students to get help early, to stay on top of concepts, and to avoid drowning when incorporating previous concepts to new topics such as stoichiometry. Supplemental Instruction (SI) is a program that provides peer-led sessions that helps students to obtain the tools necessary to avoid sinking into the “chemical ocean.” Through a multitude of techniques, SI leaders assist students in better understanding core concepts and focus on these concepts to help students build a strong chemistry foundation. Student knowledge was assessed with pre- and post-tests. Results indicate that students who attend SI sessions are able to develop a stronger knowledge base than those students who do not attend.

CHED 1482

Harmonious world of chemistry with Cathy Middlecamp

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For many years we have been discussing the importance of encouraging disadvantaged students into the field of chemistry, especially those from underrepresented groups: African-Americans, Native Americans, and Hispanics. Many of these students shy away from chemistry. It takes a committed chemist, like Cathy Middlecamp, who is ready to devote time, resources and compassion to attract these students to chemistry. Equal access to science education is a human right that belongs to all. If we do not guarantee science education to these groups, we will form a two-class society divided not by royalty and status, but by knowledge of science. Creative methods for teaching and learning must be developed for all levels, from primary school to university, and from the formal to the informal settings. These methods must utilize the students’ talents, hobbies, interests and cultural backgrounds.

A centerpiece of such a method is the development of student projects, which help them to remember and understand abstract scientific concepts. An old Chinese proverb says: “I hear and I forget; I see and I remember; I do and I understand.” These students’ projects take advantage of seeing and remembering, as well as doing and understanding. Through this process, students are active learners, instead of being passive observers. To demonstrate their understanding of scientific concepts through their projects, the students use a media of their choice, from drawing, dance and drama to computer animation. Projects can also take the form of paintings, sculptures, rap, films, and scripts for theater. These projects are used as alternative assessment methods where the whole class is involved in the assessment process. In order for these methods to be successful, workshops for teachers as well as parents must be
conducted. The cooperation of all of these units allows for there to be an educational harmony.

CHED 1483

Award Address (ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences sponsored by the Camille and Henry Dreyfus Foundation). Award address: Four-part harmony (or disharmony)

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No single factor insures student success in an undergraduate chemistry course. Rather, success involves a complex interplay of the faculty, the students, the curriculum, and the campus climate. When all four "harmonize" to encourage learning, the resulting "melody" brings joy to all who hear it. However, when one player strikes a dischord, students suffer and the disharmony is heard through the wider community. This awards address weaves together stories of harmony and disharmony, ones that can help us to better work together to minimize the dischords for all involved.

CHED 1484

Disadvantaged students: A faculty perspective

Marion H. O'Leary, moleary@csus.edu. Dean, College of Natural Sciences and Mathematics, California State University, Sacramento, Sacramento, California, United States
Teaching chemistry is easy when our students seems to be just like us—if we share culture, history, and experiences, communicating chemistry takes advantage of that shared history. Conversely, it is more challenging to teach when we have less common community with our students.

In the first three decades after World War II, this commonality was high. The GI Bill brought a large collection of bright, ambitious (mostly male) veterans into America’s universities; this was followed by the Sputnik era, in which our classrooms were focused on a bright, talented group of future faculty and researchers.

But the Civil Rights Movement of the1970s brought a more diverse community into the college chemistry classroom. Existing teaching strategies didn’t always meet the needs of this new group of students, nor the needs of other disadvantaged students. The educational establishment was slow to confront the new educational challenges brought on by these new students.

Academic problems encountered by a group of minority nursing students enrolled in a general chemistry course at the University of Wisconsin-Madison in the early 1970s led to the formation of the Chemistry Tutorial Program (now the Chemistry Learning Center). Faculty were slow to come to terms with the kinds of changes in teaching strategy that would help these students succeed, and as a result much of that effort fell to the Chemistry Learning Center.

This is the first of three talks about the Center. This one focuses on the cultural history of the teaching of chemistry in the second half of the twentieth century, with particular attention to the events leading up the formation of the Chemistry Tutorial Program. The second and third talks focus on teaching strategies and student responses as the educational paradigm gradually acknowledged the need for change.

CHED 1485

Disadvantaged students: Who are they and what prevents their learning and achievement

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Educational disadvantage does not lie exclusively in SAT scores, number of AP courses taken, or the race/ethnicity of students. Disadvantage lies at the nexus of the educational system (its instruction, curriculum, culture and context) and the student learning within that system.

In the early years of the Chemistry Tutorial Program, we found that educational disadvantage shows up in multiple contexts: when students don’t understand how to
use the course teaching elements (e.g., lectures, text readings, problems sets,) to identify what needs to be learned and at what level or when they lack the skills to process information to reach the expected level of mastery. The multiple causes of student disadvantage in learning chemistry meant there would be no magic bullet to lessen the barriers to learning and achievement. We needed cognitive, personal, affective, and socialization goals if we were to help all students learn.

Over time we developed many additional strategies beyond one-on-one tutorials. We offered group tutorials in which students could learn from one another about content and how to learn it. Problem-solving sessions taught algorithms for simple problems and taught students to write their own algorithms. We offered pre-/post-laboratory sessions, teaching students to prepare well for labs and write them up accurately. Practice exams were held before course exams, to lessen text anxiety and help students anticipate the level of test questions; by semester end, students would write their own practice exams. Post-exam critiques allow students to correct their errors and also to plan improvements in their study for the next exam.

After 4 years, Cathy Middlecamp joined the Program. In this session I will tell stories of how we put our knowledge of chemistry, computers, and of students to create a learning community for staff and students, one based on mutual respect and celebration. We live in a world where there will always be some students who are initially disadvantaged, but the Tutorial Program taught us how to empower them to ultimately succeed.

CHED 1486

Disadvantaged students: The whole is more than the sum of the parts

Anthony Jacob, atjacob@wisc.edu. Univ of Wisconsin, Madison, Wisconsin, United States

Students are more than a collection of at-risk data points. They are the sum of their academic background, family life, financial situation, and personal drive and enthusiasm. What puts a student at-risk for failure in an introductory chemistry course; can we identify the primary factors? For example, if a student’s math background is weak will this be the deciding characteristic for success or failure? How do we or can we quantify some of the less quantifiable characteristics such as a student’s social networks, the academic climate perceived, or an individual’s confidence. Is a young freshman who is still “learning the ropes” and doing poorly the same as an at-risk student? What are we missing that might be fundamental to identify an at-risk student, and should we consider the course itself as creating some of the risk? This presentation will try to answer some of these questions but will probably raise more questions than answers.

CHED 1487

Disadvantaged students: Undergrad to grad - a personal view
Derrick R. Arnelle, darnelle@alum.mit.edu. Alkermes, Arlington, Massachusetts, United States

My attendance at very good chemistry institutions has given me a particular and perhaps unfashionable view of chemical education. While chemistry topics are presented, they are often not taught. The student is expected to already have the tools to learn the topic, expected to understand the workings of their brain and stumble upon techniques to enable effective and efficient learning. Navigating science and math in college does not have to be a Brownian motion exercise vacillating between frustration and begrudging understanding. As natural scientists and students, we know a lot about the brain and how to learn; we know what works for us and research has found techniques which work for students of all ages. I argue that chemistry as a central topic in science is also able to deliver essential lessons in learning which are far more useful than the subject matter which MOST of the students will forget. If we want to encourage STEM engagement and training, I argue that we as chemistry students and teachers should be viewed as enablers of learning rather than gatekeepers in a torturous endeavor to be endured.

CHED 1488

Disadvantaged students: Mentors come in many shapes and notes

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Few, if any, successful careers develop without mentoring. The large variety of roles along the way necessarily means that different mentors must play a role along the way. A 6th grade teacher, a high-school chess coach, a college research adviser, a peer, and a member of the National Academy of Science can each play a critical but different role to the success of a professor. For the lucky few, such mentors seemingly appear just at the right time. For most, and particularly for disadvantaged students, such mentors are hard to find. Given that the demographics of the academy remain far from those of our student body, we must also recognize that differences between mentors and mentees will naturally exist. Like in the compositions of modern atonal music, such differences can be used to advantage. We will discuss examples and suggestions for implementing mentoring structures deliberately.

CHED 1489

Disadvantaged students: Diversity in many shapes and forms

Tehshik P. Yoon, tyoon@chem.wisc.edu. Chemistry Department, Univ of Wisconsin Madison, Madison, Wisconsin, United States

Diversity issues in science are difficult to address for a variety of reasons, but one important difficulty is that the needs of various constituencies are themselves so
diverse. The tools and strategies that are appropriate to work towards dismantling institutional biases against women and racial minority groups may not be the same (and indeed are clearly not the same) as those appropriate for increasing inclusivity for (inter alia) LGBTQ, disabled, or non-traditional students in chemistry. How might we craft a nimble, engaged activism that embraces the needs of all of these disparate groups without unintentionally putting them in tension? I will examine this question through the lens of LGBTQ identity and reflect upon some of the emerging scholarship around the specific challenges facing LGBTQ scientists.

CHED 1490

Disadvantaged students: Mentoring and place-based engagement in Alaska

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Where they live can disadvantage students. Where students live should have something to do with what they are taught. In Alaska, an explant of the USA, this concept of place-based education, i.e. teaching and sharing knowledge that is needed to live well, has a very long tradition. This cross-cultural tradition is central to connecting with diverse students, and engaging disadvantaged students in science topics that relate to their communities and career goals. Disadvantages can be related to many different factors, such as culture, race, family, society and financial barriers. In Alaska, students can experience the disadvantage of living in small rural villages that practice a subsistence life style with an associated holistic world view. The large size of the state with little infrastructure makes the large distances to the few education centers a barrier not often experienced in developed countries. The long and extreme Arctic winters can exasperate the travel and communication barriers. Alaska educators have learned over the last few decades from elders potential approaches to overcoming some of the barriers.

Use of traditional and local knowledge to enhance connectivity to community life and values can be coupled to mentoring.

Similar to a guide assisting a sailor or hunter in navigating an unfamiliar region, teachers as mentors can assist and encourage the student in their navigation of an unfamiliar university culture. In this discussion, I will draw upon several case studies to illustrate how students overcame obstacles to move forward in their lives.

CHED 1491

Disadvantaged students: Jumping into the deep end

Linda Nicholas-Figueroa, lnicholasfigueroa@alaska.edu. Ilisagvik College, Barrow, Alaska, United States
I teach at Ilisagvik College, the only tribal college in the State of Alaska. Ilisagvik draws students from many parts of Alaska, including the region of Alaska that lies above the Arctic Circle, the North Slope. It is comprised of eight villages with Barrow being the largest of 4500 people, Point Lay with 700 and the smallest village with 200 people. Educating the youth on the North Slope in STEM became a passion of mine. In my talk and in the discussion panel that follows it, I will describe how both I and my students have “jumped into the deep end,” telling stories that reveal the nuances in the term “disadvantaged.”

CHED 1492

Disadvantaged students: The view moving forward

Matthew A. Fisher, matt.fisher@email.stvincent.edu. Dept of Chem, St Vincent Colg, Latrobe, Pennsylvania, United States

As chemists, we understand the importance of context – acidic vs. basic pH, nonpolar vs. polar. Our students also function and learn in a variety of contexts, some of them involving complex, ever-changing relationships. Whether a student or group of students should be viewed as disadvantaged can be profoundly influenced by context. Drawing on ideas from other presentations and comments in this symposium, this talk will look at what ideas we can use as we collectively work together to move forward in the goal of engaging ALL students in learning chemistry for “the benefit of Earth and its people.”
Implementing ASCIv2 to measure students’ attitudes towards chemistry in large enrolment chemistry subjects at an Australian university

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With an institutional shift towards implementation of significant teaching and learning methodology changes in the first year chemistry subjects at the University of Technology Sydney (UTS) it was desirable and timely to institute an externally developed and validated measure of students attitudes towards chemistry, in addition to the general University survey and classroom feedback survey given each semester. 220 students were enrolled in Chemistry 1 and 624 in Chemistry 2 spring 2014 (July-November). The tool Attitude toward the Subject of Chemistry Inventory version 2 (ASCIv2) was administered to Chemistry 1 and Chemistry 2 sections. ASCIv2 was modified from ASCI and tested for reliability and validity in the US by Xu et al., followed by evaluation with a cohort of about 100 students at an Australian University. ASCIv2 has now been administered in large enrolment subjects at UTS, providing a significantly larger data set than previously available to analyse reliability and validity of this tool in Australia. It is desirable to utilize an attitude inventory each semester in first year chemistry as a monitoring device of emotional satisfaction of students and intellectual accessibility of material to students to assess impact of major teaching and learning changes in the subject.

Developing a curriculum for an international service learning (ISL) program in artisanal and small-scale gold mining (ASGM) communities

Adam M. Kiefer, kiefer_am@mercer.edu. Chemistry Dept, Mercer University, Macon, Georgia, United States
International service learning (ISL) programs combine experiences from study abroad, service learning and traditional education to generate a new and meaningful experience for students. These programs are designed to take students outside of the classroom and their comfort zone, and integrate traditional coursework with real-world applications to serve others in developing nations. Although ISL programs are rapidly becoming more common in undergraduate education, the development of chemistry ISL programs has lagged. Over a 5-week summer semester students enrolled in Mercer on Mission, an international service-learning program unique to Mercer University, participate in two classes while carrying out a service project in a developing nation. Over the last 5 years we have developed a Mercer on Mission program focusing on addressing chemical pollution related to artisanal and small-scale gold mining in both Ecuador and Mozambique. Artisanal and small-scale gold miners in these nations often use mercury and/or cyanide to concentrate and isolate the precious metal. During gold processing and purification these chemicals are released into the environment contaminating the air, soil and waterways while placing members of the local communities at risk. This rigorous program directly engages Mercer University undergraduate students in chemistry research, while providing miners with presentations on how to “safely” work with the chemicals associated with ASGM. This presentation will highlight the development of the curriculum for this ISL program, specifically as it relates to the chemical component of the program. The author will specifically discuss efforts to get undergraduate science majors to reflect upon their education in chemistry in the context of the cultures of the miners.

CHED 1495

Good CoP: A successful community of practice in a faculty of science

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We have established a community of practice (CoP) focused on improving student learning in first-year science. It is recognised that transition, whether from school to university or other possible transitions, is an issue of concern for the entire higher education sector - this has been acknowledged at Faculty and University level within University of Technology, Sydney (UTS). A group of both permanent and casual academic staff with significant membership from the wider university community such as student services staff and the central learning and teaching group of the university have met on a regular basis. The members all recognise that making the first-year experience as rewarding as possible is critical to student retention and student success. It is this common understanding that is probably the most important element in the success of the CoP. The typical format of a session is that two or three members make a short presentation, with each presentation being actively discussed by the group – the engagement of the members and the energy in the discussions are remarkable. Other factors to which we attribute the success of this CoP include: that we are working within the context of a well-established set of transition pedagogues which have been strongly promoted and supported within UTS; that the CoP is the creation of its membership and
has not been commissioned from on-high; that there is institutional support for the CoP; that there is leadership and active engagement of a senior staff member; that the recently appointed academic developer in the Faculty of Science has contributed significantly to the life of this CoP.

CHED 1496

Role of internationalization in the development of pedagogical content knowledge of pre-service chemistry teachers

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Pedagogical Content Knowledge (PCK) has been defined as a form of practical knowledge of how to teach a specific content (Shulman, 1986). It is a synthesis of pedagogical knowledge (knowing about teaching) and content knowledge (knowing about what they teach). PCK was first defined by Shulman (1986) as a theoretical construct, later empirically supported by qualitative data which helped identification of its components in a 'knowledge quartet' (Rowland, et al., 2005). Even though PCK starts to develops when teachers begin teaching in their regular classes, the development can be fostered during pre-service teacher education through experience and reflective practices (Nilssen, 2008). The role of feedback from peers has been found to be essential in teacher education (Wilkins, et.al., 2009). Recent studies have shown that pre-service teachers who receive feedback from their peers found to improve their reflective and critical thinking skills (Wu & Kao, 2008). This process can also be enriched by including international perspectives. The aim of this study was to investigate the effects of getting feedback from international and local peers in pre-service chemistry teachers' understanding of PCK. In this study, an eight-week international collaboration was designed between Turkey and Holland while pre-service chemistry teachers in both countries were taking the teaching methods course. In the beginning of the program, students watched a video of experienced science teacher and determined the practices and knowledge that the teacher had. Then, they read articles on PCK, specifically on Rowland's knowledge quartet, did group jigsaw activities, and class discussions. Next, students were randomly assigned to have international or local feedback peers; leading to 7 Turkish-Dutch and 6 Turkish-Turkish peer groups. Then, students watched a 20 minute practice teaching video of a Turkish pre-service chemistry teacher, and identified the specific dimensions of PCK in knowledge quartet and give feedback to their peers. After revizing their analysis based on the feedback of peers, they wrote a reflection on their experience. This procedure had been repeated for a Dutch pre-service chemistry teacher. At the end, as post assessment, students watched the first video again and answered the same questions. The results of the analysis showed various the effects of internationalization and peer feedback practices on pre-service teachers' understanding of PCK.

CHED 1497
PolyWhat? What in the world is a polymer

Sherri C. Rukes, scrukes@comcast.net. Libertyville High School, Libertyville, Illinois, United States

For many teachers teaching elementary and even middle school do not have the background in science let alone chemistry. Even for High School teachers the idea of teaching polymers can be rather difficult to do because they never really understood them or never was taught that. Polymers are more than just plastics and the concepts behind them are not difficult to understand, but can be intimidating. This session will give teachers many ways of introducing what a polymer is, understand what a polymer is and be given many different activities to do for their classrooms. Giving teachers the basics and ways to present the material will help them be able to add this to their classroom. Being able to simplify the concept for many to understand will allow the teachers to get a better understanding and will give them tools to use as well as being able to know what a polymer really is. The uses of polymers are many in today’s society and many debates are coming up about the use of them. By giving teachers information about polymers will help them inform the students, so they can make an informed decision.

CHED 1498

Polymers: New twists on old favorites

Debbie Goodwin, Sherri C. Rukes, scrukes@comcast.net. (1) Libertyville High School, Libertyville, Illinois, United States (2) retired, Chillicothe High School, Chillicothe, Missouri, United States

The presentation will be beneficial to those teaching polymers for the first time and those wanting to beef-up traditional polymer labs. Polymer activities are often used for "fun" lab days and learning opportunities are not maximized. We will show how to add variables and science process skills to make labs more inquiry-based.

A common polymer activity is making slime. We have added the variable of changing the amount of borax solution used. Students investigate the difference that hydrogen bonding makes in the properties by comparing the different slimes. They select the "perfect" slime and defend their choice in terms of properties and uses. Other lab extensions are provided.

Shrinking plastic is a popular polymer activity. We have enhanced the lab by adding math calculations which lead to making a student product. Geometric figures are cut from polystyrene, measurements made, and area calculated before and after the shrinking process. Percent reduction is calculated. Students design a product, draw it actual size, and use their measurements and calculations to determine the proper dimensions for the beginning piece of plastic.
CHED 1499

How are plastic toys made? The manufacturing of plastics

Andrew Nydam², Sherri C. Rukes¹, scrukes@comcast.net. (1) Libertyville High School, Libertyville, Illinois, United States (2) Teacher, ASM International Foundation, Materials Park, Ohio, United States

Every wonder how things are made or how plastic could be formed into my different shapes, sizes, films or blocks? This session will go through the manufacturing process of some of the worlds most favorite toys and other items. Discussion on picking out the right materials for the toy and where some places find the materials to use. Also there will be talks about the process of manufacturing the toy to the packaging of the toy and other favorite items such as a water bottle. However, it does not stop there. The discussion will also include what happens to the toy after the child does not want it. Why recycling plastic is a good thing, if it is able to be recycled. This will include how some toys that are made out of various plastics could be turned into something else. Ideas for incorporating this into the curriculum will also be discussed as well as activities and demos that could be used to teach it.

CHED 1500

Bioplastics: From the farm to the store shelf

Edmund J. Escudero², Sherri C. Rukes¹, scrukes@comcast.net. (1) Libertyville High School, Libertyville, Illinois, United States (2) Summit Country Day Schl, Cincinnati, Ohio, United States

As society has evolved, the use of plastics has evolved with it. Plastics have been a fundamental material for many of the devices and day to day items that we use. There are many types of plastics around and those various types are plastics are needed for the many different uses that society depends on. With the push to become greener, bioplastics are emerging more and more. This talk will discuss the various components to what makes a bioplastic, how they are made, the difference between compostable and biodegradable, the various types of bioplastics, properties of these plastics, as well as, learn how to make various types of bioplastics. The idea of making bioplastics as an inquiry lab will be discussed, as well as, how to actually test the material to see the various properties.

CHED 1501

Reaching out through outreach to the DFW community

Caleb Ashbrook, c.q.ashbrook@tcu.edu, Scott Mathis, Sydney DeSpain, Austin L. Green, Emily Fung, Prabesh Patel, Michael Chandra, sarah price, Tung Le, ryan itoh, Kevin vu, Kaitlyn Upton, claire simmons, Thomas A. Schneider, troy gurney, Julie Fry,
TCU Chemistry Club has established a series of programs in the Dallas-Fort Worth Region to provide local teachers with support for K-12 education. These activities include science clubs, college experience days and materials for teachers in the community. The TCU Chemistry Club provides this support through pre-made kits and organized modules that focus on TEKS components in the state of Texas and thereby compliment and enhance the curriculum of the teachers we work with.

CHED 1502

Passadena City College Student Chapter: Successful activities on campus and in the community

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The Pasadena City College Chemistry Club pursues to promote the field of chemistry by actively engaging the undergraduate student body, conducting outreach activities with elementary schools, and encouraging green chemistry awareness to the general public. In order to inform our members about different fields of chemistry, we invited professionals such as university professors and researchers to host talks about their scientific contribution to the society. This also informs members about possible career paths as speakers reveal their own education and career experience. Our outreach activities allow us to teach our members the importance of educating the younger generation in chemistry, provide a unique educational experience to all students involved, and encourage younger students to pursue a STEM related educational path. Our club is currently involved with CalTech and their S.E.A.L. program. We are conducting research in discovering metal oxides that will act as catalysts for photo electrolysis of water. The opportunity to conduct research and participate in club activities provides a fulfilling educational experience to students involved in our club.

CHED 1503

Expanding our community involvement

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The Illinois Valley Community College section of the American Chemical Society has been focused on expanding our community involvement. Our poster will focus on our activities with a major focus put on the now Annual Sci-Fest we hold. Last year we had over six hundred people attend our science related chemistry show and hope to keep it growing. Other side topics on the poster might include our National Chemistry Week activities, speakers we have gotten to speak to the club, and small chemistry shows that we do at local shows and at events within the college.

CHED 1504

Student chapter events and activities done at Tennessee Tech University

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The amazing number of events and activities done for outreach, for service, for networking, for fun, for education, and to promote ACS and green chemistry by the Student Members of the American Chemical Society.

CHED 1505

Non-Newtonian fluids as a student affiliates chapter event: Chemistry, logistics, and outreach

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The Pepperdine University Chapter of the ACS Student Affiliates held a “walk on water” event as a part of our community outreach for National Chemistry Week. The nugget of an idea to make the suspension of cornstarch in water commonly known as Oobleck, a non-Newtonian fluid, grew into making the event a campus and community-wide outreach event where people could play with the Oobleck, walk on it, and learn about fluids. Hosting the event required significant planning, attention to detail, communication within the club and with the college student affairs department, coordination of group members, and overcoming other logistical hurdles. We held a work day to prepare for the event where we built the wooden frame, practiced making hundreds of pounds of Oobleck with a commercial cement mixer, and considered the details to make the event both safe and fun. As the day of the event approached, we turned our attention to the specifics of our corn starch and water sources, event publicity, and developing an educational placard. Our event was a huge success where hundreds of people played with or walked, ran, or danced on Oobleck. We present information that made our event successful and observations that would improve future events such as this.

CHED 1506

ACS student affiliates chapter of Seattle Pacific University

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The Seattle Pacific University ACS student affiliates chapter is active and thriving. We have five major objectives: to promote appreciation of chemistry, foster student-faculty camaraderie, serve the community, earn funds, and send students to chemistry conferences. Our club activities that met these objectives include: voluntarily tutoring local public high school students, paying fees for student presenters at research conferences, hosting "Bowling with the Professors", serving at the Annual End-of-the-Year BBQ, inviting the community to social functions, going on laboratory tours at local labs, and doing volunteer community service in our city. All of these activities were funded by selling lab coats, lab notebooks, and ACS exam study guides throughout the year.

CHED 1507

American Chemical Society Student Chapter at The University of Texas at Tyler

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The American Chemical Society Student Chapter at The University of Texas at Tyler has been an active and rewarding chapter. In addition to learning more about chemistry, we have developed leadership skills in planning and carrying out multiple chapter activities. We are extremely proud of our chapter for receiving various chapter awards
during the past 15 years and the Green Chemistry Award for the past four years. Our chapter exemplifies what it takes to be a successful student chapter. We wish to demonstrate to other chapters the many things we do to maintain a successful chapter in the hope that others may find new ways to reach their members, campus, and community. Our poster will therefore feature segments on: campus outreach, community outreach, professional involvement, K-12 activities, community service and social events.

CHED 1508

Activities of Ferris State University student affiliate chapter

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Ferris State University's Student Affiliate Chapter of American Chemical Society strives to promote green chemistry, to be involved with the community, and to improve the intellectual atmosphere at the university. It is felt that these are key objectives in maintaining a successful student chapter. We do this by keeping a section of a nearby national forest clean, biannually cleaning up highway mileage, inviting speakers for seminars, visiting the local section's meetings, attending family events to promote chemistry among the youth in the community, being science fair judges, offering tutoring on a weekly basis, sending representatives of the university to the National Conference, and even more. This chapter has just received the Commendable Chapter Award and Green Chemistry Award for the academic year of 2013-2014. However, the chapter has been awarded these high accolades in the past. Ferris State University registered student organization awards have also been awarded to the chapter in the past.

CHED 1509

Discover gold with the Alchemist Club at Missouri Western State University

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The Missouri Western State University American Chemical Society Student Affiliate will present our club poster showcasing the various activities and events our club participated in over the past academic year. The mission of the Missouri Western State University ACS Student Affiliate is to inspire lifelong learning, advance knowledge, and foster interest in chemistry at MWSU and throughout the local community. In conjunction with the Department of Chemistry, the ACS Student Affiliate has been able to host several speakers for seminars, hold webinars and discussions to enrich the academic experience of its members, connect with the local community through outreach events for grade school children and high school students, provide opportunities for research presentation, and hold networking activities through fun,
social events. It is our goal to share our positive experiences and network with other ACS Student Affiliates from other undergraduate institutions like ourselves to get new ideas that will better our organization, university, and community.

CHED 1510

NSF Community College Innovation challenge: A proposal

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NSF has invited teams of community college students to propose an innovative solution to one of America’s most daunting challenges: broadening participation in STEM and improving STEM education. NSF leaders in undergraduate education are expecting to see new ways for students, faculty, community and industry to work together. The students at Stark State College in North Canton, OH have proposed the following solution:

Stark State College Student Affiliates of the ACS (SSC Chemistry Club) have identified a local high school that does not have a chemistry club. The SSC Chemistry Club officers have reached out to the faculty and administration at the high school to offer assistance in initiating a chemistry club with the current chemistry students. With the successful initiation of the new club, the SSC Chemistry Club will directly involve the new HS chemistry club to collaborate in their STEM outreach activities in three areas. The first area is mentoring younger students. Both chemistry clubs will work together to offer science demonstrations and tutoring to Stark State College’s “STEM in the Middle” students who are in grades 6-8. The second area is community outreach. Both clubs will collaborate with their industry partner, Lubrizol and with local Library Youth Program Coordinators to provide continuous, quarterly science outreach events at three local libraries. The third area is collaboration across the STEM areas. By partnering with other college clubs on campus such as Society of Women Engineers, Tri Beta Biological Honors Society, Physics and Astronomy Club, and the Software Development Guild, our group hopes to expand interest and participation in STEM activities.

CHED 1511

Saint Francis University Chemistry Club: Safe but fun

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The Saint Francis University Chemistry Club has maintained a high level of student involvement through different social and service events. The Chemistry Club hosts a welcome picnic, wiffleball games, camping trips, holiday gatherings, and farewell
events. Each semester, the club hosts a T-shirt design competition to enhance club visibility on campus. In addition, the club engages in service through the Rural Outreach Chemistry for Kids (R.O.C.K.) program. The R.O.C.K. program has been in operation for 20 years, annually hosting over 3000 K-12 students through a number of outreach activities, both on and off campus. The focus of the R.O.C.K. program is to have K-12 students actively involved in chemistry-related activities. Students within the club also serve as peer tutors for various science courses on campus and also actively serve the community. The Chemistry Club fosters environmental awareness and the use of green practices both in the lab and in the community.

CHED 1512

Discerning student interest in science activities

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To coincide with National Chemistry Week, the Delaware-ACS Section hosts a Family Science Adventure program at the Independence School, Newark DE. A goal of this program is to build awareness of chemistry at the local level. Every year Wesley College STEM students participate in this event and they conduct a series of "fun" hands-on experiments that explain various chemical principles. This year, we surveyed the participants (parents & kids) before and after the event, to demonstrate any measureable increase in student interest after program participation.

This poster details all hands-on experiments that were conducted and provides unambiguous data from our study on students’ attitude towards science and science topics.

The Wesley College Directed Research Program is supported with grants from the Delaware INBRE program with an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences - NIGMS (8 P20 GM103446-14) at the National Institutes of Health (NIH); a National Science Foundation (NSF) Experimental Program to Stimulate Competitive Research (Delaware-EPSCoR) grant EPS-0814251; an NSF S-STEM grant 1355554; and the State of Delaware. A number of the Wesley STEM participants are Cannon Scholars (NSF-DUE 1355554). Matt Love is a graduate student in the MAT program. Ariel & Alora are undergraduates in the biological chemistry program.

CHED 1513

Wayne State University ACS Student Affiliates
After reactivation in September 2011, the Wayne State University Student Affiliates (WSU ACS-SA) have worked very hard to become an active, enthusiastic, and energetic chapter. This year, the WSU ACS-SA will be participating in multiple social, scientific, volunteer, and outreach activities. The WSU ACS-SA has increased its on-campus presence, boosted its membership, and strengthened its relationship with the WSU Chemistry Department. The WSU ACS-SA has continued its relationship with the ACS Detroit Local Chapter, expanded its outreach and volunteering activities, and participated in ACS Local, Regional, and National Meetings. The highlights of the last year will be presented.

CHED 1514

Belmont SMACS: Engaging in awesome science

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Belmont University’s Student Members host two week-long events each year designed to draw attention to the discipline and make connections with the “real world”. During the fall semester student members participate in two types of events. One type of event is a presentation of chemistry (Awesome Science!) to the students of Belmont’s campus. The other type of event involves going to the Boys and Girls club of Nashville and providing both hands-on and demonstration experiences. In the spring, Belmont students organize a week-long series of events focusing on several aspects of forensic science. The week begins with a discussion of the realities of data collection and analysis during forensic fieldwork. The week ends with an opportunity for students to put their sleuthing skills to work to solve a staged crime after observing the evidence. Throughout the year our chapter also hosts seminars focused on exploring careers in the sciences and “next steps” for graduates.

CHED 1515
Molloy Chemical Society

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At Saint Joseph’s University in Philadelphia PA, Molloy Chemical Society has reestablished itself as an active ACS accredited student body club. Molloy consists of student associates of the American Chemical Society and is involved in campus and community outreach, educational guest lectures, fundraising and monthly club meetings. In the 2013-2014 academic year we had guest lecturers, including Dr. Kadine Mohomed who discussed the contributions of modern thermal analysis in materials science and the application of these techniques to problems of interest in the industry. Our commitment to campus and larger community involvement is embodied in student members of Molloy attend both regional and national ACS conferences to present research as well as volunteering in the Philadelphia Science Carnival. Our main fundraising campaign is the Valentine’s Day Test Tube sale where all profits benefit activities such as the Franklin Institute field trip, a booth at the Philadelphia Science Carnival, and travel costs for ACS regional and national meetings. The ultimate goals of Molloy Chemistry Society are to encourage undergraduate scientific involvement, establish a university and community presence and provide students with opportunities to learn and experience the wonders of chemistry.

CHED 1516

SIUE Chemistry Club: Promoting science education on campus and beyond

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The SIUE Chemistry Club is committed to sharing our passion for chemistry with our community. Our primary goal is to prepare members for careers in science through educational activities, professional development experiences, and a diverse, supportive network of peers. Members organize a large number of educational and social events each year. Recent educational events include hands-on demonstrations for preschool children, a celebration of National Chemistry Week, a tour of a local industrial chemical facility, and volunteering with local ACS section events. A subset of the group, Cougars Volunteering for Science, travels to local schools to lead interactive chemistry-related lessons throughout the year. Each year, SIUE Chemistry Club joins with the SIUE Department of Chemistry to support visiting speakers from academia and industry, as well assisting with our annual Probst lecture. We are continuing to incorporate activities related to green chemistry and sustainability, as well as increasing volunteer efforts in our area.

CHED 1517

American Chemical Society Student Chapter at Peninsula College
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In 2015, the student chapter of the American Chemical Society at Peninsula College will celebrated its third anniversary. Events during the first year focused on community outreach such as Science Saturday at the library and chemical demonstrations for elementary school children. During the second year, the chapter attended a regional conference and assembled a GC/MS instrument donated to the department. Details of the activities will be presented and future goals for the chapter will be discussed.

CHED 1518

Gruen Chemistry Society: Student affiliate activities at Olivet College

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Gruen Chemistry Society at Olivet College was reactivated as a student affiliate chapter in 2009. We have named ourselves after Dr. Fred Gruen, the 1970 faculty advisor from the initial student affiliate chapter. Our chapter's activities have included participating in Chemistry Day at Impression 5 organized by our local section, hosting Chemistry Day at our home institution, participating in Science Night for local elementary children, Service Day projects, and participating in Battle of the Chem Clubs with other Michigan chemistry clubs hosted by our local section’s YCC. Our fundraising activities have included edible periodic tables and holiday chocolate sales which have allowed students to accompany the current faculty advisor to the past four spring ACS national meetings. This year's plans include continuing participation in these activities, new fundraising activities, and hosting more social events for our members.

CHED 1519

Millersville University ACS Student Chapter 2014-2015

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The Millersville University ACS Student Chapter does a variety of activities throughout the year. Some of our biggest activities include celebrating National Chemistry Week and sending students to the ACS National Meeting to present their research. We also try to spread the joy of chemistry to fellow college students, high school students, and younger children by participating at the local Whitaker Center and the S.T.E.M. Fair. Throughout the year we do fundraisers to help support our chapter. The two fundraisers that contribute the most to the Student Chapter are selling chemistry themed T-shirts and the Sugar Bowl fundraiser. We are a green chemistry chapter and we spread the
word of green chemistry to the campus and beyond. We also like to plan fun activities like bowling, student/faculty picnics, and more.

CHED 1520

Improving leadership and programming: Finding the balance between quality and ability

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The Penn State Berks Chapter has become well known in the community for it's programming. However, like many chapters, we have experienced vacant positions and/or the inability of officers to fulfill the duties of the positions to which they were elected. After 2013-2014 experiences, a new approach was taken - allowing students to lead where they can instead of completely adhering to the traditional leadership model. This is our experiment in finding the balance between quality and ability.

CHED 1521

Online fundraising activities to support student travel and research at Illinois State University

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Our Chemistry Club recruited student volunteers to sell department T-shirts, club mugs, faculty-developed lab manuals, safety glasses, and practice exams for chemistry courses with the help of the Department of Chemistry. As these sales involved frequent cash transactions, online sales were introduced in the Fall of 2014 in order to manage these transactions more effectively. The revenue generated was given back to our active members in the form of travel and research grants, enabling 12 students to attend ACS national meetings and supporting 2 additional students in their research endeavors. In addition to fundraising activities, significant attempts were made by our club members to engage the ISU community in chemistry-related demonstrations. Building upon the foundations of solid fundraising activities, our club seeks to provide
increased opportunities for students to actively volunteer in community outreach events to earn grants while promoting our chapter, ACS, the department, and ISU.

CHED 1522

Student Affiliates of the American Chemical Society San José State University Chapter

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The goals of San José State University’s Student Affiliates of the American Chemical Society (SJSU SAACS) are to provide a diverse and welcoming environment for students and faculty to interact, and to foster a well-educated scientific community through outreach and philanthropy within the community. SJSU SAACS provides its members many opportunities to be involved in community volunteer activities, such as National Chemistry Week, the Bay Area Science Festival, and the Regional Undergraduate ACS Symposium. Additionally, we organize seminars with the Chemistry Department to promote research opportunities with professors at SJSU. We also hold activities that encourage bonding with our members, such as bowling and holiday socials, as well as bi-annual Faculty/Student mixers in the form of the Winter Dinner and Spring Picnic. As SJSU SAACS is a non-profit organization, all raised funds are donated back to the members and the community in the form of scholarships and grants.

CHED 1523

Aquinas Chemistry Society: 2015 successful chapter poster

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The Aquinas Chemistry Society is a student chapter of the American Chemistry Society that promotes chemistry and science at Aquinas College and the surrounding Grand Rapids community. Throughout the year, our society participates in several on-campus events that not only promotes chemistry on campus, but advertises our society as well. These events include homecoming booth, Fall Fest, and Saint Stock. In addition, our society hosts several events during the year for our student members. We host speaker series, including undergraduate summer research students; conduct monthly meeting with fun activities such as experiments and games; coordinate a volunteer-based tutoring program that is available on a weekly basis for all chemistry students; organize a banquet at the end of the year to celebrate all science graduates and recognize their achievements; and organize events for National Chemistry Week, including selling Periodic Table of Elements cookies, chili cookoff, and find-the-mole competition. We promote science to the community through various events such as chemistry-in-the-
mall and St. Albert's Day. Our society is particularly proud of St. Albert's day because every year, we host this science day for nearly 100 local fourth grade students for a day of fun scientific experiments that encourages students interest in science. Our student chapter is committed to working with other members of the American Chemistry Society West Michigan Chapter as well. Our society collaborates with other chapters by participating in events such as Program-in-a-box and Battle of the Chem. Clubs. Our student chapter has attended the past three National ACS meetings and has been recognized at the National meeting with awards for the past nine years.

CHED 1524

ACS Student Chapter of the University of St. Thomas: At the center of the energy and medical capital of the world

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Since its inception in 2000, the ACS Student Chapter of the University of St. Thomas in Houston, TX, the energy and medical capital of the world, has received Honorable Mention, Commendable, and Outstanding Chapter awards. For the past two academic years, we received Outstanding Chapter awards and received a Green Chemistry award for 2013-2014. Our accomplishments are a result of publicity, regular meetings, planning activities of interest for the student members, and by interacting with the local ACS section. For 2013-2014, we organized a career tour to visit the new neurology lab at Texas Children's Hospital in Houston. We started a weekly tutoring program for both ACS and non-ACS members. We organized the annual career forum for STEM fields. We performed chemistry demonstrations at the Houston Museum of Natural Science and the Houston Children's Museum for National Chemistry Week. During Black History Month, we held a screening of the PBS documentary about Percy Julian, "Forgotten Genius". We held a spaghetti dinner at the Hospitality Apartments and Ronald McDonald House where patients stay during treatment at the Texas Medical Center. We also hold social events, such as barbeques where students can come tie-dye their lab coats. Because of the enthusiasm and support of our members, we are a very successful club on campus.

CHED 1525

Florida Southern College student chapter growth 2014-2015

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The American Chemical Society Student Chapter (ACS-SC) at Florida Southern College (FSC) aims to promote chemistry on campus and in the community and to promote chemistry education in K-12. To do so, the ACS-SC has needed increased participation from its members. This year, the ACS-SC focused on leadership and recruitment techniques. With respect to leadership, the chapter updated and passed new by-laws to more clearly define executive officer roles. With respect to recruitment, we visited freshman and sophomore chemistry classes, hosted events early in the semester, and encouraged each functioning member to bring one new functioning member into the organization. With more functioning members, we were able to host more events to meet our goals of promoting chemistry, advancing member careers and improving chemistry education in the community. Activities included traditional chapter events, such as inviting speakers from academia and industry to campus for the Chemistry Lecture Series, performing chemistry demonstrations for students on campus and at local K-12 schools, and hosting Advanced Placement (AP) Chemistry Labs for area high school students on campus. New activities included ‘professional development’ events such as the Program-in-a-Box webinar ‘Speaking Simply’ and social activities, such as a ‘Candy Party’ for National Chemistry Week and science movie nights. In addition, our chapter has provided networking opportunities to members by hosting dinners for members and invited speakers. Overall, the FSC ACS student chapter’s goals and achievements have reflected those of ACS as a national society.

CHED 1526

Small but mighty Centenary College Chemistry Club

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This year, the Centenary College Chemistry Club has the mission to strive for the three pillars set by the American Chemical Society: Service, Professional Development, and Chapter Development. We prioritized these pillars through the annual programs that our club presents along with a variety of new programs to be implemented this year. Our large annual programs that work towards the pillars of Service and Professional Development are National Chemistry Week and the Annual Chemistry and Physics Circus. During National Chemistry Week we have at least one program every day of the week to benefit both members of our organization and students across the campus. The week always ends with Chemistry Club members volunteering at SciPort, Louisiana’s Science Center, to facilitate hands-on activities for kids in upper elementary and middle schools from around the area. For the Chemistry and Physics Circus, we partner with the Centenary College Physics Club and the Centenary College Admissions Department to perform a variety of demonstrations for prospective students visiting the college. During the event, prospective students are able to watch chemistry and physics undergraduate students perform the demonstrations to the crowd. The new programs to
be implemented this year will focus on the Shreveport community located around the
college. We hope to build relationships with local high schools, as well as local alumni
who work in various industries in the town of Shreveport. Being a small chapter from a
small school leaves the Centenary College Chemistry Club with some limitations, but it
also allows for many unique opportunities for our members and more freedoms for our
officers to plan events. With this mindset, the Centenary College Chemistry Club sees
ourselves as a small but mighty club doing great things both on campus and in the
surrounding community.

CHED 1527

NCW 2013 at UPR Humacao: A sweet celebration

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The chapter of student members of the American Chemical Society at UPR Humacao
details their enthusiastic participation in the celebration of NCW 2014. Ending with a
successful “Festival de Química” where ACS student chapters of all Puerto Rico united
with Chem Clubs and the ACS Local section to celebrate chemistry's influence in our
lives and promote the NCW theme of "Candy: the sweet side of chemistry" among our
communities.

CHED 1528

Speaker series at Northeastern: Inspiring the next generation of chemists

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and Chemical Biology, Northeastern University, Boston, Massachusetts, United States

One of the main goals of the Northeastern University Student Affiliates of the American
Chemical Society (NUSAACS) is to foster an environment where undergraduates can
explore their interests in the growing and exciting fields of chemistry. A central piece to
achieving this goal is the speaker series that we organize throughout the entire
academic year. Thanks to Northeastern's world-renowned experiential learning
cooperative education (co-op) program, NUSAACS has been fortunate enough to
successfully reach out to influential and prominent members of industry and academia
to speak at our meetings. As a larger organization we understand that there are varying
interests among our members and a countless number of possible career paths with a
chemistry degree, so we are always very conscientious about what types of speakers
we invite to our meetings. In the past year, we have had speakers from varying ares of
industry and academia including green chemistry, forensics, biotechnology,
neuroscience, cosmetics, and radiochemistry. In addition, our own members and alumni
of the chemistry department have shared their experiences with wine chemistry, beer
chemistry, graduate Ph.D programs, medical school, and more. Our presentation will
detail the various speakers and events of the past year and the incredible impact they have had on our members. We firmly believe that this exposure to diverse career paths provides our members with a sense of purpose as they continue their chemical education. The objective of this presentation is to showcase to other groups the importance of such events and how they can be tailored to fit the needs of the organization as a whole.

CHED 1529

American Chemical Society University of New Mexico Chapter

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The University of New Mexico Chemical Society chapter is a successful student organization composed of over 20 active members. Many of these students are currently conducting laboratory research in chemistry, biology, chemical biology, and biochemistry related fields. ACS-UNM provides funding, networking, and local research opportunities to our active members; we seek to aid our friends and peers in the chemistry-related fields so as to enrich their undergraduate experience and strengthen their future careers in science. We have a proud outreach program that helps to expose children in local elementary schools to the wonders of science. Our members regularly volunteer in chemical demonstrations aimed at teaching children the scientific method in addition to basic chemistry concepts. Through laboratory notebook sales and fundraising, we donate money to local charities and mentoring organizations. Our chapter at UNM believes that enthusiasm and passion are essential trademarks for a successful researcher.

CHED 1530

ACS Wilkes Student Chapter applying green chemistry principles

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The ACS Student Chapter at Wilkes University utilizes “green” chemistry principles while promoting science education in the local school districts, grades K-12. Several events such as WEBS (Women Empowered by Science), Pre-Med Day and Passport to Science bring in young students from local schools to participate in lab activities and demos. These activities often use household items to practice do-it-yourself experiments and expose participants to basic chemistry. The members of the Wilkes Student Chapter also participate in the majors/minors fairs, open houses and host an annual lecture featured by a renowned scientist. In October 2014, the Sterling Professor
of Chemistry at Yale University, Dr. William Jorgensen, presented his research on drug-design using computational chemistry. All these events involve chemistry and non-chemistry students who share their passion for science and chemistry with others.

CHED 1531

SMACS attacks chemistry

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Frostburg State University's Student Members of the American Chemical Society (SMACS) are excited to present their activities in public outreach through chemistry demonstrations. SMACS performs demonstrations for local schools and the general public. Our experiences include FSU's STEM Festival and a National Chemistry Week presentation on the science of candy.

CHED 1532

Events and outreach of the University of Colorado Denver SAACS Chemistry Club

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The Chemistry Club at the University of Colorado Denver aims to express the invaluable role that chemistry shoulders in everyday life to the community and students of all ages. By educating freshmen, sophomores, and transfer students on the importance of undergraduate research and showing our colleagues about the wonders of chemistry during our fundraising events, we strive to incorporate chemistry and science education into all the activities we strive to do in our organization. Every year during National Chemistry Week, we sell safety goggles and liquid nitrogen ice cream while engaging students about the importance of green chemistry and education. All demonstrations we perform are chemistry focused and environmentally friendly as we appreciate the importance that environmental consciousness plays in the world of science and chemistry. For example, the liquid nitrogen ice cream that is made for National Chemistry Week is delicious, demonstrates phase changes, and only produces an innocuous gas. We perform demonstrations like this during university open houses, for elementary school students, and during seasonal tabling events, which not only gives us an opportunity to talk with students about chemistry but also to discuss the advantages of choosing chemistry as their major, and a potential career path. These types of interactions benefit everyone involved because the chapter acts as a friendly interface between students and faculty. We continuously work to expand and improve
our chapter through outreach events and educational opportunities for the benefit of our community.

CHED 1533

Restarting the student affiliate in the oldest town in Texas

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Stephen F. Austin (SFA) State University is located in Nacogdoches, Texas. Nacogdoches has the distinction of being “The Oldest Town” in Texas. The ACS Student Affiliate at SFA was restarted in October of 2014. With a renewed vigor the section trained 6 undergraduate students to safely conduct classical chemical demonstrations. Thereafter, we brought the demonstrations to local schools. In the process, the student members honed their presentation to younger students which lead to a greater appreciation of chemistry by all. In the poster we will present a description of the demonstrations given, and a teaching tools we developed to follow up with the students. Images of the children enjoying chemistry will also be shared.

CHED 1534

University of Central Arkansas ACS chemistry chapter: Using an inter-chapter relations grant to increase chemical outreach

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Our chapter has an avid interest in interacting with our community to develop a public appreciation for chemistry and science. To share and learn from other chemistry clubs, we applied for and received an ACS Student Inter-Chapter Relations Grant to host
Demo-Palooza, an afternoon of demonstrations by UCA’s Jerry Manion and Louisiana Tech’s Bill Deese. With over 60 attendees from our own campus, local community, and four other nearby universities, the demonstrations and explanations of their chemistry concepts educated and delighted the audience. Our chapter plans to implement what we learned into our regularly scheduled events, such as Science Nights at local schools, a community-wide environmental EcoFest, and Kids’ Club at UCA football games. Performing these demonstrations and participating in these events has not only contributed to our community, but benefited club members via volunteer opportunities, professional growth in organizational and communication skills, as well as networking with our peers.

CHED 1535

Leading a successful ACS Student Chapter

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Being an active member of an ACS Student Chapter provides many benefits for the student such as increasing the quality and number of professional contacts, developing leadership capabilities, building career knowledge, and increasing the opportunities to experience tours and technical presentations. Recruiting and keeping members is one of the most important endeavors for any student-run organization. Once students have joined, there are many ways to keep them involved in the chapter. Knowing the members’ needs is important. Many students need tutoring and so are willing to go to tutoring sessions. It is also important to be flexible. There should be several chapter meetings at various times. Each one could occur twice a week at various times so that the students are more likely to be available and attend at least one of them. The time that the members put into the chapter should be worth the effort. The meetings and activities should be interesting and worthwhile. If attendance is declining, requesting that chemistry professors give extra credit for participation in chapter activities can be very fruitful. The use of social media helps keep the members engaged. Using a combination of mass e-mails, on-campus bulletin boards, LMS, and classroom announcements helps to spread information about activities. Providing successful chapter activities is a great way to keep the members interested and engaged. Field trips give students the chance to spend time together as a group away from the campus. Providing an opportunity for travel to a regional or national meeting has helped to motive the Chapter to successfully fundraise toward a goal. Chapters should also take advantage of ACS grants which are a great way to direct energy around their mission.

CHED 1536

Cultivating and communicating chemistry on campus and in the community
The Ouachita Baptist University ACS student chapter hosts a variety of events designed to target both the community and our chapter’s members. The main focus of our community outreach has been to share a love of science with the children in Arkadelphia as well as our fellow students. We also participated in Tiger Serve Day which is an event that allows Ouachita students to serve elderly or disadvantaged residents of Arkadelphia. Last year at Peritt Elementary School, we began performing Fusion Science Theater, a skit that uses the scientific method as a teaching tool. Because it was such a success, we applied for and received a grant to perform the skit at our local children’s hospital.

We also host events that target our chapter’s members. Examples of events include attending lectures, hosting grant proposal workshops, and organizing classes, such as ceramic glazing, to connect science to other areas of study. To give our members an opportunity to showcase their research and to learn about other advances in the field of chemistry, we attend spring national ACS meetings. We sent thirteen of our chapter members to attend the 247th National ACS Meeting. While at the national meeting, our chapter participated in the Speak Simply competition and received six of the fifteen awards given. Currently, our chapter has 40 members, 14 of whom are national ACS members.

CHED 1537

New Mexico Highlands University Chemistry Club: Starting a student chapter

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In 2013, NMHU reactivated a long dormant student chapter. The club's outreach in both the academic and social areas will be presented. Activities with local high schools and university students that raise the profile of the group and excite the student members have been instrumental in establishing and growing our chapter.

CHED 1538

Successful student chapter, Suffolk University 2014

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The purpose of the Suffolk University chapter of the American Chemical Society is to allow an opportunity for students studying chemical and biological sciences to enjoy the intellectual stimulation that arises from being a member of a professional association. In order to create a professional drive among the members interested in scientific and chemical careers, we held events involving professional talks and engaged in our community through our involvement with middle school and high school students. To further strengthen our community involvement, chapter members have volunteered in various regional events, such as in museums for the National Chemistry Week and for the celebration of Earth’s Day sponsored by ACS.

CHED 1539

Eastern Oregon University ACS Student Member Chapter: Promoting community outreach and professional networking

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The EOU ACS Student Chapter has continued its tradition of community outreach and high involvement on the EOU campus in the past year. Club members have served as ambassadors of chemistry in events including Girls in Science, Saturday Science, and chemical magic shows. These events were hosted with the goal of sparking an interest in science among a group of young, diverse students. The popularity of EOU ACS Student Chapter activities has become evident, as demonstrated by the growing number of elementary through high school aged participants each year. In addition, seventeen club members presented undergraduate research spanning a multitude of chemical and biochemical applications at the national meeting of the American Chemical Society in Dallas, Texas. This opportunity was made possible thanks to funding from the ACS Richland section, EOU Senate Allocations, and club fundraisers.

CHED 1540

Saint Louis University brings the wonder of chemistry to local Saint Louis students

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The theme of this 249th ACS National Conference and Convention is “Chemistry of Natural Resources” emphasizing the importance of utilizing the environment wisely. The ACS Student Chapter at Saint Louis University has taken full advantage of their environment in the city of Saint Louis. Because the campus is located in an urban setting, club members get the chance to volunteer with inner city youth and tour various types of laboratories and chemical companies. One of the Chemistry Club's lead projects this year is a partnership with an after school program in North Saint Louis called North Campus. There, Club members teach 6th-8th grade students various chemistry topics through hands-on demonstrations and lessons. SLU Chemistry Club also takes advantage of the University environment through innovative ways of recruiting new members, such as liquid nitrogen ice cream and encouraging fellowship and learning amongst students with similar interests in chemistry. To foster learning, Chemistry Club provides its members with the unique opportunity to become a “demo captain” and perform an experiment for the Club while explaining the chemistry behind it. SLU Chemistry Club has also added a chemistry honors society, a chapter of Gamma Sigma Epsilon, to Saint Louis University. Through all of these academic, service, and fellowship pursuits, SLU Chemistry Club has promoted the importance of chemistry on campus and in throughout the Saint Louis area.

CHED 1541

Surface modification to impact our community

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Surface modification is the action of transforming the surface of a material by changing physical, chemical or biological characteristics different from the ones originally found on the surface of a material. As a young chapter we are always modifying our work to ensure that our community will be positively affected. Through our amendment as a chapter we have focused on community service, helping homeless people and making an impact on educating children (K-12) through the power of chemistry. Our community has been impacted through activities as “Back to school”, where public housing residents received basic materials for the new academic year. We have supported non-profit organizations as "GoGo Foundation" to help children with cancer and "Amor que Sana" that serve daily food to homeless people. Also we collaborate with the administration of our college in several activities to raise funds for scholarships. The K-12 activities have been improved this year. We changed the chemical demonstrations in order to allow every child to learn and enjoy chemistry in a green way. We have had the opportunity to see the results of this immense reaction and the good we are making to our community. Also we visited more schools than past years. We are prioritizing the recruitment of new members to create a larger change that will impact more surface
area. Professional development of our member has been successfully achieved through conferences, research meetings and hands-on activities. The National Chemistry Week and Earth Week has become an important activity where we involved the entire academic community at our campus. We are willing to be part of a surface modification if that will make a transformation in people. We like to be a chemical force that facilitating good things to everybody through our chapter.

CHED 1542

Ecofriendly chapter: education and implementation for a sustainable world

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As habitants of a planet which is surprisingly deteriorating by the hazardous effects of the misuse of its resources, it is with honor and enthusiasm that the Green Division of the ACS Chapter Inter American Ponce engages in the movement towards a green mind set applying the principles of Green Chemistry. We are aimed to conserve a healthy and green environment exploring and promoting the design and implementation of products and processes that minimize the use and generation of hazardous substances. We believe that Green chemistry ultimately is a more eco friendly way of doing chemistry without hurting our environment. As members of the Division of Green Chemistry we are being part of the overall movement towards a better and sustainable world. Likewise, our Chapter pursues the awareness among campus and off campus population to promote education on how to reduce environmental hazardous damages produced by chemical products and or processes related with the human health and also the environment. Among the initiatives adopted by our chapter, are a go Green vision implemented through recycling programs of plastic and aluminum, as strategies to prevent the generation of pollutants. Also, we have been actively promoting the correct use of chemistry through demonstrations and creating awareness of the usefulness regarding green chemistry. Our planet’s resources are being over-used at a slow replacement rate; we must act now to conserve for sustainability. Chemistry is responsible for essentially everything that surrounds us, we as green believers need to procure that the materials or substances are as benign and environmentally friendly as possible. Our passion as members of ACS Green Division is to encourage green chemistry and promote safer practices.

CHED 1543

PCUPR student affiliate chapter celebrates a summer festival

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The Student Affiliate Chapter of the American Chemical Society at Pontifical Catholic University of Puerto Rico organized a Summer Festival for the second consecutive year. The festival was celebrated at La Guancha in Ponce, Puerto Rico. Being in the south side of the island, sometimes our region is left behind when larger activities are organized in San Juan, PR. Our chapter decided to impact the south area by organizing this festival in La Guancha, a recreation area for children, adults, and tourists of the south region. Chemistry demonstrations were performed from 2:00 PM to 6:00 PM. Presentations included the areas of materials (polymers), the environment (recycling), and acid-base demonstrations. Some of the demonstrations included: Secret message and Color changes (acid-base), Snow creation and Slime production (polymers), Cleaning water and using plastic for decorations (environment). Students were organized by topics and faculty helped as supervisors. This idea was developed by one of our members, Nilza Negron. The activity was for the general public and we impacted near 100 people. This is the second year we celebrate the festival and our chapter already had established this festival as part of our academic year activities. Next year we plan to invite students accepted at PCUPR in the College of Science to involve them in our chapter activities before entering the university.

CHED 1544

Metamorphosis: Our chapter evolution

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Ten years ago we started a new course, opened our wings to a new world: to renew our engagement with the American Chemical Society. Our association has undergone a metamorphosis and evolved in its ideas, vision and goals to produce a highly recognized student organization inside and outside our University. Through the years and experiences, we have grown as students, professionals and human beings. We have grown intellectually, as social entities and have started to open the doors to successful futures.

Our association’s success strives in our community and professional engagement. We work hard to help individuals and groups in need. Those experiences has helped us to grow as a group and as better persons.

Each year we recruit new members and make them an integral part of it. We promote fellowship and share activities, stories, and even dreams. We are all a family. By planning and participating in many activities such as demonstrations which encourage the love of Chemistry, and community work we have become more responsible and have developed leadership skills within each of us. It has been ten years of hard but
successful work, but most important is that together we stand tall and the sky is the limit.

CHED 1545

ChEmory: Emory University's undergraduate chapter of the American Chemical Society

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ChEmory is Emory University’s undergraduate chemistry club and American Chemical Society chapter. The mission of our organization is to spread the passion that all of our members have for chemistry and science. Our goal is to involve members of the community in educational chemical demonstrations, participate with undergraduate and graduate students at Emory University, and work with the American Chemical society at a local, state and national level. We are actively involved in the Atlanta community with our outreach programs at elementary, middle and high schools. We help to excite students about chemistry in the hopes that we can spark the same passion for science that we carry. Not only that, but we are also involved with Atlanta-wide events, such as the Atlanta Science Festival, to reach as many people as possible. The inaugural Atlanta Science Festival in spring 2014 was a very exciting opportunity. The event drew thousands of people from all over Atlanta and our organization helped to create a booth explaining polymer chemistry and non-Newtonian fluids. We also performed science as a keynote event show utilizing many of the typical experiments we perform as a part of our outreach. ChEmory has been invited to participate again in 2015. On campus, we train students in chemical demonstrations, help disseminate information about career options in chemistry, and assist with the pursuit of higher education. We work with graduate students to assist with everything from undergraduate research to graduate school applications. Furthermore, with the help of the Chemistry Department, we find speakers to discuss careers outside of the laboratory or academia. We have many goals and missions that we pursue each and every year. We succeed in all of our arenas, and we are currently growing to become a very involved organization at Emory University and in the Atlanta Community.

CHED 1546

Exploring chemistry through candy at Carroll University

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The main goal of our chemistry club this year was to become more well-known around our campus community by demonstrating the importance and prevalence of chemistry in our daily lives. To do this, we took advantage of the American Chemical Society’s
theme for National Chemistry Week: The Sweet Side of Chemistry—Candy. Candy is typically universally enjoyed, so this was a good theme to catch campus’ attention. We hosted campus events to accomplish our goal of demonstrating chemistry in daily life, including candy-making, candy demonstrations, and a flavors and fragrances contest. To celebrate the theme, free candy was offered to the attendees at every event while they took part in our chemistry-related activities. Through the theme of candy, we were able to attract more of the campus population and provide them with related chemistry knowledge.

CHED 1547

Successful student chapters abstract: Hofstra University student members of the American Chemical Society

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Hofstra University’s Student Members of the American Chemical Society (SMACS) provides a professional yet social environment in the Chemistry department. Students of any major with an interest in Chemistry are welcome to join, as most of the events held are Chemistry related. To promote a sense of community in the department, SMACS offers social events open to both professors and students such as an ice cream social, a movie night, bowling, and a trip to the Museum of Natural History. Members also have the opportunity to participate in community-service based events that SMACS hosts including a Jones Beach clean-up and Relay for Life. SMACS also promotes Chemistry in the community by hosting chemistry events for the Girl Scouts and performing experiments at the NY Hall of Science for National Chemistry Week. Last but certainly not least, SMACS invites three guest lecturers per semester to present their research for professional development. A handful of members have the opportunity to have lunch with the guest lecturers and ask about their research or how to succeed in graduate school. This presentation will describe the events mentioned and their success.

CHED 1548

Student Affiliate Chapter of the American Chemical Society: Minot State University

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The Student Affiliate Chapter of the ACS at Minot State University received its Charter in 2008. It is a fairly small organization with an average annual membership of 8 to 10 students. Working closely with the campus’s Science Club, the students interact with the community through events such as the MSU at the Mall event, chemistry demonstrations at local schools and our biggest event, the annual Science Open House. At the annual Science Open House, almost 1000 students from local elementary and middle schools come to our department for the day while we do a variety of science demonstrations for them. All members of the Chapter have been very active in conducting research in chemistry and in presenting the research results at various science meetings including the National Meetings of the American Chemical Society. Since 2008, the students have made over 130 original research presentations at the national, regional, and local level. Four times now (2009, 2010, 2013, and 2014), MSU chemistry students were selected by the national Council for Undergraduate Research to present their research results to members of the United States Congress at the Posters on the Hill Session.

CHED 1549

Georgia College's outstanding student chapter: "Sweeter" than Georgia peaches

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Georgia College's ACS Student Chapter is community service oriented, while also emphasizing professional and academic development. A large component of the organization’s activities involves engaging students and families in the middle Georgia area in order to show the public how exciting chemistry can be. Some of these activities include peer tutoring on campus, visits to the Georgia War Veterans' Home and several local nursing homes, participating with hands on activities with local K-12 schools via magic show demonstrations, and volunteering as science fair mentors and judges. Through partnership with the Middle Georgia Local Section, the student chapter has been able to successfully coordinate National Chemistry Week-enhancing the community’s knowledge of the sweeter side of chemistry-and Earth Day along with various other events. Professional development workshops are offered to assist the chapter with career choices, résumé writing, and interviewing skills. Beyond all the organization's hard work, the club spends just as much time promoting new friendships among its many members. The organization plans many social activities such as movie nights, trivia nights, cookouts, and bonfires. This poster highlights some aspects of the organization through its accomplishments.
CHED 1550

Miami Chemical Society from Miami University (Ohio)

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The Miami Chemical Society welcomes all students with interests in chemistry at Miami University by providing social, academic, and professional opportunities to members. MCS also sponsors educational events for other Miami students and for the public. MCS provides a great opportunity to meet students with similar interests, gain exposure at national events, grow as scientists by meeting with visiting researchers and faculty from around the country, and share a passion for science both on campus and in the Oxford community.

CHED 1551

SMSU Chemistry Club: Activities of an outstanding student chapter of the ACS

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The chemistry club at SMSU strives to maintain an active chapter in a variety of ways. One of our primary activities is outreach with area K-12 schools. We love sharing our enthusiasm for science and trying to inspire future scientists. We do this in part by performing large open-to-the-public demonstration shows on-campus followed by liquid nitrogen ice cream. We do additional on-campus shows for specific school groups, with hands-on activities when possible. We also take our show on the road and travel to area schools for demonstration shows and hands-on activities. Additionally, we participate in the SMSU Homecoming Parade, attend ACS-sponsored webinars, visit graduate programs of universities in our region, invite area chemists and alumni to speak, and attend the Spring National ACS Meeting. We try to keep our activities fun and interesting and continually try to recruit new club members from our existing and incoming student population. We hope they love sharing and doing chemistry as much as we do!

CHED 1552

First Loras College chemistry carnival: The chemistry of candy
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The Loras American Chemical Society Student Chapter hosted their first ever Chemistry Carnival. In this event, middle to elementary aged children learned about the sweet side of chemistry with over a dozen hands on activities and demonstrations, such as learning how to make rock candy. Some of the themes for these demonstrations included learning about the chemistry of the body, environmental chemistry, and the chemistry of candy! In addition to the chemistry carnival, the ACS student chapter hosted the Chemistry Olympics – an event where high school students participate in various chemistry competitions, such as titration races. Finally, other activities of the student chapter, such as mole day celebrations and guest speakers, are presented.

CHED 1553

Stimulating interest and enthusiasm for chemistry

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In collaboration with the FIU Chemistry department we hosted two workshops for undergraduate chemists– “Careers in Chemistry” (Spring 2014) and “Chemistry Graduate School Symposium” (Fall 2014). It was exciting to be part of the “Geekiwood” event, aimed at increasing interest in STEM fields among middle school and high school girls. On Mole Day, we discussed Avagadro’s number and distributed chips and Gauco-mole. Members also did demos on the “Family Day” at the Museum of Science and Discovery in Ft. Lauderdale as part of National Chemistry Week. Free tutoring is provided for General and Organic chemistry during the semester and for the first time this summer we hosted a Final Exam study session. The club also attended a roundtable to raise awareness about the looming threat of antibiotic resistance. As part of outreach, high school students will be invited to come on-campus to participate in interactive lecture-demonstrations and perform inquiry-based experiments.

CHED 1554
Successful chapter activities of the Monmouth University Chemistry Club

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Monmouth University’s Chemistry Club has a history in offering educational and professional development to those who are attracted to the field of chemistry. With the use of different events to broaden students’ mindsets about the field of chemistry through its various applications, students have the ability to be subjected to innovative research, graduate panels and attend guest speaker seminars. We highly recommend that students learn about different career paths through the visitation of graduate schools or chemical companies. In addition to a focus in professional development, the Chemistry Club partakes in various community service events, such as doing demonstrations at local schools. As another asset to students who are involved in the club, we encourage them to remain an active member in the Student Affiliate Chapter of the American Chemical Society. Thus, the purpose of Monmouth University’s Chemistry Club is to sculpt students during their development of becoming young scientists through the various range of events offered.

CHED 1555

University of Puerto Rico- Río Piedras ACS Student Chapter: A role model to our society

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As an ACS student chapter our mission is to improve the quality of life through the transforming power of chemistry; educating about the relevance of chemistry in our daily life. This is achieved during various activities that our chapter led all the way through the academic year; conferences, hands-on demonstration, chemical demonstrations: “The Magic of Chemistry”, community services, among others. Our performance has allowed us to be an Outstanding Chapter for more than 20 years and a role model to emulate. This has been possible due to the commitment that our members have with the chapter and their interest in helping and contributing positively to our society. The trajectory of our chapter members, as Chemistry Ambassadors, demonstrates that the future generation of chemists is one that cares about society. Our members are taught to use their passion for chemistry and the knowledge they have, to contribute positively for a better society, one that benefits all alike. Our successful pathway will be elaborated.
Reactions to increase the yield of involvement

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The Student Organization of the American Chemical Society at the University of Arkansas at Little Rock (UALR), with support from the Chemistry Department, has continued to increase involvement both within the university and with the local community. Our organization has continued a long standing tradition to improve campus involvement, and to provide free tutoring for our fellow chemistry students. Our monthly meetings provide an opportunity for the students of UALR to connect with faculty and graduate students in the Chemistry Department. The organization's focus, this year, has been to promote interest in Chemistry within the local community. This includes students at the college as well as local high schools, middle schools, and even elementary students. Through our activities, we strive to inspire students to someday engage in the Chemistry community.

Tethering community and academic pursuit: A story of success

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As a Student Chapter of the American Chemical Society, the Stonehill College Biochemistry and Chemistry Society is committed to maintaining and fostering an academic community to cultivate the development of a population of independent thinkers. In addition to supporting society programming, many of our members serve auxiliary roles within the Department of Chemistry as laboratory assistants, research assistants, and teaching assistants. Through a complex interaction of social and academic pursuits, we strive to embody our chapter’s mission of generating an equilibrium between fellowship and scholarship.

Arkansas Tech University Chemistry Club: Encouraging and broadening participation through outreach and on campus activities
ATU Chemistry Club was founded in 1974. It is one of the most active student organizations on campus. The members organize a variety of activities on and off campus to: 1) engage and support chemistry students in their academic endeavors, 2) share their passion for chemistry with the community and 3) enhance faculty-student interaction. This poster is a presentation of some the activities ATU Chemistry Club has conducted in recent years. The challenges encountered, and impact of the activities on the academic success and professional development of the students will be discussed.

CHED 1559

Promoting science with the “Chemistry CirCus”

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It is a challenge to demonstrate and get children involved in the science field. Our solution is "The Chemistry CirCus": an experimental outreach program for communicating chemistry creatively offered by the American Chemical Society (ACS) student members of the University of Texas at El Paso. Our group has given performances of the Chemistry CirCus to the El Paso community for over 25 years. The Chemistry CirCus consists of a dozen activities and presentations engaging the audience in inquiry-based learning via experimental and demonstrative activities. These activities range from: explaining acidity via pH indicators, demonstrating endothermic and exothermic reactions, testing different combustion reactions, presenting hydrogen balloon explosions, and utilizing liquid nitrogen to teach about extreme low temperatures. The Chemistry CirCus has been proven to be an efficient method for educating the basic concepts of chemistry for all ages at different levels of education.

CHED 1560

Outreach, teaching, and university connection programs for two-year college students

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For the 2014-2015 academic year, the Pima Community College student chapter started new activities and programs. We received both Community Interaction Grant (CIG) and Innovative Activities Grant (IAG) from ACS to establish a teaching program with topics in the chemical sciences with a local K-8 school. We also have a program that conducts field trips and invites speakers from various science and engineering departments from our local university. The student affiliates have been conducting innovative outreach activities for children, high school students and the general public this year. Finally, PCC student affiliates have started working on new green chemistry activities. All these activities and programs will be discussed.

CHED 1561

Traditions and innovations guiding the way to success for Nittany Chemical Society at Penn State

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The student chapter at Penn State University, Nittany Chemical Society (NCS), has undergone a lot of change and growth over the past several years. While holding onto traditional chapter activities and events, we have strived to develop new and innovative activities for our organization in order to help increase membership retention and involvement. We would like to highlight the events that have lead to our recent success, both new and old.

CHED 1562

Onward and upward: Revitalizing a small student chapter

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Our chapter has had an exceedingly busy year, and after attending the Spring 2014 national meeting, we have implemented new recruiting methods, community service programs, and outreach activities and programs. We were integral in the implementation of the pilot program, Imagine: Your STEM Future, for the Girl Scouts targeting middle and high school girls, encouraging them to follow a STEM pathway. Additionally, we have developed a new outreach program that emphasizes the applications of chemistry in forensic science. Furthermore, we hold campus wide events, promoting creative expression through science. An example of such an event is our tie-dye day, where we provided free tee-shirts to college students and families and taught them about the chemistry of the coloration process. We are continuing to expand our club and are excited to exchange ideas with other student chapters.
Western Washington University Student Chapter of the American Chemical Society

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The Student Chapter at Western Washington University is very active chapter that has been in continual operation since 1969. The goals of our chapter include: 1) create an engaged learning community for students and faculty, 2) serve as a resource for students in their educational experience, and 3) serve as ambassadors for chemistry in our community by offering meaningful service opportunities. Social activities such as the department picnic and bowling night bring students and faculty together in informal settings. Informational seminars, professional development workshops, industry tours, lunches with speakers, conference travel, GRE study groups, and Scholar’s Day help students gain practical knowledge and experience in the chemical fields. Community outreach efforts include: mentoring elementary school science fair students, Wizards @ Western program, and tutoring underserved groups in the community. This year the chapter performed its first-ever bilingual science demonstration at a local community college. Recently, the chapter has been involved in diversity outreach events for increasing diversity in STEM fields. Fundraising events that support our activities include t-shirt and beaker mug sales. The activities organized by the chapter have made an impact on the department, college, and surrounding community.

CHED 1564

Priory of Biology & Chemistry at East LA College: Organically fun

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East Los Angeles College (ELAC) is home to one of the most diverse body of students in the U.S. Here, the Priory of Biology & Chemistry Club (POBC) seeks to attract and ignited student’s passion for science, bringing science and non-science major’s students together in fun, community engaging activities. Regardless of our majors and career goals we meet to share our common interest for the chemical sciences. As a club, we provide students with leadership experiences through various scientific education initiatives and, are always in the lookout for opportunities to be Chemistry ambassadors. During the last year we implemented an ACS Community Grant, which allowed us to visit several high schools and the East LA farmers market. At these places we engaged with the community in the “organic chemistry of smelling,” by using aromatic compounds found in common fruits and vegetables.
Members also get together for social gatherings and biweekly meetings that consist of student presentations/demos as well as presentations from invited educational speakers. As an ACS affiliated chapter, we are always looking forward to do outreach activities in our very diverse community via chemistry demonstrations and hands-on activities. We celebrated Chemistry Week: Candy! with some pretty cool talks and activities in the Hollywood area. We continue to support and maintain our club activities by holding various fundraisers on and off campus. Please come visit us to learn more about our wonderful community and our even more amazing club!

CHED 1565

Getting your chapter involved the community: Examples of community involvement by the Elmira College ACS student affiliate chapter

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One of the major goals of a student affiliate chapter is to get involved in community service. This presentation will focus on the efforts of the Elmira College student chapter of the ACS and the type of community involvement projects they established. The focus of the presentation will be finding the right organizations off campus to work with, developing an activity that promotes both organizations and involves the local community as well as delivery of the activity. The presentation will look at the case study of three different community events created by the chapter and include their development and lessons learned for each activity.

CHED 1566

Instilling chemistry into our biggest natural resource

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Our chapter’s main goal is to educate the community in the sciences. We are very focused on the children and the community and direct many of our programs toward them. Our big accomplishment is instilling a focus on green chemistry and the environment within these children. In order to achieve our goals, we hosted a large variety of events some of which included chemistry speakers, researchers, and professions who had come out to speak to the student body and community and share their professional experiences. We get to do a few large programs in each year, which happened to be Taste of the Sciences, where we took a group of 150 girl scouts and taught them different aspects of chemistry, biology, and forensic science. A STEM Girl Scout program where we took another large group of girls and taught them the different ways that green chemistry and conservation can be accomplished through sciences.
Eco Fun Day where we take a local middle school who is focused on conservation, and we taught them all about the environment at our local Angelica Park on campus. Science Day we brought in 50 5th and 6th grade students from a local inner city school and taught them chemistry, biology, and forensic science for a day to get them interested in furthering their education someday. We hosted a summer camp where we partnered with Carpenter Technologies to bring out 150 kids for 5 days in the summer to learn about chemistry, engineering, and physics. We ended our summer camp with a trip to the Franklin Institute in Philadelphia. We also did many smaller scale events all semester long with 10-50 kids which ranged from girl scouts events involving forensic science, water and air, and home chemistry, also we have a partnership with Muhlenberg and Berks Parks where we do events with their local children on chemistry and the environment. Our club was successful in connecting with our local grade schools, Girl Scout troops, and college students by teaching them about the basics of all fields of science through National Chemistry Week. We also hosted our second annual Green Chemistry Week. During these events, make-your-own-novelty events, green chemistry and household chemistry information booths, guest speakers, and service projects. Overall, our chapter successfully increased the awareness of and interest in the sciences, and promoted community relations.

CHED 1567

Central Washington University SA-ACS 2014-2015: Development of standard operating procedures (SOPs) for the safe, educational and fun performance of chemistry demonstrations

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Chemical demonstrations have played a large part in creating interest in the CWU Chem Club (CWU SA-ACS) and drawing in new members. Although the nature of demos are fun, these various phenomenon lead to a variety of serious hazards that must be well understood to perform in a safe manner. To ensure safety is our top priority, our club devised a 3-part demonstration standard operating procedure (demo-SOP) that includes (1) chemical preparation in the stockroom, (2) chemical presentation in front of the audience, and (3) differentiated learning that explains the demonstration at a K-8 or 9-12 level that align with Next Generation Science Standards (NGSS). This 3-part demo-SOP provides an excellent quick guide for safely preparing and delivering the demo, the equipment needed, how to properly dispose of the chemical waste, and
an age-appropriate explanation of the chemistry involved so that the performed demonstrations are as safe and informative as they are fun!

CHED 1568

Importance of community outreach and encouragement of the sciences

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The Temple University Chemical Society (TUCS) will be discussing the various outreach programs we perform throughout the year. Setting the Spike for Science, our annual volleyball tournament fundraiser will be discussed, along with our 8th and Diamond Community Center trips and fundraising events such as Alex's Lemonade Stand. As a chapter, we believe that reaching out to the community and spreading a love for chemistry is a great way to make a difference, and we would like to share our methods with our fellow Student Chapters.

CHED 1569

Barry University Chemistry Club: Celebrating twenty years of excellence

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Chartered by ACS in 1994, the Barry University Chemistry Club has been an award winning ACS Student Chapter for 20 years, by providing service to the university and surrounding community as well as professional development activities for our chemistry students by hosting guest speakers from other institutions and even our alumni, and providing peer tutoring. We present Chemistry Magic Shows at local elementary schools and day-long chemistry programs with hands-on activities and demos for middle-school-aged students, supported by a Community Interaction Grant from ACS. Our National Chemistry Week (NCW) was voted the Best Event of the Year (2013) by our Student Organization Council. Chapter members set up a chemistry display table and handed out a variety of chemistry-related items, such as Chem Matters, wallet-size periodic tables and sold chemistry t-shirts, bumper stickers, Avogadro- Milli- and Nano-mole dolls. We also participated in the South Florida ACS NCW event at the Ft. Lauderdale Museum of Discovery and Science where we performed intriguing demos for over 400 children and parents. We celebrated Mole Day by making liquid nitrogen ice cream and sold cookies decorated with element symbols. On Earth Day the club emphasized the importance of green chemistry and created awareness in the Barry University
community about proper safety and waste disposal systems. Several free green chemistry items were handed out as part of the event. In addition, the club has participated in other community events such as the annual coastal beach clean-up, the Miami Heart Walk, and collecting toys for sick children for Christmas. Our members enjoy semester kick-off pizza parties and end of semester luncheons (food provided by department faculty). The chapter activities have largely had a positive impact on member recruitment and retention, contributing to the overall success of the chapter.

CHED 1570

How to retain members and make them feel included

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A reoccurring theme for the Central Michigan University ACS student members is retaining members after that first “kick-off” meeting of every new academic year. There seems to be a steady exodus of non-executive board members as the year wears on. Is this because the new members do not feel like they are an important key player in the group? Is the e-board micromanaging or not sharing the planning responsibilities? The primary goal for the 2014-15 campaign is to reverse the recent group trend of member decline throughout the year. Early efforts are showing a doubling of active members this year (relative to last). This poster will present ways implemented to retain members, student interviews, and group progress towards membership retention/involvement.

CHED 1571

Chemical demonstration program for continuing education

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The Adrian College Student Chapter of the American Chemical Society sponsored a new event in conjunction with the Lenawee Intermediate School District (LISD) to provide continuing education for local elementary and middle school teachers. Funded by an ACS Innovative Activities Grant (IAG), this project contained two parts, an all day work shop for the teachers and creation of chemistry demonstration kits for local schools to check out from Adrian College.
For the all day workshop teachers were invited to Adrian College’s campus to be taught about each demonstration kit, including the state objectives behind the kits and the proper procedures for their use. The workshop was split into two sessions. In the morning classroom session the ACS Student Chapter members explained each demonstration in detail, including its procedure and safety hazards and how it fits into the state’s science curriculum. In the afternoon laboratory session the chapter members performed each demonstration and then allowed the teachers to practice the demonstrations themselves. The Chapter worked with the LISD to design the workshop so that the hours spent at the event could be counted as continuing education hours for the teachers.

Demonstration kits were created to be loaned out to the teachers on an as-needed basis to be used in their classrooms in accordance with the state objectives. The kits contain all that is needed to successfully run each demonstration, including instructions, reagents, glassware, and safety equipment. When the teachers are done using the kits, they are returned to the Chemistry Club to be restocked and lent out again.

CHED 1572

SAACS Is Au(l) at SHU

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Our club is focused on spreading chemistry education to the community. Through numerous outreach projects and campus demonstrations we have brought chemistry to children and adults. Our goal is to present the basics of chemistry in a fun way that encourages people to learn more about the subject. Our liquid nitrogen demonstrations have been a huge hit on campus that engages people in the topic of flash freezing. We have also gone to community schools and presented chemistry in an age appropriate setting that engages children to become more interested in science. Our club is funded through donations from the campus and community as well as fundraisers both on and off campus. We participated and organize campus events, raffles, and other activities to gain funds as well as exposure for our club. We are a constantly growing club and are continually improving our efforts for spreading chemistry education. This poster will outline all of our activities.

CHED 1573

Forensic chemistry division; A new outreach in our campus
Forensic sciences is one of the most well-known programs in our campus. As promoters of chemistry we created the forensic chemistry division of ACS Inter Ponce, in order to enhance the impact of applied chemistry in our community. We are in a constant reaction to make stronger structures to help us promote understanding of chemistry even though our campus does not have a major in chemistry. We are committed to combine chemical methods and techniques of research for the development of exciting and applied experiences. We have conducted demonstrations to public and private schools applying forensic chemistry. In addition, several activities on and off campus were developed. Those activities include strategies for professional growth and community services. Professional growth activities include organized workshops, forensic science conferences and participation in the Puerto Rico Forensic Institute Annual Symposia. Our commitment to the mission and vision of our Institution is shown through our participation in the Open House, promoting our forensic science program. We serve our community in various ways such as; participation in activities of charitable organizations and in the recollection of toys for Operation Christmas child boxes. As future forensic scientists, we are developing skills through chemistry to become scientific citizens and promote excellent career opportunities.

CHED 1574

Xavier University of Louisiana’s student chapter: Enriching the legacy

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Over the past several years the Xavier University of Louisiana Chemistry Club has worked to build connections within the New Orleans community. One goal was to foster intercollegiate collaboration with other students in the city of New Orleans. This goal helped to create new ties and partnerships with university students from different backgrounds. Another past goal was to promote community interaction amongst the Chemistry Club members. This goal helped club members connect with children in New Orleans and serve as role models. This year the goal has evolved to not only maintain previously established connections within the New Orleans community, but to help serve as facilitators to help pass the torch to others so that the Chemistry Club can set the groundwork for what would become an interstate of STEM and community outreach. Xavier’s foundress, St. Katherine Drexel, and the sisters of the Blessed Sacrament had a vision for Xavier’s students to promote a more just and humane society by preparing the students to assume roles of leadership and service in the global society. The XULA
Chemistry Club continues to embody every aspect of that mission since its inception. Our members have worked within our university, as well as our community, as chemistry ambassadors. The club has helped foster a love and joy for chemistry and learning with each person we encounter. The Xavier University of Louisiana Student Chapter is a club that will continue our commitment to service. XULA Chemistry Club aims to execute this mission by: fostering innovation amongst youths, speaking simply and communicating about STEM to various audiences, and providing help to others who hope to start their own clubs.

CHED 1575

UTPB Chemistry Club: Promoting chemistry in west Texas

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The UTPB Student Affiliate of the ACS is mainly focused on community outreach, as well as getting the public involved in activities that promote chemistry. In addition to having a positive and visible presence on the campus through the active participation in university-sponsored events (such as the Halloween Carnival, the Big Event, Falcon Days…), as well as on-campus fundraisers (bake sales, date with a book…), our community outreach activities include volunteering our time and energy at the regional science fair as judges for elementary and middle school science projects. Students volunteer in elementary schools throughout the Permian Basin, bringing chemistry demonstrations to kids as a way of showing them an accessible way into science, as well as emphasizing the importance of safety when dealing with science. Overall, the Student Chapter focuses its energies into promoting the field of chemistry in the Permian Basin community.

CHED 1576

Successful activities of the Waynesburg University ACS Chapter

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The Waynesburg University ACS student chapter seeks to bring a knowledge and appreciation of chemistry to not only our University, but also the surrounding community. Our chapter utilizes several events, such as our Homeschool labs and Science Day, to spread interest, information, and experience in the field of chemistry. Our homeschool lab event brings in local students to participate in a hands-on experience in a controlled laboratory setting which is run and organized by our members. Science day allows high school students interested in the STEM fields to visit
our campus to participate in lectures, demonstrations, and activities hosted by faculty. They also have the opportunity to discuss with undergraduate students the benefits of majoring in science at the college level. Our chapter has recently added a new activity, the Coffee Lab, in which we invite a local barista to campus to discuss various coffee brewing methods and work with him to test various properties of the brewed product. This event is open to the entire campus.

CHED 1577

Lock Haven University Chemistry Club

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The Lock Haven University of Pennsylvania Chemistry Club is comprised of students who look to advance chemistry knowledge in their school and local community. The club holds many activities to help spread chemistry appreciation and learning. Demonstration shows, held several times a year, allow students to perform interesting experiments for local members of the community and educate people on the science behind the demonstration. The club also offers an annual Chemistry camp, a day long program where local middle school children are taught and shown interesting concepts in chemistry. They perform experiments such as launching pop rockets made with film canisters, water, and antacid tablets. They learn the concept behind the propulsion and what reaction is taking place to cause the rocket to launch. These are just a few of the activities the club holds in order to bring chemistry to the community. Recently the club was also awarded an honorable mention as a student chapter from the ACS.

CHED 1578

Student Chemists Association at The College of New Jersey

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The Student Chemists Association (SCA) at The College of New Jersey (TCNJ) is an American Chemical Society Student Chapter dedicated to professional advancement of members and service to the local community. Webinars, as well as a variety of speakers from different fields of chemistry, are hosted throughout the year, and many upperclassmen members attend lectures, give talks, and present posters at the ACS National Meeting. To facilitate the professional development of freshmen and more generally their acclimation to college life, SCA holds “Happy Hour” events in the fall where freshmen, upperclassmen, and faculty can interact. In terms of service, the club hosts “dry ice bubbles,” “elephant toothpaste,” and “red cabbage indicator” demonstrations at several local elementary and middle schools, as well as at the Ewing
Township Community Fest. SCA also volunteers at the Trenton Area Soup Kitchen, for the Ewing Green Team, and during TCNJ Finals Fest, giving out pretzels to stressed-out students whilst explaining the chemistry of lye! Students in need of a study break enjoy “stressbuster” events such as rockclimbing, lasertag, and paintballing all sponsored by the chapter. Perhaps the most successful events are the social activities. Our most popular events are the Departmental Thanksgiving Potluck and Chemistry Semiformal. Here, we detail what we believe are the best practices for an Outstanding ACS Student Chapter.

CHED 1579

Erskine College ACS Chapter: Not just winging it anymore

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The Erskine College Student Chapter has grown and matured in many ways in between the 2011-2012 and 2013-2014 school years. Our chapter has gone from Honorable Mention for 2012 to Outstanding and Green for 2014. In a school of only 600 students, our 30-member chapter is flourishing, and has been able to make a mark not only the college but also the community. We have learned to diversify our leadership core by pushing project leadership beyond just the chapter officers. We have also incorporated a leadership mentorship process into our officer election cycle. Collectively, these changes, our passion for teaching, and our diverse membership have helped the Erskine College Chapter achieve new heights without feeling like we are “winging it” afresh each year.

CHED 1580

PLU Chemistry Club: Redistributing knowledge according to Le Châtelier’s Principle

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With a continuing theme of green chemistry, the Pacific Lutheran University ACS Student Chapter (PLU Chem Club) has increased its focus on community outreach in the 2014-2015 academic year. In pursuit of a fifth ACS Green Chemistry Award, our club now uses compostable paper plates and utensils during events and avoids environmentally-harmful chemicals during demonstrations. In the interest of spreading chemistry awareness in the general community, club members presented a tri-fold display at a local farmers market event (Plastics: The Good, The Bad, The Ugly) to educate the public about polymer chemistry, the use of BPA in food packaging, and plastic micro bead pollution from personal care products. A direction toward outreach
has also targeted increasing the audience we reach. Since the 2014 Spring National Meeting, our annual "Desserts and Demos" event in the spring hosted nearly 100 local K-12 school students and other community members. The National Chemistry Week (NCW) "Mole Day Eve Spooktacular" attracted a new record of over 120 visitors, bringing together PLU students, faculty, schoolchildren, and families from the local Tacoma region. The 2014 "Chemistry of Candy" NCW theme was celebrated with a live cooking demonstration of caramel-making by PLU Dining Services. In addition to increased attendance to our events, the Chem Club has begun to do outreach opportunities for younger audiences. Group members have presented safe demonstrations multiple times at a local daycare center to groups of about 15 children, and they will facilitate a series of 25-minute hands-on chemistry sessions with 130 fifth-graders visiting the PLU campus in November 2014.

CHED 1581

Collegiate Chemistry Bowl, Demomania, Chemagic show, eminent speaker and networking luncheon part of UT-Martin hosting the undergraduate program at SERMACS

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The University of Tennessee at Martin chapter of SMACS received a grant from the Society Committee on Chemical Education to host the undergraduate program of the 66th Southeastern Regional Meeting of the American Chemical Society (SERMACS) meeting at Nashville from October 16-19. The program included 344 research papers
(out of a total of 1,110) presented by undergraduates, an eminent scientist lecture by Dr. Albert L. Wiley, of Oak Ridge, on Medical Preparedness and Response to Nuclear Power Plant Accidents, a “Chemagic” show by Dr. Al Hazari of UT Knoxville, “Demomania” presentations by SMACS from five universities, including one by UTM SMACS, a networking luncheon and the College Chemistry Bowl. Eleven universities from a five-state area competed in the bowl patterned after the former “The G. E. College Bowl” television show. Concord University in West Virginia won the championship, the University of Alabama at Birmingham was the first runner-up, with Fisk University and Tennessee Technological University as second runners-up. Recognition plaques, trophies, and SERMACS undergraduate program T-shirts were presented by UTM SMACS to winners, judges and oral sessions emcees. Fourteen SMACS spent about two hundred man-hours getting ready and executing this project.

CHED 1582

Career development and networking for chemistry, biochemistry, engineering, and pharmacy majors: KU Chem Club

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The University of Kansas Chemistry Club (KU Chem Club) has over a century of history participating in outreach projects in the Lawrence area, and is known particularly for excellence in K-12 STEM outreach within the Lawrence community and beyond. Officers actively plan and conduct outreach events with new audiences that will lead to a larger awareness of the club’s objectives. During the past year, the KU Chem Club has successfully enhanced its impact on campus and in the broader community: the club has increased its reach in communication by strengthening its online presence; participated in more events with its charter organization, the American Chemical Society (ACS); and communicated with other ACS student chapters. The officers have made the club more attractive to prospective members to increase membership and participation, and therefore, increase community impact. Club members are committed to developing events that promote networking among students, and to forging collaborations with other organizations to promote the growth of all involved parties.

CHED 1583

Saint Vincent College Chemistry Club

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The members of the Saint Vincent College Chemistry Club are dedicated to spreading knowledge and love of chemistry on our campus and to the community. Many of our events involve teaching children about chemistry. These events include helping Cub scouts earn their science badges, hosting a science day for local gifted students, and sponsoring a National Chemistry Week booth at the Carnegie Science Center in Pittsburgh. For National Chemistry Week, the club also participated in “The Periodic Table of Cookies”, where St. Vincent students were able to decorate cookies with their favorite elements. In addition to that, we volunteered to judge a local home school science fair for 8-16 year old students. The members conducted an extremely successful fundraiser by selling safety goggles to chemistry and biology students. The club is also very proud to be able to send members to the Spring ACS Conference every year.

CHED 1584

Green chemistry: Prevention for a cleaner future

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Our student chapter ACS-UPRAg has taken up the mission to educate the community about the importance of Green Chemistry. Due to lack of awareness, we have allowed a great deal of pollution to our ecosystems. This year our green chemistry division started things off by visiting elementary schools and teaching the basics of the green concept. By guiding today’s young students to a greener lifestyle, they will become the professionals that we need in the future. Furthermore, we can’t forget the rest of the community if we want a meaningful change in our society. We organized and hosted the first “What is Green Chemistry?” Workshop in our campus. In this way we can impact the college community, members and non-members alike. We also took the initiative of placing “green” posters around the Natural Sciences Department, not just for the disclosure of the Green Chemistry Principles, but also so that our presence in the department is representative of the importance of the green initiative. Each year, with the same goals in mind, we publish our green journal “La Idea Química”, giving us a way to keep the community updated with news about Green Chemistry. Our chapter is always looking for new ways to reach out and raise awareness. In the past spring semester of 2014, we organized the 1st ACS Green Chemistry Fair: Scavenger Hunt Sustainable Future where the community participated in a campus wide scavenger hunt. Our goal is to make this a recurrent activity each year to continue promoting the events message “Be the change you wish to see in the world”. These are just some of the ways our chapter has played a part in the green chemistry movement. In the future, we will continue trying to fulfill our mission of promoting the spread of the green philosophy.

CHED 1585
Forging leaders: Diamonds for society

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Our chapter has pledged its commitment to our student members to guide them to improve as future professionals and productive social entities. While majorly composed by biology students, the ACS Student Chapter at the University of Puerto Rico at Aguadilla (ACS UPRAg) excels at chemistry. We are biologists that love chemistry. We celebrated the 2014 International Year of Crystallography and just like carbon turns into diamonds, an organized crystalline structure, when exposed to pressure and heat, our members, with the help of ACS UPRAg as a catalyst, will be transformed into leaders in society and mentors for next generations. Our success as an Outstanding Chapter comes from the hard work, motivation, and dedication of our active members. It is their enthusiasm, creativity and versatility that, year by year enhances the Chapter’s formation into a well organized diamond.

One of our main goals as a student chapter is to transform people’s lives with the power of chemistry. We work for our members but specially, we work for our community. From teaching children about the exciting world of science and experiments to bringing joy to the elderly by spending quality time with them, ACS UPRAg encompasses the whole community to help improve their lives. By improving our community lifestyle, we ensure an interaction with the local and college community. An example of our commitment with the community is the celebration of our first Health Fair. The Health Fair is for the open community and we'll have the participation of several health organization. ACS UPRAg is also part of the first Analytical Chemistry and Green Chemistry Symposium organization committee in which our members have the opportunity to develop presentation skills.

We will continue working with our members to improve their formation as diamonds for society while becoming leaders in our community.

CHED 1586

Stay calm and get your grizzly growl on: Georgia Gwinnett College chemistry outreach

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Our two year old chemistry club is making a big impression on Georgia Gwinnett campus. This year, we had two big events during NCW on campus: student chemistry demonstrations with exploding pumpkins, burning ice, screaming gummy bears and lots more; and another food day of dragons’ breath and liquid nitrogen ice cream. Our outreach has expanded to include an all day Saturday event for middle school girls, which combines chemistry with technology. Events include soap making, experiments
with liquid nitrogen, tye dye, uncut vs. cut gemstones and crystal lattice energies, paper making, and assorted hands-on chemistry experiments.

CHED 1587

Catawba College Chemistry: The fuel that will stand the test of time

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The Catawba College ACS chapter values the fuel of education. This year activities have ranged from campus-wide activities to community involvement. Our chapter participated in activities this year including outreach programs in the local middle schools, campus celebrations of chemistry, and travel to the 247th ACS National Meeting in Dallas, Texas. Our chapter has participated in community service events such as hosting a blood drive and judging science fair contests. The Catawba College ACS chapter has enhanced the chemistry knowledge of others by diverse interaction with the community.

CHED 1588

Chemistry outreach efforts at North Dakota State University

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Educating the public about chemistry is an important part of the ACS Student Affiliate Chapter of the NDSU Chemistry and Biochemistry Club. Community outreach programs permit the chapter to get involved with our community and show how chemistry is impactful, fascinating, and fun. At NDSU, the club participates in outreach programs throughout the year and interacts with students of all ages. Our main targets for outreach activities are students ranging from the primary to postsecondary levels. Our goal is to demonstrate how enjoyable chemistry can be in hopes that students will pursue a career in science. Activities range from presentations on campus to chemistry demonstrations at local schools. This year the chapter has also worked to increase the number of elementary schools impacted by our organization. Green chemistry education is also a major part of our outreach activities. These activities help to increase public awareness and show that science can be fascinating and fun, all while enabling the club to engage in teaching experience.

CHED 1589

Fundraising methods at North Dakota State University
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Fundraising plays a major role in the ACS Student Affiliate Chapter of the NDSU Chemistry and Biochemistry Club. Fundraising allows us to be an increasingly active chapter and boost awareness of chemistry in the Fargo-Moorhead area. The fundraising is done both on and off campus. Some on-campus fundraising includes goggle sales for chemistry labs and selling practice chemistry tests in intro level courses. One of the valuable sources of off-campus fundraising opportunities includes networking with local companies. The majority of the funds raised go to the community outreach projects for the purchase of chemicals and supplies for demonstrations. The funding also supports inter-club activities and student attendance at the National ACS meeting. Fundraising enables the NDSU Chemistry and Biochemistry Club to get students more involved in research, community outreach, and networking opportunities.

CHED 1590

Modeling a successful student chapter

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With every year, the Fresno State CHEM Club looks to improve and increase their efforts. Whether it is reaching out to the younger generation through outreach or refining the experience of its members through professionally relevant seminars, the club is always self-reflecting to see how they can improve the experience for students at Fresno State. We also increased our efforts of growing our club through a number of informal social events. The club continued to utilize social media to stay in touch with members as well. The Fresno State CHEM Club not only reached out to other clubs on campus, but we also received an ACS Inter-Chapter Relations grant and held an event with the CSU, Stanislaus ACS student affiliate.
The University of Utah ACS Student Chapter is a group dedicated to exciting and educating youth about science. Three chapter projects and activities will be highlighted: an environmental awareness campaign, a program at a local children’s hospital, and an event co-sponsored with the University of Utah School of Medicine. With the assistance of an Innovative Activities Grant from the National ACS, the chapter has partnered with local high schools with the goal of educating students about an environmental issue that is particularly important in our region, air pollution. We will present on our efforts to educate these students through Science Power. At Science Power, the chapter introduced demonstrations and hands-on activities in order to raise awareness of environmental issues. The group will also engage students in activities that explain the multi-faceted topics related to green and traditional energy sources. The group’s ultimate goal is aimed at helping children find passion and fun in science, while promoting the idea that their unique minds can influence the future of chemistry. This goal is accomplished by being very active in the community, participating in numerous outreach events throughout the Salt Lake Valley and the University of Utah Campus. At these events, such as the Science Power event, children are able to involve themselves in hands-on chemistry experiments as well as see more complex chemical reactions with demonstrations given by undergraduate students. Another program we wish to highlight a unique outreach program at Primary Children’s Hospital. Each week a group of students from our ACS group visits the hospital to participate in a weekly science show, which includes demonstrations and hands-on activities. Some of these include: culinary chemistry, acid/base food reactions, clothing dyes, polymers, and DNA extraction.
Truman State University is proud to consistently be an outstanding ACS Student Chapter. Our purpose builds from within our organization to the TSU campus and extends to the local community. Our student chapter meetings include informational mini-talks about chemistry and social events to promote networking within our chapter. We invite the campus to learn about chemistry and with our seminar series and green chemistry and National Chemistry Week events. Finally, our efforts extend to the community via our partnership with local schools to perform chemistry demos for elementary students. We also raise money to provide a scholarship for local students, advancing education opportunities.

**CHED 1593**

**Successful student chapter of the American Chemical Society, South Dakota School of Mines and Technology: Promoting chemistry and reading**

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Our chapter focuses a lot of its energy on outreach. We hold demonstrations for middle school science classes on Mole Day during National Chemistry Week, host large groups for our Magic Show during Engineering Week, and held another Magic Show for Girl’s Day. Over the summer we tried a new adventure by putting on numerous events at local libraries. The theme for the local summer reading series was science. Dr. Meyer, our chapter adviser, along with our student members traveled to seven locations in the area to promote science and reading. Our section has also held numerous other successful events including a chemistry week scavenger hunt, mini golfing, and additional fundraising activities.

**CHED 1594**

**Science of service: Gordon College’s student chapter of the American Chemical Society**

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The focus of the Gordon College student chapter is to facilitate the intersection where building of relationships with fellow students, faculty, and chemists both on and off campus meets a philosophy of service through science outreach. Throughout all of our activities and events, we are working to fulfill our chapter’s mission to provide professional development and service opportunities to our student members. Over the
past year, our chapter has both grown in membership and in our community involvement, while still participating in many of the same activities we do each year. Our members are heavily involved in service projects that help students at the elementary, middle, and high school levels, including weekly tutoring for a local high school honors program. Other community engagement events, such as hosting a science carnival during Homecoming and Parent’s Weekend on campus, as well as volunteering at the Boston Museum of Science during National Chemistry Week and Earth week, help to develop interest in chemistry among children and families. To foster interdisciplinary campus community, as well as interest in science throughout the general student body, we hold a variety of events such as science cafés for students in between lab classes, Green Chemistry lectures featuring major researchers in the field, and an all campus science outreach event for students and families called Chemistry on the Quad. This year we have also continued to hold our annual fall cookie jar fundraiser, which raises money for first year student entering Gordon the next fall and helps to establish an endowment to secure the future of this scholarship. Throughout the year, our chapter has also begun to host a variety of new events, including the inaugural “Academic Pie” Contest, a series of chemistry webinars, and industry tours at local laboratories. In all of these events, our members have been embodying what it means to serve the community through shared scientific appreciation while building valuable relationships with other students and professionals in the field.

CHED 1595

Chemistry: the final frontier: These are the chronicles of the Chemistry Club at South Texas College, its enduring mission — to spread knowledge, educate the unknowing, serve its community, and go where no chemistry club has gone before

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The Chemistry Club at South Texas College has fulfilled their mission with many community service projects and their outreach program “The Traveling Chemists”. With each of our demonstrations, we gained the curiosity and interest of the children in every school we visited. It means the world to us that we can show kids that science is amazing and fun. Along with being invited to schools, our club has been invited to do other events throughout the Rio Grande Valley at parks, libraries, museums, and community centers. The members of the ACS chapter also participated in the local community activities such as Keep McAllen Beautiful, Breast Cancer Awareness Month, and Spooky Science Fest. Our club held events on and off campus to celebrate National Chemistry Week, Nano Days, and Earth Day. We owe our success to our devoted members who are passionate and dedicated to our clubs success. We wouldn’t be able to do it without their dedication and support.

CHED 1596
MTSU SMACS activities 2014-2015: Turning 40 isn't so bad

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Our poster’s theme is a celebration of the past forty years of MTSU SMACS. Over the past four decades, we have maintained a presence on campus that keeps everyone interested. Pizza and chemical demonstrations react to yield what can only be described as a youth serum that energizes our members and increases curiosity of chemistry. Meeting bi-weekly during the school year keeps us engaged and informed, which is another of our anti-aging secrets. By selling safety goggles to students, our chapter raises money to pay for social events and for transportation to and from ACS meetings. For National Chemistry Week, we reached back into our youth and indulged our sweet tooth by creating and distributing marshmallow molecules and by sharing our love of chemistry with young children through demos. Rounding out the celebration of our big 4-0, we have our invitational Golden Goggles Lecture—a lecture in which a nationally known speaker unveils the secrets of a long, healthy life, through the study of chemistry. It has been quite famously stated that life begins at forty, and if that’s true, MTSU SMACS is just getting started!

CHED 1597

Exploits of the UM-Flint Demo Squad: Dragons, duties, and dewars

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The University of Michigan-Flint Chemistry Club prides itself on being involved in the community and campus by interacting with people and teaching them about the wonderful world of chemistry. We have developed a series of interactive, hands-on demonstrations designed to teach students, adults, and teachers about chemistry and are performed at most of our events. This year was considered a transition year for the club, which meant a lot of new members learning all the demos. To develop members’ understanding and presentation of demos we continued our Demo Squad program. The program allows members to learn demos by presenting them at meetings, and then present them at events while earning prizes and Demo Squad Status. We held events
at the Early Childhood Development Center on campus, local area schools, and on our

campus with Super Science Friday, which brings about 600 middle schoolers in to learn
about science. Some of our favorite demos include “Dragon in a bottle”, exploding
pumpkins, and packing peanuts with liquid nitrogen.

CHED 1598

Park University C.H.E.M. Club: Using sweets to promote chemistry and
conservation in the community

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The Park University C.H.E.M. (Chemists Have Explosive Minds) Club chapter has taken
advantage of the 2014 NCW theme of "The Sweet Side of Chemistry" to inspire events
and encourage interest in chemistry throughout the campus and community. Outreach
events pertaining to the science of sweets allowed us to promote chemistry through a
common interest. Activities involving candy and sugar were used to demonstrate
important ideas such as energy, nutrition, and environmental conservation. Educational
demonstrations were performed during National Chemistry week, at the school's annual
public Halloween carnival, a local pumpkin patch, local elementary and middle schools,
and on-campus student activities.

CHED 1599

Journey of ACS student members at Duquense University

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The Duquesne ACS Chapter continues to be an engaging and exciting resource for its
119 active members. Faculty-student relations were fostered through events on Mole
Day, including both professors and students in a human whack-a-mole game. A new
student-student mentoring program was envisioned and carried out. The Chapter made
strides with its community involvement, reaching out to local high schools, offering
seminars on majoring in science, as well as providing novel demonstrations. An
emphasis was placed on incorporating green chemistry activities into the usual
schedule of events. The student members organized hundreds of volunteers to host a region-wide STEM competition for middle and high school students. A new Chapter website was developed, offering up-to-date information about Chapter activities. The website also includes a section where the executive board offers advice to other student member chapters.

CHED 1600

Increasing participation in the Chemistry and Biochemistry Club at Minnesota State University Moorhead

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After a few years of declining interest and participation in the Chem & Biochem Club at Minnesota State University Moorhead, a new core of energetic and organized student leaders emerged and have made the Club an active contributor to the activities of the Department of Chemistry & Biochemistry and the broader campus and local communities. This poster will present an overview of the methods used to revitalize the Club and highlights of the activities in which the Club participated during the 2013-2015 academic years. Examples of contributions include the campus-wide “Dragons After Dark” program and outreach to elementary students.

CHED 1601

University of Central Florida's student chapter of the American Chemical Society

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The UCF student chapter provides as many programs as possible to foster members' personal and professional development. Through outreach within the community, the chapter is able to form partnerships with community leaders who advise members on how to succeed during and after college. This chapter is very keen on service to its members by hosting workshops for success and socials to provide a more communitarian atmosphere. Lastly, this chapter has significantly increased activity related to green chemistry and, as a result, has been named a green chemistry chapter by National ACS. This chapter has hosted green activities in most of their events in the hopes of creating a more eco friendly chemistry environment by stressing the importance of reducing waste and increasing recyclability. Outreach to the university has become an important part of what this chapter does. This chapter has dramatically increased in active member size mostly in part to its enthusiastic members' constant presence in university outreach opportunities. This year the chapter launched a student tutoring service for the university in which ACS members assist students who struggle in
STEM courses. During each day of National Chemistry Week the chapter runs activities, which creatively apply chemistry while engaging with students of the university. For example, this chapter creates a Periodic Table of Cupcakes to receive monetary donations as well as teaching students about the periodic table and the elements. Lastly, this chapter is heavily involved in the community. Outreach to the community involves partnering with nearby ACS chapters including student chapters and the Orlando chapter. The Orlando Science Center is this chapter’s largest outreach venue where members are able to teach individuals of all ages from all over the world about chemistry through hands-on experiments. This chapter provides many services to the community. Most recently, it has developed a program, Bonding with Bithlo, through which ACS student members provide a place for youth in a struggling city to succeed academically. This program is helping at-risk youth to achieve, and it lifts the morale of the whole community. Finally, this chapter provides chemistry awareness through each service opportunity namely Earth Day, where this chapter, along with members of neighboring student chapters and the Orlando Section, teach the people of Orlando about chemistry through experiments, games, and pamphlets to take home.

CHED 1602

Community outreach projects of the ACS: RUM Chapter

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The American Chemical Society has been in the University of Puerto Rico, Mayagüez Campus since 1954, making this year its 60th anniversary. Since then, we have been helping our members develop their academic and professional skills. During this past year, our focus has been to develop our members’ awareness on the importance of community service. As students we have great potential for creating solutions for the communities in which we live in. For this reason, our chapter has been involved in activities such as “Out into the streets for Hope”, which is an event of the Muscular Dystrophy Association in Puerto Rico, The International Coastal Cleanup and volunteer work at animal shelters and other charity organizations as foster homes. We are grateful for our academic education, which is why we feel the responsibility to share our knowledge as well as our skills with others. One way that we have done so, is by visiting public schools to present chemistry demonstrations and sparking a science curiosity in them. Along the journey, by serving those who need us in our community, we have enriched ourselves.

CHED 1603
Successful activities of SAACS at the University of Central Oklahoma

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The University of Central Oklahoma Chapter of the Student Affiliates of the American Chemical Society (UCO-SAACS) has continued to develop a group of dedicated and active members through collaboration with the other science-related organizations. A new committee of chairs and method of event organization has increased our possibilities for events. Keeping the tradition of old events, UCO SAACS teamed up with the Tri Beta Biology Club, Society of Women Engineers and other engineering organizations for events including a Halloween bash, Science Prom, Tie-dye events, and many more. In addition, the club plans to spread excitement for chemistry in the community by performing demonstrations at the Oklahoma Science Museum’s Science Day and provide members with information about graduate schools and summer undergraduate research opportunities. By utilizing Facebook and OrgSync groups, the club has been able to maintain more communication with members.

CHED 1604

University of Kentucky Students of the American Chemical Society: Expanding undergraduate chemistry involvement at UK

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The Students of the American Chemical Society (SACS) affiliated with the University of Kentucky has focused this year on expanding membership and finding ways, like cooperating with the Office of Undergraduate Research at UK, to creatively integrate research opportunities into the undergraduate experience. Our chapter has used the resources available to SACS to expose more undergraduates to the research opportunities available with faculty at UK as well as at world-class facilities within driving distance of our campus such as Oak Ridge National Laboratory, with the ultimate goal of encouraging much more involvement of students in undergraduate research. Our monthly chapter meetings have focused on aspects designed to appeal to undergraduate students with varied interests, such as educational opportunities and a variety of topical issues. Other chapter activities this year have included fundraising, membership expansion efforts, re-chartering a national honor society, and outreach events to encourage scientific engagement among students in primary and secondary schools.
Angelo State University ACS Student Chapter

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The local student chapter of the American Chemical Society at Angelo State University continues to pride itself on community service and outreach programs for the beautiful city of San Angelo, Texas. Our chapter participates in hands-on events that promote chemistry, such as the Santa Rita Science Enrichment program and the annual Eco Fair at the San Angelo Museum of Fine Arts. We also take part in Science Days an event where local fourth grade students visit ASU as an opportunity to learn and gain interest in the sciences. We participate by providing Chemistry Magic Shows where we demonstrate chemistry in fun and inventive ways in addition to the hands on activities we provide. We also provide demonstrations and hands on activities for local elementary schools for Math and Science Nights to help spark an interest in chemistry. For fundraising activities, we sell lab notebooks, goggles, and lab coats. We hold bi-weekly student chapter meetings that include speakers from visiting institutions, field chemists, and local research students. Our primary goals involve bettering our community, spreading a positive influence of science, and furthering the careers of our members.

Angelo State University Green Chemistry Student Chapter

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At Angelo State University, our Green Chemistry Student Chapter of American Chemical Society has continued in its endeavor to promote green chemistry and all of its benefits to the great town of San Angelo, Texas. We do so by encouraging our members to attend lectures from experts in the field to gain a better understanding of green chemistry. We also participate in the city-wide events such as the SAMFA Eco Fair where we provide green chemistry demonstrations and bring green chemistry awareness to the city. We also hold Green Chemistry Magic Shows where we demonstrate green chemistry for all to attend. All demonstrations involve green chemistry and most activities included can be done at home.

Sweet success: NCW 2014 at Tarleton State University
A long standing tradition of the Tarleton State University Student Affiliate Chapter is promoting the science of Chemistry. Accordingly, during National Chemistry Week each year a banner is displayed in the lobby of the Science Building and a Bake Sale is held on Mole Day (which netted approximately $100 for Chemistry scholarships this year). Since the theme for NCW 2014 was “The Sweet Side of Chemistry”, events were planned in association with Dublin Bottling Works – a facility which has been bottling sodas for more than 120 years using exclusively pure cane sugar. A company representative presented a seminar comparing cane sugar to high fructose corn syrup and demonstrated some of the quality control techniques used at the plant. On Saturday, members were treated to a special tour of the bottling facility and associated museum. As an extra treat, members also had the experience of bottling their own “special” sodas.

CHED 1608

Student members of the American Chemical Society: University of Arizona chapter

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The University of Arizona Student Members of the American Chemical Society aims to foster passion for science, promote the importance of higher education, and provide professional growth to members. Chapter meetings incorporate an invitational speaker series where guests from academia and industry can present research, networking opportunities, and insight to our members. The speaker series and our Household Hazardous Waste volunteer program, in which members sort and collect environmentally harmful waste, highlight the chapter’s “green chemistry” efforts. Additional chapter outreach includes aiding the University’s recruitment process, and performing Chemistry Magic Shows for our local community as well as being active in University Residence Life having been invited to perform at events and Residence Halls. Additionally, our chapter has pioneered a “Chemistry Discovery” outreach program that invites middle school students to our campus to engage in hands-on activities with university students as activity station leaders. Chapter members have presented at several ACS National Meetings and are proud recipients of the Outstanding Chapter and the Green Chemistry Awards for the 2008-2009, 2009-2010, 2010-2011, and 2011-2012 school years as well as Commendable Chapter 2012-2013 and 2013-2014. Chapter members also regularly enjoy social events, such as bowling, barbecues, dessert outings, and the SMACS Fiesta at the semester’s end, which help to encourage friendships between club members.
Confectionary chemistry: Spreading the sweet joys of chemistry to Bristol, RI

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The Roger Williams University Affiliates have engaged in several projects throughout the year to enhance the presence of chemistry on campus. Club members were actively engaged through bi-weekly chemical demonstrations that took place during our Monday meetings. Members hosted a campus wide event, Roger After Dark, an alternate form of weekend entertainment for university students. The event consisted of chemistry demonstrations, trivia, games as well as raffles for molecular model kits and t-shirts. On Mole Day the student affiliates hosted the Gagliardi Distinguished Seminar Series by Dr. Marcetta Darensbourg from Texas A&M University. For Thanksgiving, the club members organized a division wide food drive donations delivered in a chemically themed box with periodic table place mats. The affiliates provided guidance to the students of Mt. Hope High School in Bristol RI and helped them achieve success in their annual science fair. Furthermore, members visited their chemistry classes and performed demonstrations as well as round table discussions on deciding which college to attend and the many paths a chemistry major can lead to. Chapter members availed themselves at student advisement and open houses to talk directly to incoming and perspective students about opportunities at RWU in chemistry. The affiliates co-sponsored several events with other clubs and organizations on campus, for example Tri-Beta Biology Society and the American Society of Biochemistry and Molecular Biology for the end of the year barbeque, sport challenges and freshman welcome tables. During the 2014-2015 academic year, the club has sponsored and organized 12 students to present their research at the National American Chemical Society Meeting. Club members also participated in several regional conferences held at Bridgewater State University, Providence College, and Roger Williams University. Members participated in fund raising selling periodic table labeled cupcakes prior to morning chemistry lectures, blue and yellow M&M’s in test tubes, decorated round-bottomed flasks and organized the study guide drive for students taking general and organic chemistry.

Newberry College Chapter of the American Chemical Society

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Included are details explaining the types of activities and events members plan and attend. Some of these activities and events are as follows: CSI Night, Western Carolina
ACS Meetings, SERMACS Meeting, Junior and Senior Science Olympiad, Demonstrations at an after-school program, nursing home, Newberry College, and social events.

CHED 1611

**Texarkana College Chemistry Club, 2013-4 Activites Poster**

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The Texarkana College Chemistry Club presents a poster that details the club activities during 2013-2014.

CHED 1612

**Chemistry and community outreach**

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The University of Southern Maine Chemistry Club makes it a priority to educate and attempt to draw the next generation of students into the many fields of chemistry. A variety of demonstrations designed to be both stimulating and educational were performed in combination with more hands on activities to raise interest in the fields of chemistry. These workshops were held in the Children’s Museum (Portland, ME), the Crusher's Kids Concert in the Park (Portland, ME), a STEM exposition hosted by Portland Public Schools, and for the New England Association of Chemistry Teachers Annual Conference so they could perform the same demonstrations in their classrooms. Demonstrations included showing the effect of surface area on flammability and the enormous hygroscopicity of sodium polyacrylate. Interactive activities include the mixture of polyvinyl alcohol and borax to make “Slime” and the effect that soap has on a mixture of oil and water.

CHED 1613

**Making a better student chapter**

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With a growing number of active members, the Missouri State University (MSU) section of student affiliates took advantage of many great opportunities in 2013-2014. The
return of many successful programs, such as Water Pong for Pure Water allowed the new and returning members to once again work together with non-chemistry students and demonstrate that chemistry is interesting and can be found in everyday settings. The student affiliates worked closely with the Ozark local section to help plan the undergraduate portion of the 2013 Midwest Regional Meeting with such events as Chemistry Jeopardy and a graduate school fair. With help from an Innovative Activities grant, the group planned and hosted a green chemistry conference with speakers from all over the state of Missouri. New social programs, such as Chemistry Bingo, were added to give newer members an opportunity to meeting veteran members in a casual setting. Finally, through a continued emphasis on charity work, including the Sertoma Chili Cook-off, Relay for Life, and Adopt-a-Street, the group continued to be involved in the greater Springfield community. Through the group had many successes, it faced challenges in an abrupt change of leadership and a large graduating class. Despite those challenges, a year of hard work combined with new and old ideas resulted in the chapter earning honorable mention student chapter award status.

CHED 1614

PLNU chemistry club is involved in San Diego

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The PLNU ACS Student Chapter encouraged and developed interest in chemistry in the youth of the greater San Diego area by visiting a Middle School, performing interactive chemistry demonstrations at the very large science fair at Balboa Park, and instructing the students at the middle school on the concepts of chemical and physical changes, chemical properties, and the periodic table. We have been actively collaborating with UCSD and were able to participate in the Annual ACSSA Undergraduate Chemistry Research Symposium. On campus, we hosted a graduate school information night where a panel of PLNU alumni who are currently in graduate programs in chemistry answered questions from our students. We have also organized a career fair where different professionals came to campus to discuss their careers in the field of chemistry.

CHED 1615

Honoring our professors and faculty: 75 years as a student chapter and 40 years of service from Jane Schley

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In the Fall of 2013, the Chemistry Club of the University of Detroit Mercy (CCUDM) decided to honor the faculty and staff of our Department in conjunction with our student chapter’s achievement as the longest standing student organization at UDM. It was the 75th anniversary of our Club’s founding and we wanted to honor the faculty and staff’s positive contributions to our Club. We also honored the administrative assistant of our Department, Jane Schley, who has served the faculty and students for over 40 years. The CCUDM organized a small dinner party with beverages, hors d’oeuvres and cakes, celebrating both occasions. We unveiled a dedicated sign in front of the Chemistry Building, honoring Club members past, present and future. We also honored Jane Schley by dedicating the new Chemistry Building lobby to her; a plaque was hung to mark the dedication. Our celebration brought her to tears and our Club shared our appreciation for the department and the university. Other student chapters can implement this type of event as recognition of and appreciation for faculty and staff’s efforts to provide a better learning environment for students.

CHED 1616

Cleaning up Belle Isle: A UDM chemistry club project

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Belle Isle is a Michigan State Park found between the borders of the US and Canada on the Detroit River. The park has many acres of green land and beaches, and the Chemistry Club of the University of Detroit Mercy (CCUDM) decided to be a part of its restoration. In January of 2014, our green chemistry chair helped CCUDM to adopt one beach on Belle Isle through Michigan’s Adopt-a-Beach program. The plan was to utilize the beach for possible events for our student chapter, but the beach was extremely dirty and the water was polluted due to civilians’ wasteful habits and sewage dumping into the Detroit River. At the end of UDM’s final exam week, the CCUDM went to Belle Isle to clean up the beach. Club members picked up different types of trash such as plastic and glass bottles, fast food bags, wrappers and an assortment of different types of waste. While we cleaned the beach, our green chemistry chair was trained to use an instrument that could monitor E. coli levels within the Detroit River. With all the effort from our student chapter and the project leadership, we were able to leave our Belle Isle Beach much cleaner than it started. For future events, more students plan to become trained in water refining techniques and to return to maintain the beach.

CHED 1617
St. Edward's University American Chemical Society Student Chapter

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Our student chapter hosts guest speakers, has a chemistry picture of the month contest, and participate in volunteer activities. We collaborate with the local ACS section with national chemistry week and with the Austin community. We are currently volunteering at a local elementary school to promote science and perform chemistry demonstrations. Other activities we have are socials with our club members and with other science clubs at the university.

CHED 1618

Propagating education in chemistry

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Through the 2014-2015 academic year, the Utah State University ACS student chapter has maintained a focus on two primary goals: to propagate interest in chemistry and knowledge of basic chemical principles as widely as possible, and to provide our members and students in the USU Chemistry and Biochemistry department with opportunities for networking and professional development.

Historically, the vast majority of our efforts addressing our first goal have been focused on performing after-school demonstrations at local elementary and middle schools. This year we have enjoyed a fruitful collaboration with USU’s College of Science by performing demonstrations at their Science Unwrapped events. We strive to select vivid and memorable demonstrations. Our demonstrations are performed with an emphasis placed on safety, and on an explanation of the relevant chemical phenomena. The Science Unwrapped events reliably attract a large number of curious students and our demonstrations at these events have been particularly successful.

As part of our second goal, we recruited several graduate students and undergraduate researchers from the Department of Chemistry and Biochemistry to present in a poster session which we held in the Chemistry building during National Chemistry Week. We received funding from the department for the preparation of a periodic table of cupcakes, consisting of 118 cupcakes decorated with a corresponding elemental symbol. We distributed cards for each of the elements to our presenters which they gave out to those who stopped to listen to the presentations.

This year we have restructured the leadership of our chapter to include a branch devoted to community outreach and one devoted to campus activities in order to more efficiently focus our efforts. We strive to seed a desire in young students to pursue careers in chemistry. We also work to encourage the general public to learn more about chemistry and chemical research and to provide students in our department with opportunities and experience to further their education. These efforts are made possible
through the tremendous support we receive from Department of Chemistry and Biochemistry, the College of Science, and the faculty.

CHED 1619

Starting a Successful Student Chapter 101

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The University of Massachusetts Lowell ACS Student Chapter submitted its first year-end chapter report in the 2013-2014 academic year, and subsequently received an Honorable Mention Award for its activities and events in its inaugural year. The founding officers attended the 247th National Meeting in Dallas with the intention of meeting other officers who had recently started a chapter to gain advice, but had little success in finding officers who had been involved in the actual founding of a chapter. This poster outlines the steps prospective founding members could take to launch a successful student chapter, and provides a sampling of events that were profitable to the new chapter.

CHED 1620

Organelle bioelectrocatalysis

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Over the last 5 decades, bioelectrocatalysis has been classified as either enzymatic bioelectrocatalysis or microbial bioelectrocatalysis, but there are biocatalysts that are neither proteins nor living cells. This talk will detail the use of organelles (specifically mitochondria and thylakoid membranes) for bioelectrocatalysis at carbon electrode surfaces. Both organelles are capable of direct electron transfer with carbon electrodes and can be used for both energy conversion applications (biofuel cells and biosolar cells) as well as self-powered sensors. This talk will detail the mechanistic investigation of organelle direct bioelectrocatalysis, as well as applications in energy conversion and pesticide and explosive sensing.

CHED 1621

Designing artificial metalloenzymes and their applications in biocatalysis for alternative energies

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Metalloenzymes play critical roles in sustainable energy, such as in photosynthesis, biofuel cells and water oxidation. Designing metalloenzymes is an ultimate test of our knowledge about metalloenzymes and can result in new biocatalysts for practical applications. In this presentation, we provide three examples to demonstrate that, while reproducing the primary coordination sphere may be good enough to make structural models of metalloenzymes, careful design of the non-covalent secondary coordination sphere interactions is required to create functional metalloenzymes. In the first example, we demonstrate the fine-tuning of reduction potentials of azurin, a member of cupredoxin family that are involved in long-range electron transfers (ET) in many biological processes such as photosynthesis, to span ~1 V through carefully design of hydrophobicity and hydrogen bonding networks around the primary coordination sphere, and the use of these proteins to address fundamental questions in biological ET such as reorganization energy and Marcus inverted region. In the second example, we have shown that the roles of two conserved glutamate in converting myoglobin into nitric oxide reductase (NOR), one through binding to a non-heme iron and the other through hydrogen bonding interaction. Such a model system allowed elucidation of reaction mechanism of NOR. Finally, we show that the presence of waters as part of new hydrogen-bonding network in myoglobin is necessary to confer oxidase activity in reducing O₂ to water with minimum release of other reactive oxygen species and with > 1,000 turnovers. A combination of the above approach with rational tuning of redox potentials have recently resulted in new oxygen reduction reaction (ORR) catalyst with a very low over-potential and activity approaching to that of native enzymes. Recent results and their implications for designing novel biocatalysts for alternative energies will be discussed.


CHED 1622

Design and development of metal-metal bonded catalysts for transforming small molecule

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We seek to unravel how metalloenzymes convert small molecules using inorganic chemistry. Our approach is to develop, investigate, and exploit unusual structure-function motifs that are found in nature. For example, Fe-Fe hydrogenases may utilize metal-metal bonding for activating hydrogen. By preparing model coordination complexes featuring reactive metal-metal bonds, we can extract a detailed picture of their physical and electronic structures that may elucidate the underpinnings of their function. We can then apply this understanding towards new systems that improve on the natural counterparts in activity, selectivity, and substrate scope.

CHED 1623

Assessing the effectiveness of POGIL-PCL workshops

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POGIL-PCL (Process Oriented Guided Inquiry Learning in the Physical Chemistry Laboratory) was developed in order to improve student learning and encourage students to be active learners in the laboratory. This presentation will give an overview of the structure of past and future workshops designed to create guided inquiry physical chemistry experiments and to facilitate the adoption of these experiments in the laboratory. The final experiment structure, which included two 'data-think' cycles, was shaped by the community of workshop participants. The presentation will also include the results of a recent survey designed to assess the workshop model. Survey results will be compared to workshop assessment collected immediately following the workshops. The workshop model and the results of the survey will be discussed in light of change theory, which describes the process by which instructors adopt and implement new teaching methods. We will also discuss how we are building a community of instructors who collaborate on generating and using POGIL-PCL experiments.

CHED 1624

How instructors and materials influence the development of scientific arguments and conceptual understanding of thermodynamics in POGIL classrooms

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The Process Oriented Guided Inquiry Learning (POGIL) instructional approach is designed to help students learn chemistry while encouraging the development of
process skills such as communication and critical thinking. POGIL materials are designed to guide the students through the chemistry concepts, but facilitation can influence the students’ conceptual understanding of the content and the development of process skills. This case study focuses on how an instructor’s implementation of the POGIL materials influenced student argumentation and conceptual understanding of thermodynamics. Data was collected by recording student and instructor interactions and conversations. This data was then studied with an analytical approach that examined how the class translated between macro/submicro/symbolic levels of representation, Toulmin’s Model of Argumentation and the Inquiry Oriented Discursive Moves framework. Analysis of the POGIL materials using the levels of representation helped to identify which questions encouraged which representational level of conceptual thinking, and the extent to which they prompt meaningful collaborative discourse. Analysis of the instructor’s implementation, student interactions, and the materials provided insight regarding the nature of small group and whole class conversations, the nature and quality of student generated arguments, and students’ conceptual understanding of thermodynamics.

CHED 1625

Development and implementation of the enzyme-substrate interactions inquiry activity for a biochemistry survey course

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Previous research has indicated that biochemistry students have a particularly difficult time with enzyme-substrate interactions and the Enzyme-Substrate Interactions Concept Inventory has been developed to determine the most common misconceptions in relation to this topic. Using the concept inventory, misconceptions were identified from a one semester biochemistry course and an activity was constructed for use in the classroom as a replacement for the traditional lecture-based method of instruction. This activity will help students to better incorporate enzyme-substrate interactions into their long-term memory as well as giving students the chance to discuss their idea with fellow students. Results from the national implementation of the activity and corresponding ESICI evaluation will be presented.

CHED 1626

Topic-specific pedagogical content knowledge (PCK) in chemistry: A characterization of chemical bonding PCK in high school teachers

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Pedagogical content knowledge (PCK) is a complex and multi-faceted concept. Broadly defined, PCK allows teachers to transform subject matter knowledge, knowledge of context, and pedagogical knowledge into instruction so diverse learners can achieve conceptual understanding in the classroom. Due to its complexity, PCK is difficult to observe and document. The purpose of this study is to optimize the data collection process and characterize high school chemistry teachers’ topic-specific PCK. This study proposes a model of PCK synthesized from the literature, as well as a four-stage data collection method aimed at improving PCK data quality. This method employs interviews, classroom observations, observational protocols, and guided teacher reflections, and seeks to elucidate data from three measurable indicators: explication — what teachers state about their mental frameworks and planning; enactment — classroom instruction; and reflection — teachers’ responses to their instruction, which informs changes in their PCK. Data collection and analysis were coupled with a novel data reduction technique employed to map data from the four-stage method onto the six PCK components: Orientation to teaching chemistry, teacher self-efficacy, chemistry curriculum, students’ understanding of chemistry, instructional strategies in chemistry, and assessment. Five teachers participated in the main study focused on chemical bonding, a crosscutting and foundational topic in chemistry. Results include emergent themes which characterize chemical bonding PCK in the context of chemistry PCK components. Results and implications for future research, pre-service teacher education, and professional development will be presented.

CHED 1627

Investigating the tutor-learning effect: Identification of predictors of tutors’ productive behaviors

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It has been established that both tutors and tutees gain from tutoring sessions. However, tutors’ benefits may be enhanced or limited depending on the type of behaviors they are performing during the sessions. Although productive behaviors can be promoted by training, generalized tutor training models that are often used do not take into account tutors’ preexisting perceptions of tutoring. The theory of planned behavior highlights the tight connection between one’s attitudes toward a behavior and the enactment of that behavior. The goals of this multiple-case study of four chemistry tutors are to characterize their perceptions of tutoring, their behaviors during tutoring sessions, and the connections between their perceptions and behaviors. Data was collected through interviews in which tutors’ perceptions of tutors and tutoring were probed and through video recordings of three to four interview sessions for each tutor. Interviews were analyzed using a thematic analysis approach. Video recordings of sessions were analyzed using a list of codes corresponding to different types of behaviors that had been reported in prior tutoring studies. Analysis of the interviews indicate that tutors perceived tutoring as a one-on-one learning experience that
supplemented lecture and/or recitation sections. All highlighted the need to address and adapt to the needs of the tutee. Their perceptions of tutors included qualities such as knowledge, flexibility, and communication skills. Cross-case analysis indicates that tutors' behaviors derive from their perceptions of their students' needs and that tutors' level of comfort with the content knowledge being taught influences their behaviors. The results of this study may be used to improve tutor training, particularly through examining individual tutor's perceptions of tutoring and their role as tutor to create more targeted training programs.

CHED 1628

Investigating student perceptions and opinions regarding recitation techniques in general chemistry

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Recitation sections in undergraduate chemistry courses can be an effective tool for improving students' problem-solving skills and understanding. A variety of techniques are used in recitations that can significantly impact students' learning as well as their perceptions of classroom effectiveness. Here, general chemistry students at Colorado State University participated in a variety of recitation activities throughout the course of the first semester of a 2-semester general chemistry sequence, including peer-led exercises, games, and scaffolded worksheets. Through weekly surveys, students were asked to evaluate and assess recitation activities for both interest and effectiveness as part of their course homework assignments. Also included in homework assignments were content questions relevant to the weekly themes, which provided a measure of student learning of recitation topics. Student opinions are correlated with content retention while also providing insight into the role of peer and TA interactions on perceived successes. Both qualitative and quantitative data from these surveys will be presented. These data will also be compared to student responses to a pre-survey administered before the first recitation session, providing a baseline measure for students' expectations of recitation courses and how well those expectations are met through the various types of activities employed.

CHED 1629

Metamorphosis: Transforming a general chemistry lab to a blended course

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Missouri University of Science and Technology (Missouri S&T) piloted blended lab sections in the fall of 2014 to improve learner outcomes, decrease instructional costs, and increase enrollment capacity. This presentation reports the first semester results, identifies the modifications implemented for the scaled up spring pilot, and identifies potential challenges for the full scale deployment of a blended 1,000 student lab course for the fall of 2015.

A comparison of “in-the-commons” and traditional labs will be presented. Topics that will be covered include a review of EHS participation, campus compliance, waste management, as well as the experiential nature of the “in-the-commons” activities that were chosen, lecture to lab content synchronization, and other logistical challenges of the redesign. Information gathered from pre- and posttest, lecture grades, and student feedback and surveys will be included.

CHED 1630

Sustainability and undergraduate chemistry education: How far we have come, and what work remains

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In 2002, when I joined CEI, bringing green chemistry into undergraduate education was just starting to be discussed. The term “sustainability” wasn’t used that often in ACS, and it certainly wasn’t talked about in the context of education. For the next 11 years I consistently and passionately advocated for the importance of incorporating sustainability into undergraduate education, seeking to inspire others to engage in meeting this challenge with me. My work has largely focused on:
1) the importance of viewing undergraduate chemistry education as involving Sullivan’s three apprenticeships of professional education – head, hand, and heart;
2) approaching this challenge as ultimately about BOTH content AND context, not either one or the other locked in an antagonistic relationship;
3) highlighting the work of colleagues already incorporating sustainability in their chemistry classes so that the wider community could benefit from these examples.
In many ways we have made a lot of progress in bringing sustainability into undergraduate chemistry education. But there is also work that remains to be done

CHED 1631

It’s about connections: Sustainability in a liberal arts curriculum

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To make sustainability topics come to life, students in a liberal arts chemistry course engage in the Connections Project. As part of this semester-long project, students create an annotated outline from a chapter not covered in their text. In the outline they
weave together new chemistry content, apply recently learned concepts, and apply a sustainability topic such as the Triple Bottom Line, shifting baselines, and cradle-to-cradle. Other aspects of the project include student peer review of the outlines and an oral presentation. It is during this presentation that students teach us about a chemistry concept and how it links to a sustainability topic. It is rewarding to see them make the connections between chemistry and sustainability.

CHED 1632

Empowering undergraduates for sustainability research and education

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Since 2006, I have challenged undergraduates to engage sustainability in the classroom, in the teaching laboratory, and in the research laboratory, resulting in six articles in The Journal of Chemical Education to date. Juniors and seniors have written papers critically comparing the greenness of industrial or academic syntheses of pharmaceutical drugs. Freshmen, sophomores, and juniors have developed new laboratory experiments that focus on green principles and have resulted in eight poster presentations at national meetings and an invited talk at a 2011 national meeting of the Two-Year College Chemistry Consortium. These sustainability efforts have impacted advanced organic synthesis students, introductory and intermediate organic chemistry students, general chemistry students, high school students, and elementary school students. Future plans target undergraduates in biochemistry, analytical, and inorganic courses. In every case, an emphasis is placed on students taking an active role in sustainable education.

CHED 1633

Incorporating Green chemistry and sustainability into the undergraduate curriculum at UC Berkeley

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The Berkeley Center for Green Chemistry (BCGC) seeks to bring about a generational transformation in the design, production, and use of chemicals, materials, and products. Initiatives at the center integrate the chemical sciences, environmental health sciences, and the study of public and private governance into a cohesive educational program that includes innovations in education, research and engagement. This approach has been applied to the redesign of the introductory chemistry labs which serve over 2500 students per year as well as the development of an interdisciplinary graduate curriculum. The effort to redesign the undergraduate introductory chemistry curriculum in the classroom and laboratory has been a collaborative effort between John Arnold,
Angelica Stacy, Anne Baranger, Michelle Douskey, and MaryAnn Robak. Over the past three years they have redesigned the introductory curriculum to show students how chemistry can be used to meet society’s sustainability challenges.

CHED 1634

Using the chemistry curriculum as the starting point for engaging students and their families in pro-environmental behaviors

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The chemistry curriculum is a logical place to describe and discuss our world’s natural resources: water, earth, air, and energy. After all, three are made of chemicals and the fourth is involved in chemical transformations. The NSF-funded Families, Organizations, and Communities Understanding Science, Sustainability, and Service (FOCUSSS) program is an instructional project created to make connections among various learning environments – the chemistry classroom, the home, and the community. It uses natural resources as its contexts, and instructional units start in the classroom and extend into out-of-school experiences for students with their families. By blending these environments, the project has provided opportunities for students and family members to learn the science behind sustainability principles. Data from this project support that cutting across these learning environments and expanding the notion of curriculum do foster pro-environmental behaviors both for students and their family members.

CHED 1635

Using TUES funds to create undergraduate scholarship

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In August 2013, the Chemistry Department at Metropolitan State University of Denver was awarded a TUES Grant (NSF #1245666). The funds from this grant made an immediate difference in the educational experiences of undergraduates enrolled in organic chemistry laboratories and those involved in undergraduate research. The title of the Grant, \textit{NMR Spectroscopy: Introducing the Modern Chemist’s Toolkit to Undergraduates} aptly describes the success that the installation and broad use of a high-field NMR has had on the pedagogy at our PUI. These include a transition to inquiry-based labs and project assignments that introduce research. This talk will describe the outcomes of the use of the instrument, the intellectual merits that have been measured after the first year of the grant, as well as additional assessments being obtained. The broader impacts of this grant will also be summarized, as the instrument
location in a building shared by three higher educational institutions makes it very accessible to broad usage.

CHED 1636

Implementing Raman spectroscopy into the chemistry curriculum

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We have developed and tested Raman spectroscopy experiments and experiences for the undergraduate chemistry curriculum that address key course-specific student learning outcomes (SLOs) and more fundamental anchoring chemical concepts or “big ideas”. We are using the Raman spectrometer to introduce and reinforce increasingly more complex chemistry concepts as part of a restructured chemistry curriculum implementing a “spectroscopy-to-learn” approach. In this approach, we present Raman spectroscopy as a practical tool to teach concepts such as molecular structure, quantitative analysis, elucidation of reaction mechanisms, equilibria and applications of spectroscopy for research.

To date we have developed experiments and experiences for five courses. Examples include: 1) “Raman investigation of the dissociation of a strong acid” in General Chemistry 2 Lab; 2) “The analysis of vitamin C in tablets” in Quantitative Analysis Lab; 3) “Investigating the polymorphism of acetaminophen” in Instrumental Analysis Lab; 4) “Functional group analysis of products of organic reactions” in Organic Chemistry Lab and 5) “Monitoring the kinetics of imine formation with Raman spectroscopy” in Physical Chemistry I Lab. We are assessing both student’s attitudes as well as their progress in understanding chemical principles as a result of these experiences. This work is funded through a National Science Foundation (NSF) Transforming Undergraduate Education in Science, Technology, Engineering and Mathematics (TUES) Type I grant (#1244807).

CHED 1637

PhET interactive simulations: Using research-based simulations to transform undergraduate chemistry education

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The growing suite of over 30 free chemistry simulations from the PhET Interactive Simulations project (http://phet.colorado.edu/) represents a rich online resource for undergraduate chemistry students and faculty alike. These research-based, student-tested simulations (sims) are interactive, game-like environments in which students learn chemical concepts through exploration and experimentation, connecting real life
phenomena with the underlying sub-microscopic and disciplinary representations. Here we outline the latest NSF-supported developments in PhET sims for college chemistry, particularly in instructional materials development and research on sim use in instruction. Collaborating with experienced college chemistry faculty teaching in diverse undergraduate classroom environments, we have developed a series of classroom-tested sim-based teaching resources. These resources, including sim-based interactive lecture demonstrations, clicker questions, and guided inquiry activities, support faculty in effectively leveraging the sim in alignment with pedagogically sound teaching practices. Recent research findings on PhET sim use in college chemistry classrooms offer insights into how activity design and guidance in the classroom affect student usage and engagement and how chemistry sims can afford development of both student conceptions and practices.

CHED 1638

Active learning project of the Analytical Sciences Digital Library

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Faculty members from over 20 institutions are collaborating on an NSF-funded project to develop active learning materials for use in the undergraduate analytical chemistry curriculum. Materials are being designed for use in a variety of formats (e.g., classroom activity, homework assignment, laboratory project) and in a form that can be modified to suit the particular needs of an instructor or institution. Each module consists of a series of inquiry-based activities or problem-based exercises. Learning objectives, appropriate textual material and an instructor’s manual that support the activity or exercise are provided as well. Materials developed in this project will be disseminated through the NSF-funded Analytical Sciences Digital Library (ASDL), http://www.asdlib.org. When finished, the classroom activities and laboratory experiences will span the range of topics normally incorporated into the undergraduate analytical chemistry curriculum. Work completed to date, ongoing activities, and future plans for topic development will be described.

CHED 1639

Student learning and attitudes in real world vs. virtual laboratories

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Students in a second semester general chemistry lab performed two experiments in either the physical laboratory (control) or in the virtual world of Second Life
Virtual lab experiments were designed to mimic the analogous real world experiments as much as possible. Students in both groups performed all other experiments in the physical laboratory. Pre- and post-semester surveys measured changes in students' attitudes about chemistry and pre-/post-experiment quizzes measured gains in knowledge. Students from both groups performed a short practicum after one experiment in order to determine if the virtual environment affected students’ kinesthetic lab skills. Finally, students in the experimental group completed a survey in which they compared various aspects of the real and virtual experiments.

Although students in both groups held a lower opinion of chemistry at the end of the semester, the views of students performing the virtual experiments were less negative. Overall, both groups of students showed similar gains in knowledge and similar kinesthetic skills, although interesting differences between the control and experimental groups are noted for some aspects of these assessments. Students performing virtual experiments expressed more positive views of the lab curriculum, indicating a preference for a mix of the two types of experiments. Women showed more positive attitudes about the virtual experiments than male students. This project began in 2013 and is ongoing. Results from fall 2014 will be presented also.

CHED 1640

How things were then, and why history matters

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Teaching is a very complex human activity. If the purpose of teaching chemistry is to help students learn chemistry content, improve their critical thinking skills, appreciate the world about them, and develop or maintain a positive attitude toward science, steps must be taken to assure that the strategies teachers use do this for every student. A great deal of research has been done on devising and improving these strategies, particularly with respect to content learning and problem solving. Bywords in the past were “information processing,” “constructivism,” and “conceptual change models.” The focus was on effective classroom strategies such as questioning, using analogies and models, concept mapping, collaborative learning, real world applications, and demonstrations. However, during the last few decades of the 20th century, chemical education underwent a paradigm shift the likes of which had not been seen since the days of Lavoisier and Liebig. The drastically changed needs of students, coupled with the demands of the chemical profession and of government, chemical educators realized that they could no longer rely on strategies that seemed no longer to be effective. Whole new ideas, concepts, technological tools, communications possibilities, communities of change, etc. opened up the challenge of putting chemical education research into practice at every level. Concomitant advances in parallel disciplines, such as the cognitive sciences, have served to enrich and enhance understanding of how students learn and how we can find out how and what they learn. This paper will review the
history of how things were and why understanding this history can help to chart a trajectory into the future.

CHED 1641

Getting it right: A paradigm for the education of chemists

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The 1957 Soviet launch of Sputnik launched the United States on “catch-up” science and mathematics curriculum reform pathways at all educational levels. The two major chemistry secondary level projects, the Chemical Education Materials Study (ChemStudy) and the Chemical Bond Approach (CBA) both involved teams of secondary and tertiary faculty and were intended to expose high school students to a modern understanding of chemistry. At the tertiary level, the launch coincided with the appearance of Sienko and Plane’s textbook, perhaps the most influential general chemistry text ever published. It ushered in an era of theory-first presentation (“baby p-chem”) that became the norm for most other general chemistry texts and courses for at least two decades. An overriding principle of all these developments was to get the science right and rigorous, so students would get a good foundation and not have to “unlearn/relearn” later. This presentation will focus on the consequences: a staggering amount of material and effort in the form of texts, secondary texts to explain primary texts (study guides), topical monographs, audiovisual aids, more quantitative laboratory work, computer-assisted instruction, redesigned courses, and more, almost all aimed at getting students started on a pathway into the chemical sciences.

CHED 1642

Chapter 6: New models for teacher preparation and enhancement

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This paper will take a brief look at the history of teacher preparation and the factors that have influenced its focus. High school chemistry teacher preparation in the United States has been influenced by changes in the student audience and the implications of research on learning. High school chemistry is no longer limited to those who plan to pursue physical science careers; classrooms are now populated by students with a wide range of interests and goals. Since Sputnik, programs have shifted from teacher directed lecture in the classroom to models that are more student-centered with emphasis on a strong laboratory component. Models that emphasize active student participation in their own learning require new approaches to teacher preparation. Due to the nature of the chemistry laboratory, future high school chemistry teachers require specific training to address the logistics and safety of choosing and supervising an appropriate laboratory program. New programs, enhanced by new technologies, have
expanded beyond traditional teacher preparatory programs. Evaluation of the wealth of data available from the Internet as well as traditional textbooks and lectures creates additional challenges. The availability of the new technologies has played a major role in these changes in emphasis. This in turn has led to educating students to understand and address the issues and needs of society. Programs will face the challenge of stimulating creativity in new teachers of chemistry. Teachers will need support and encouragement as they design strategies to introduce students to current topics involving chemistry by weaving wide ranging issues such as air pollution, GMOs (Genetically Modified Organisms), and climate change into their curriculum. Time will tell which programs prove to be the most effective in inspiring teachers to achieve their best practice goals.

CHED 1643

Access and diversity: Role of the two-year college

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Considered one of the most important 20th century higher education innovations, the two-year college has been responsive to the needs and demands of our society. Since the first two-year college was founded in 1901 as a less-expensive means of access to higher education, two-year colleges have undergone various transformations that lead students to transfer to other institutions of higher education or to employment.

These open-access institutions, with little or nothing by way of entrance requirements, have become the higher education entry point for a large and diverse population of U.S. students who otherwise may not be able to afford such an opportunity. Today, two-year colleges educate about half of the students in higher education, and over half of the underrepresented populations. This talk will highlight the uniqueness and some of the major changes that the two-year colleges have undergone over the last half-century.

CHED 1644

College chemistry for non-scientists

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Few of the immediate post-Sputnik education reports and recommendations addressed science for nonscientists. The major challenge was perceived as increasing the quantity and quality of Americans professionally trained in science, mathematics, and engineering. Enhanced scientific literacy for the general public was not a significant priority and often treated with not-so-benign neglect. In many college chemistry departments, a one-size-fits-all approach was followed: what’s good for the majors is good for the masses. When this proved to be ineffective, another non-ideal solution was
proposed: chemistry at infinite dilution. The next attempt was to present chemistry with a heavy emphasis on its intellectual history, but this strategy was primarily employed at liberal arts colleges. Textbooks and courses emphasizing the applications and misapplications of chemistry were more interesting to students. The next step was to lead with issues and applications and imbed the chemistry in its social context. Over the years there has been a gradual recognition that a scientifically informed public is essential for modern society, and as the needs of this audience have been addressed, certain of the pedagogical innovations developed have emerged as effective in the education of chemists and other scientists as well.

CHED 1645

What can the learning sciences tell us about teaching chemistry?

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Over the past few decades a growing body of work has emerged that speaks to how people learn and how we might better structure learning experiences; it also includes the multiplicity of affective components that impact learning and a better understanding of the neural mechanisms that underlie learning. In addition the recent National Research Council report on Discipline Based Education Research (DBER) synthesizes what we know about student learning at the college level in various Science, Technology, Engineering and Mathematics (STEM) disciplines. However, it is quite surprising that relatively little of this understanding has made its way into the design of chemistry curricula offered at most colleges and universities. While there is much discussion of evidence based reform, most of these efforts are focused on incorporating “active learning” techniques, rather than redesigning the curriculum in light of evidence from research. This presentation will focus on the need for evidence based curriculum reform, the research findings that can guide such reforms, and how we might assess the results of these reforms.

CHED 1646

Enhancing and assessing conceptual understanding

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Teaching for conceptual understanding was a new thought not so long ago. Chemistry knowledge had been thought to be best measured by mathematically-based problem solving. If students could calculate the molarity of a solution or the grams of product produced by a limiting reagent, it was assumed that they understood what dilute and concentrated meant on a particulate level or how reactions take place between individual atoms and ions. It wasn’t until research demonstrated that many students could solve achievement measures based on their math ability rather than their
understanding of the chemistry involved that chemical educators took note. The revolution in chemical education shifted the emphasis in teaching and learning from producing a correct numerical answer to understanding the process that was being described by the numbers. This presentation will describe the revolution highlighting the research that sparked it and the changes that were implemented in teaching pedagogies, textbooks and standardized tests as a result.

CHED 1647

Visualization: The key to understanding chemistry concepts

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Chemistry is a science that operates at many levels, including the invisible molecular level. Over the years chemists have devised ever more useful and complex representations of molecular-level structures and interactions. The introduction of computers in the latter half of the twentieth century led to the development of powerful visualization and modeling tools that have enhanced chemistry research capabilities. These techniques allowed more accurate and informative images of the molecular level to be generated for use in education and animations were developed to show how atoms and molecules interact. At the ACS Examinations Institute Dwaine Eubanks led some of the earliest efforts to enhance assessment of conceptual understanding through the use of visualizations. Because scientific visualizations and animations can be complex and difficult to understand, multidisciplinary teams are now studying how the use of visualization techniques in the teaching of chemistry can be optimized. These collaborations are revealing how students perceive and interpret various kinds of molecular animations and are showing how best to develop and use static graphics and dynamic visualizations for the learning of chemistry.

CHED 1648

ACS’s role in improving chemistry education--synergism between governance and staff

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The objects of the American Chemical Society (ACS), according to its 1938 national charter, include “The improvement of the qualifications and usefulness of chemists through high standards of professional ethics, education, and attainments”. Education is core to the Society, making ACS unique among scientific societies. The Society, through its partnership between governance and staff, has made a significant impact on
the teaching and learning of chemistry during the last half-century. Several of the educational activities and materials developed by ACS were groundbreaking and paved the way for many other changes in chemistry education. After sharing a brief history of the evolution of the Society’s Committee on Education, the Division of Chemical Education, and the Education Division, a variety of programs that were developed and implemented by governance and staff, working synergistically, will be reviewed. From developing curriculum, publications, and textbooks to establishing teacher training and supporting two year colleges and green chemistry, the Society—it’s governance and staff—has been a major player and a true catalyst for change in chemical education.

CHED 1649

Climate change: Opportunities and challenges for ACS and its members

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This symposium highlights efforts undertaken by ACS local sections to disseminate climate science information to the public. These activities were undertaken as a result of the ACS climate challenge grant program, following the posting of the ACS Climate Science Toolkit on the ACS website. These efforts can be scaled up and further expanded by local sections and divisions. The ACS Committee on Environmental Improvement has taken the lead in reviewing and articulating strategies for dissemination of climate science information to school teachers; college and university faculties; industrial science and business leaders; civic and religious groups; professional, scientific and educational organizations; and elected public officials at all levels and in all branches of government. These strategies aim to enrich and expand on the ACS leadership and advocacy on matters related to climate change.

CHED 1650

Communicating science in the public sphere: An elective course for science and engineering majors

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Traditional curricula provide few incentives for science and engineering undergraduates to converse with the public about contemporary scientific issues. But such dialogue can improve student learning and enliven socially pertinent discussion among non-scientists. We thus designed a one-semester Communicating Science elective course for students to practice persuasive communication strategies; global climate change, energy sources, and environmental impact were recurrent themes. Students learned
from invited experts with prior successes engaging non-technical audiences. Scientist-contributors included an ecologist, evolutionary biologist, biochemist, engineer, pathologist, immunologist, and an environmental historian. Enrollees practiced communication skills throughout the semester with live and mock audiences ranging from elementary school-age children to the elderly. Students were coached on best practices in communication by a rhetoritician, storyteller, and a creative writer, and by journalists with experience in video, audio, and print. Instructor assessments and student surveys indicated that at least three-fourths of enrolled students developed skill at promoting science concepts with ethical persuasion and advocacy. At a free, two-hour capstone event at a local natural history museum, students framed discussions of climate science and energy with hands-on activities for attendees. Course design and content will be discussed, and the results of several course assessment tools will be described, including attendees’ reactions to the museum outreach event, instructor assessment of student improvement, and pre- and post-course surveys. The potential for formal coursework and service learning to incite dialogue on contemporary scientific topics, especially climate change, will also be addressed.

CHED 1651

Facilitating chemistry club climate change outreach

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Through the ACS Presidential Climate Science Challenge grant we set the goal of helping the Illinois Heartland Section’s chemistry clubs raise awareness and understanding of climate change in our communities. At Illinois College one of the ways we are achieving this goal is through granting Community and Civic Engagement general education credit to chemistry club members that participate in climate change workshops and demonstrations. The requirements for this credit ensure that the students are both knowledgeable regarding climate change and prepared to address differing viewpoints. Allowing students to receive this credit gives them a strong incentive to participate in these activities. This talk will describe the requirements Illinois College students must meet to earn this general education credit; share the reading materials and assignments that are used to prepare our students; describe the science demonstrations that we use at public venues; and describe our efforts to publicize our outreach experiences through public presentations and on our website in an effort to encourage others to engage in this important form of community service.

CHED 1652

Infrared radiation and greenhouse gases: An introductory chemistry laboratory experiment

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The science of climate change is complex, but it is fundamentally linked to the chemical phenomenon of absorption of infrared radiation by certain types of molecules, collectively called greenhouse gases. We have created a general chemistry laboratory experiment for introducing students to the phenomena of absorption of infrared light radiation by various gases. The laboratory experiment employs a three phase learning cycle. In phase one, a simulation (for URL, see PhET below) is used to explore the interaction of infrared light radiation with gases. In phase 2, each group constructs a “simple” homebuilt infrared spectrometer using a hot plate (source), infrared thermometer (detector), and various gases (sample). Each group is asked to design an investigation in response to this scientific question: comparing the absorption of infrared light radiation in the presence and absence of each different sample of gas, are there any significant differences that can be observed experimentally? In phase 3, groups visit the ACS Science Climate Toolkit (for URL see below) in order to think about climate science and interpret their results. Each group reports their findings in a poster, which is present to their lab section. The laboratory experiment will be described as well as examples of student work. [PhET: molecules and light; phet.colorado.edu/en/simulation/molecules-and-light; ACS Science Climate Toolkit: www.acs.org/content/acs/en/climatescience.html]

CHED 1653

Communicating climate science by educating chemists in the Puget Sound

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The Puget Sound Section used funds from the ACS Climate Science Challenge grant to create opportunities to connect expert scientists in climate change to chemists interested in communicating climate change to the general public. Our approach was two-fold: (1) to develop a presentation that can be used by chemists in a speaker’s bureau to educate chemists and the general public (adults) on common climate change misconceptions, and (2) develop interactive informal activities that engage younger audiences and families in climate science topics in a non-confrontational way. We will discuss the planning and execution of a Climate Communication Workshop for Chemists. A total of 46 people attended or volunteered from 25 different institutions, agencies, and companies, including at least 6 people who never attended a previous ACS event. During the morning session, attendees participated in hands-on workshops with experts in climate change science. In the afternoon session, attendees completed a mindmap exercise which allowed them to organize and relate multiple facets of this complex topic. This framework can be used and modified by anyone wanting to understand and speak about climate change. The presentation will also discuss the
difficulties that arose during the planning process, including the organizational hurdles that hindered implementation of the designed activities. Strategies for avoiding these pitfalls will be discussed. After the workshop, attendees ranked themselves as proficient in climate change tools.

CHED 1654

Communicating climate science to non-science groups

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The Kalamazoo Section held three hands-on climate science workshops for non-science groups, including faith communities and secondary educators, who could earn continuing education credits. The ACS Climate Change Toolkit served as a springboard for sessions on the scientific evidence of climate change, the response of the planet and biosphere, and technological, personal, and policy decisions that have an impact on climate. Participants received a digital takeaway (USB flash drive) with workshop materials and lists. Pre- and post-workshop assessments were carried out. An examination of this approach and its efficacy will be discussed.

CHED 1655

Challenges and success factors of student run climate change demonstrations and exhibits

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Anthropogenic climate change is one of the most pressing issues facing humankind. Effective and accurate communication regarding climate change is therefore paramount. In response to the 2013 Presidential Climate Science Challenge, the Portland Section of the American Chemical Society partnered with the Oregon Museum of Science and Industry (OMSI) to provide temporary exhibits illustrating the effects and mechanisms of anthropogenic climate change. In order to address the particular challenge of communicating science concepts
to a varied audience, students also attended a workshop at OMSI designed to help develop effective science communication skills. Participating students were responsible for developing and presenting the climate change exhibits to museum visitors. Engagement, interactivity, and relatability were all important goals, and compelled us to include a hands-on experiment or activity in each exhibit. During development, we discovered that connecting the individual exhibits to one another created a stronger overall experience. Our final exhibits focused on carbon dioxide as a central theme, addressing its sources, the implications of its increasing presence in the atmosphere and ocean, and how it connects to global climate change. In this presentation we will discuss the development, implementation, and future direction of these student-run climate change exhibits, including: challenges in communication and reproducibility, factors contributing to success and positive audience reception, implementation of permanent museum exhibits and further science education outreach.

CHED 1656

Cli-Sci Teacher Workshops: Outreach activities and demonstrations in the Illinois heartland

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The Illinois Heartland Local Section was one of the eleven original recipients of the ACS Presidential Challenge Grants for climate science outreach. We have been active in direct outreach to the public at the Illinois State Fair, Heart of Illinois Fair, Wildlife Scary Park nights (the two weekends before Halloween), and a variety of sustainability fairs including one in Door County WI. These events use typically about four demonstrations, which vary from event to event. They include two participatory events for youngsters: “Ocean Acidification by Exhaling” and “CO\(_2\) is Heavier than Air”. Others include a “Reflexivity Demonstration”, “CO\(_2\) Warming Effect” using anti-acid tablets and a spotlight, “From Fossil Fuel to Ocean Acidification in 45 Seconds” and “Ocean Chemistry of CO\(_2\)” (based on a demonstration designed by Jerry Bell). These catch the attention of the public, especially the Fossil-fuel demonstration, which relates butane to
octane to make a connection to folks personal use of fossil fuels. We estimate over 2,000 observers so far. We provide URLs for the National Academy of Science, American Association for the Advancement of Science and National Climate Assessment and IPCC free downloadable booklets, which are all designed for the public. Outreach is important, but time-consuming. Teacher Workshops have the advantage of prolonged multiplication of the outreach. High school teachers can reach 150 or more students every year; elementary teachers about 30. We presented 2 workshops in 2013 and one this year with two more planned. Each workshop emphasizes the ACS Cli-Sci Toolkit and the NAS, AAAS, NCA and IPCC booklets as resources both for the teachers, and for h.s. students doing research or term papers. There is a session on classroom applications, last year dedicated to high school level primarily. This year we will run parallel sessions for elementary and high school focus, with middle school teachers choosing one or the other. An outside speaker on a biological or agricultural aspect was included last year, and this year we are adding a meteorologist. Two lab sessions are devoted to the demonstrations. The teachers leave with two loaded DVDs this year and a package of supplies for the demonstrations. A Speakers Bureau has been established recently in order to reach out further to community groups, schools, government agencies, church groups, etc.

CHED 1657

Climate Science Toolkit: A successful project in Puerto Rico

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To support the Climate Science Initiative, the ACS Puerto Rico Section proposed a series of activities to benefit our members and our community as well. Dr. Bassam Shakhashiri, ACS President-2012, states that chemists have the responsibility to understand the climate science, and to help other people, non-scientist, to recognize the relevant issues to maintain a livable climate. It is for this reason that a successful non-formal education program was developed in Puerto Rico to promote the public interest and understanding of Climate Science through ACS student chapters, ChemClubs (high school students) and the general community. The goal of the project is to inform the community about different phenomena occurring on Earth and not only warn about some changes that are happening now; but also to offer a number of actions that can be taken to reduce them and provide a common good. This program is mainly based on the materials already available at the ACS web page, including the Climate Science tool-kits. However, some hands-on demonstrations were developed to facilitate the understanding of the concepts. The program includes workshops applying the “train the trainer” approach, resources/ materials/ tool-kits (brochures, power point presentations and some materials needed for the activities). Furthermore, it also includes an outreach
component through a Science Cafe and participation in our premier outreach event known as the “Festival de Química”. Thousands of people have been impacted with the project. As a future projection, to fulfill our duty as chemistry ambassadors and make this science accessible to all kinds of people, we will adapt these interactive activities to make them suitable for persons with special needs (vision problems). The outcomes of the program will be elaborated.

CHED 1658

Energy and the environment: Exploring climate change

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A recent focus in course development has been climate change, and the role of chemistry in the sustainable world. There is an increasing concern about the impact of human activities on the earth, and a desire to learn about those effects. This presentation details the development of course content for EGEE101: Energy and the Environment. The main objectives of this course are to: provide basic understanding and appreciation of energy and environmental concepts and interconnectedness; analyze energy consumption patterns; discuss various energy resources that power the modern society; examine the energy conversion processes; explore interrelationships between energy use and industrial progress and environmental consequences; discuss future energy alternatives. EGEE101 is a hybrid course, conducted both in the classroom and on the web, which is a novel environment and has necessitated new methods of communicating information to the public.

CHED 1659

Communicating climate change: More than a message in a bottle

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Sometimes it seems as if we put the message of scientific consensus on climate change into a bottle and hope that it arrives on a beach occupied by receptive individuals. In truth, communication is about both choosing the method of delivery and about crafting the right message for each audience. For example, although a segment of the general public remains woefully resistant to the science of climate change, momentum is building behind the need for preparation, adaptation, and resilience to address the results of a warmer world. State and local governments as well as the Department of Defense are all bright spots of action towards addressing the now-inevitable alterations in the global landscape. Challenges and successes of matching messages with audiences will be discussed from the perspectives of a ACS Congressional Science Policy Fellow, Chair of the ACS Committee on Environmental Improvement, and a chemical educator reaching both science and non-science majors.
CHED 1660

Enzyme mechanisms: From physical chemistry to evolution and new drug targets

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Enzymes are fascinating catalysts from both the point of view of a chemist and that of a biochemist. They can be studied on very different levels, ranging from the “circle meets triangular to produce a square” level, to examination of “arrows pushing” organic mechanisms to the physical chemistry level (dynamics and quantum mechanics). I will demonstrate this range via recent studies of dihydrofolate reductase and thymidylate synthase, which are enzymes catalyzing the de novo biosynthesis of the DNA base T (thymine). The role of such mechanistic understanding in identifying potential targets for antibiotic and chemotherapeutic drugs will be discussed. Aspects of molecular evolution from bacteria to human revealed by those methods will also be discussed.

CHED 1661

Harnessing polyketide thioesterases to produce complex molecules

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Biocatalysts have proven to be a powerful tool in organic chemistry. Their high selectivity is a blessing, enabling stereo-, regio-, and chemo-selective reactions to be
performed efficiently, and a curse, severely limiting the substrates that can be effectively processed by the enzymes. This latter drawback has limited many biocatalysts to synthetic applications that occur early in syntheses, where substrates have reduced complexity. Unlike enzymes from primary metabolism, which have evolved to be exquisitely substrate selective, enzymes from secondary metabolite pathways, such as polyketide biosynthetic pathways, typically have relaxed substrate specificity. In this talk, we will discuss the development of macrocyclizing biocatalysts from the thioesterase domains embedded in polyketide biosynthetic pathways. Macrocyclization is a synthetically challenging reaction requiring high selectivity and greatly increasing the complexity of the substrate that is processed. It is typically the most decisive step of a synthesis and the step that defines the efficiency of a synthesis. As such it is ideal test case for development of a broadly substrate tolerant set of enzymes able to generate 12-18 member macrocycles. This would be of great value to the synthetic community as a late stage ring-forming catalyst. Thioesterase from polyketide biosynthesis selectively generate macrocycles from linear activated esters. To take advantage of this enzymatic activity, we have kinetically characterized recombinant purified thioesterases from the erythromycin, pimaricin, epothilone, zearalenone, radiciol, and bacillaene biosynthetic pathways with synthetic substrates. The selectivity of these thioesterase domains will be interpreted in light of the evolutionary pressures on the different pathways to identify ideal thioesterases for development as biocatalysts.

CHED 1662

Lov story in biocatalysis: Natural product biosynthesis and protein engineering coming together

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Many important drugs in the clinic today are natural products or semisynthetic versions of natural products. Investigations of the biosynthesis of these complex molecules have led to the discovery of new enzymes that catalyze interesting chemical reactions. For semisynthetic compounds, these enzymes can serve as candidates for biocatalytic reactions that improve the synthetic modifications steps. We have investigated the lovastatin (lov) biosynthetic pathway with an aim for finding enzymes that can improve the atom economy and cost effectiveness of the semisynthetic conversion of lovastatin to the blockbuster drug simvastatin. Although the difference between simvastatin and lovastatin is a single methyl substitution, the multistep chemica conversion process requires protection and deprotection steps and is costly overall. In this presentation, i will discuss our efforts in characterizing the lovastatin biosynthetic pathway during which we found an acyltransferase LovD; how we combined metabolic engineering, structural biology and protein engineering in transforming LovD into a powerful simvastatin synthase. The process we developed, in collaboration with Codexis Inc, is now used in the commercial production of simvastatin and replaced the multistep chemical processes. I hope the talk can illustrate how merging natural product enzymology and protein engineering can be a powerful marriage towards developing new biocatalysts.
Innovations in biocatalysis for pharmaceutical applications

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In recent years, the use of biocatalytic approaches for chemical manufacture has seen an increasing interest from industry. In pharmaceutical manufacturing biocatalysis can provide many advantages, including reduction of manufacturing costs, increasing product quality, improving safety, and reducing hazardous waste and other harmful impacts on the environment. Advances in enzyme optimization technologies and new platform developments enable the various technical aspects required to dramatically improve enzymes for commercial use. However it is the collaboration between scientists with backgrounds in various life science disciplines that integrate such advances towards the common goal of solving the complex problem of enzyme optimization for commercial use.

This presentation will describe how CodeEvolver™ Directed Evolution Technologies were used to enable a new platform for synthesis of a broad range of chiral secondary and tertiary amines.

Case studies of problem solving strategies used by college professors, graduate, and undergraduate students in chemistry

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Research studies have shown that experts and novices approach problems differently. While novices focus on the surface features of a problem under consideration experts tend to consider deep features of a problem; employ multiple strategies; and are metacognitive in their approach to problem solving. In a study conducted in a large midwestern university using a comparative case study approach, the problem solving strategies of course professors, graduate students and first year chemistry students were compared for specific problems in the domain of stoichiometry and thermochemistry. Key findings from this study will be presented along with the recommendations for metacognitive strategies that can be employed by students to approach domain specific chemistry problems like experts.

Gaining insight into visual problem solving by combining eye-tracking with multimodal data analysis
We investigated the patterns of behavior exhibited by chemistry undergraduate students in attempting to solve visual problems in stoichiometry using multimodal data. Eye-tracking provided fixation data for each problem solved and by combining cluster analysis and principal component analysis patterns of viewing were identified between and within participant video segments. Additionally we performed a qualitative analysis of the multimodal problem solving strategies used by the students. This talk will discuss the implications for teaching and the opportunities gained by combining mixed method analysis and multimodal data to yield insight into how the students solve chemistry problems with symbolic, submicroscopic, and algorithmic representations.

Gaze plots from the PhET simulation *Reactants, Products, and Leftovers* were analyzed using cluster analysis of fixation durations.

CHED 1666
Numerical comparisons of eye fixation sequences from chemistry problem solving

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A numerical string analysis method was used for the first time to examine eye fixation sequences from students asked to solve problems in chemistry. The method uses the Needleman-Wunsch algorithm, which determines the relationships among protein and DNA strands. Pairs of strings of areas of interests (AOIs) representing eye fixations were given similarity scores based on a substitution matrix and a penalty gap. Incidences of identical AOIs between two strings were scored by normalizing over the lengths of AOI diagonals. Penalties for substitution among dissimilar AOIs were assigned by normalizing over average distances between AOIs. Substitutions between highly related AOIs were also penalized to a smaller extent than those between less related AOIs. AOI strings were then separated into groups using k-means cluster analysis of similarity scores. These groupings identified students who exhibited similar visual behaviors while solving chemistry problems.

CHED 1667

Study of self-explaining skill development in college level introductory chemistry courses via latent transition analysis

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Research on the self-explaining effect has shown that careful design of activities can lead to authentic learning in the sciences. However, little direct evidence exists that self-explaining (as a learning strategy) provides a useful function in the way(s) students learn chemistry at college level. In a recent review of literature on research on self-explaining at college level only two papers (out of 57 papers) investigated chemistry content knowledge, and in the last year only two papers (out of 20 papers) did. This indicates that the study of the self-explaining effect on chemistry education at college level is an under-researched field. Also, more than 70% of the published papers were done in laboratory settings, that is, non-naturalistic learning environments. The work presented here comes to fill that void in knowledge by investigating the self-explaining effect in the natural environment of introductory chemistry courses. The study investigates the development of self-explaining as a skill using multiple activities design to promote differential self-explaining behaviors, based on prior research. The activities consisted of chemistry problems that presented students with experimental data on water solubility of different chemicals for them to explain. Data collection consisted of written explanations from +60 students at six points in the semester. The written explanations (qualitative data) were coded using published coding schemes from similar studies, to later transform it into quantitative data. The transformed data was then analyzed via latent transition analysis to investigate the development of student’s self-
explain skill along the different data points. The preliminary findings of the ongoing study will be presented and discussed.

CHED 1668

Using an interactive simulation to support student development of expert practices for balancing chemical equations

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Balancing chemical equations is a foundational chemistry skill that is most often taught traditionally, using explicit instruction paired with drill-and-practice. As such, limited research is available about how to support students in learning the meaning and practice of balancing chemical equations in an inquiry-based learning environment.

In this study, we investigated student-use of a PhET interactive simulation, Balancing Chemical Equations, in a undergraduate preparatory chemistry course. Students worked in small groups on a guided-inquiry activity that framed their learning around exploration of the simulation. Although the activity and instructor provided prompts for student interaction and discussion, no explicit instructions were given about the definition of a “balanced” equation or the process of balancing.

Through qualitative analysis of each group’s audio and screen capture data, we developed a framework for distinguishing differing levels of practice in equation balancing and investigated the ways in which the simulation successfully supported the development of increasingly ‘expert-like’ student practices for balancing chemical equations. Moreover, as the sophistication of students’ balancing practices was observed to vary not only with increasing group expertise but also in response to particular features of the chemical equations themselves, we propose that the progression from intermediate to advanced practice may depend on specific equation-level cues that are independent of the mode of classroom instruction.

CHED 1669

Students’ growth in scientific reasoning and the implications for chemistry instruction

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It is widely believed that students taking chemistry courses, even those at the introductory level, learn chemistry content as well as engage in the process of doing chemistry. This engagement in process skills is intended to help students develop the procedural knowledge of a budding scientist or a scientifically literate member of society. Given these intentions, a specific process skill—scientific reasoning (SR)—was
measured at the beginning and end of a non-science majors’ chemistry course for six semesters to determine if the goal of increasing SR skills had been met. Previously published work has shown that in a traditional lecture class (a two-semester historical control), the growth, while statistically significant, was modest at best. Four semesters of students (the treatment group) engaged with materials designed to develop content knowledge through questions cueing SR skills. Results on the growth of SR skills in the treatment semesters will be presented along with the implications the results have on chemistry instruction.

CHED 1670

Characterizing students’ explanations of energy change at the atomic-molecular level

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A central practice within STEM fields is constructing explanations for chemical phenomena by appealing to core concepts such as atomic-molecular structure, electrical forces, and energy. In this report, we describe a qualitative study aimed at characterizing how undergraduate general chemistry students construct explanations for the energy changes that occur as atoms and molecules interact. Using semi-structured interviews and an online short-answer assessment, we examined students’ explanations for energy changes in three different contexts: interactions between helium atoms, hydrogen atoms, and water molecules. Here, we present a characterization of student’s explanations in terms of increasing sophistication and connectivity between the ideas of energy, force, and atomic-molecular structure. We discuss how this characterization may be used to assess the efficacy of instructional interventions aimed at improving students’ ability to construct a coherent understanding of energy ideas across contexts.

CHED 1671

Integrating scale-themed instruction into the undergraduate general chemistry curriculum using active learning methodologies

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The American Association for the Advancement of Science (AAAS) has outlined four themes that define science literacy; these are systems, models, constancy and change,
and scale. Recently, the National Research Council has released the framework for K-12 science education that includes seven crosscutting concepts with “Scale, Proportion, and Quantity” as one. Our research has shown that scale literacy is a better predictor for success in a general chemistry course than traditional measures and integrating scale as a theme in the undergraduate general chemistry curriculum has been accomplished through a variety of methods.

The laboratory experiments previously taught in general chemistry were evaluated and updated to include specific scale-themed objectives. Student performance was evaluated using a comprehensive approach that included a laboratory survey, weekly quizzes and traditional methods of assessment. Scale concepts were incorporated into traditional general chemistry lecture content using a scale learning progression built from empirical data. This learning progression was aligned with a learning progression of general chemistry concepts and lecture content was altered accordingly to incorporate scale.

Throughout this first phase of incorporating scale into instruction, we have found that adapting laboratory experiments and incorporating supplemental instruction contribute to the greatest increase in student content knowledge. However, little to no increase was found by adapting lecture material but keeping the same teaching methodologies. For this reason, the traditional general chemistry lecture content was transformed into active learning lecture activities. Using traditional and enhanced assessment techniques the efficacy of this approach has been studied and the results of this experiment will be discussed.

CHED 1672

Exploring an inverted classroom model in General Chemistry II using POGIL style activities and undergraduate Learning Assistants

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A large lecture based introductory General Chemistry II course at Florida International University (FIU), a Hispanic serving institution, was redesigned as a fully inverted classroom. Students were expected to read, watch online lectures and complete online Learnsmart assessments to prepare for class. During class, students worked in groups on POGIL (Process Oriented Guided Inquiry Learning) style worksheets, facilitated by the instructor and trained undergraduates. Clickers and online Connect quizzes were used to assess learning during and after class respectively. Impact on student learning was measured by comparing the inverted class’ performance on a common exam to that of other traditionally taught lecture sections during the same semester and to same class taught by the instructor in previous semesters using a traditional approach. Preliminary results indicate an increase in class averages for the flipped class with a rise in As, Bs and Cs and a concomitant decrease in Ds and Fs.
Stop cheating! An evaluation of a scientific integrity writing strategy in General Chemistry I

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There is an epidemic of cheating spreading through America which has permeated academia. Since early in the 1900's, researchers have been studying cheating behaviors and the factors that influence cheating among undergraduate students at the university level. Cheating comes in many forms, but in science, there is a shared concern about scientific misconduct in research and writing in science. It is well known and accepted that the training of future scientists begins at the undergraduate level, both in coursework and the research laboratory setting. This study investigated the use of scientific writing strategy in General Chemistry I at Wright State University in Ohio. The goal of the study was to determine if providing scientific integrity and ethics training, while teaching students to write journal article-like laboratory reports, reduced the number of ethical violations committed in General Chemistry I. There were three main components to this study: 1) pre-intervention data collection, 2) intervention presentations and 3) post-intervention data collection. Pre-intervention data included both a pre-test on the Integrity Principles and Ethics in Scientific Publications and a pre-intervention laboratory report. The intervention was a training on the Integrity Principles and Ethics in Scientific Publications which occurred during the participants’ laboratory periods. Post-intervention data included post-tests and the evaluation of another laboratory report, written after the intervention. An ethics rubric was developed and used to evaluate both the pre-and post-intervention laboratory reports. The evaluation of the laboratory reports was completed using this ethics rubric that focused on six facets of plagiarism. The results showed a statistically significant increase in students’ scores on the pre-and post-tests on the Integrity Principles and Ethics in Scientific Publications. Evaluations of laboratory reports with the ethics rubric showed that there was a decrease in the number of ethical violations related to plagiarism. The study also found that students who earned A grades on the laboratory reports had the least number of ethical violations post-intervention. Finally, the study evaluated the likeliness of females vs males to engage in plagiarism. Though the incidences of plagiarism decreased throughout the study, it is evident that more training is needed in the area of ethics and scientific integrity at Wright State University.

Fracking and carbon sequestration, oh my: Connecting general chemistry students to climate change topics

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Through an NSF-funded project, we have written a series of in-class activities that link general chemistry concepts to climate change topics using the POGIL (Process Oriented Guided Inquiry Learning) approach. Within each activity we have chosen models that connect climate change context to chemistry content. We believe the direct inclusion of context models is important in activities traditionally designed to teach fundamental chemistry concepts as a way to increase student engagement. Choosing appropriate types of models helps guide students towards making connections between the content and context found in each activity. This talk will address the importance of choosing relevant models and some of the challenges we have found in linking these context models with general chemistry content. A few example models will be presented.

CHED 1675

Climate change and public health: The importance of literacy domestically and globally

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As the urgency and importance of climate change education and literacy grows, considerable attention has been given to the impact of secondary effects. One such ramification that cuts across age, race, and region is human health, which is dependent on a plethora of variables. This presentation examines the impact of literacy and education both globally and domestically of health topics related to climate change. By attending, observing, participating, and representing the American Chemical Society at the 2014 United Nations Framework Convention on Climate Change 20th Conference of Parties in Lima, Peru, I have first-hand experience with the international discussion and diplomacy of climate change. My experiences at the conference as well as social media efforts are used as data to gauge public knowledge and global perspectives. This presentation looks at how warmer climate is expected to increase the risk of heat-related diseases, result in a decrease in air quality, threaten human safety, and allow some diseases to spread quicker, while comparing and contrasting how developed and developing nations are prepared and educated about the changes to come.

CHED 1676
Climate change impacts on biodiversity and mitigation efforts

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Climate change is a hot topic in the United States—one of the only nations still debating the basic science behind whether or not climate change is happening. We know with increasing certainty that climate change is occurring and we are observing its impacts on different ecosystems around the globe and on biodiversity. As a UN accredited Observer representing the American Chemical Society at the 2014 United Nations Framework Convention on Climate Change 20\textsuperscript{th} Conference of Parties in Lima, Peru, I investigated an extensive range of direct and indirect effects that climate change can have on different species in all types of environments, the majority of which are negative and harmful. This talk will focus on impacts that climate change has on biodiversity as well as what humans are doing to mitigate these effects.

CHED 1677

Energy discussions at the 20th Conference of Parties

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The Conference of Parties (COP) is the decision-making body of the United Nations Framework Convention on Climate Change (UNFCCC). The 20\textsuperscript{th} COP will take place this December in Lima, Peru, which eight students will attend on behalf of the ACS. This COP is particularly important because the Kyoto Protocol’s agreement has been set to be adopted in 2015 at the COP in Paris, France. The COP 20 is one of the last opportunities countries will have to negotiate the terms of the Protocol and their commitment. It is vital that the general population is involved with these negotiations, especially the younger generations since they will be the main ones impacted by the effects of climate change. The goal of the eight ACS student delegates is to promote climate literacy among a broad audience, including college and university students, by employing social media as a tool and the UN as a platform for education to engage others in climate change discourse. The energy sector is one of the main areas of focus for the global reduction of greenhouse gas (GHG) emissions. Making the switch to cleaner energy technologies will play a significant role in reducing GHG emissions. I plan to use social media to engage my peers in the discussions taking place at the COP 20 about the energy sector and the changes being made to reduce GHG emissions.

CHED 1678

Effects on agriculture from climate change
Agriculture depends on climatic conditions. Changes in our climate present challenges for farmers. Important issues within agricultural development include predicted impacts on plant growth with increased atmospheric, higher UV-B radiation, higher temperatures, and changing precipitation ratios. This transforms into the world’s food production. The UN Food and Agriculture Organization is trying to understand climate change impacts to assure that agricultural output can meet the demands of the growing human population. As a student delegate representing the American Chemical Society, I participated in the United Nations Framework Convention on Climate Change 20th Conference of Parties this year in Lima, Peru to gain a deeper understanding of how climate change is projected to impact my generation. My presentation focuses on the impact climate change has on crops, livestock, and food production with special emphasis on how developing nations are preparing to deal with climate disruption. I will also give my student perspective on advances and roadblocks in climate negotiations at COP 20 in preparation for the anticipated global agreement at next year’s COP 21 in Paris.

CHED 1679

Campaign strategy, outreach, and advocacy efforts at the UN Climate Conference

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Climate change is a social justice issue, and as such requires a public commitment to think, speak and act in ways that inspire and affect positive change at the individual, community, national and global level. In the global movement for climate justice, informed decision-making is crucial to the development and implementation of successful mitigation and adaptation strategies. Yet efforts to promote climate change literacy, and engage the public in climate change discourse, are often met with resistance and indifference as advocates are faced with the challenge of a single question- Why should I care? It is the mission of the Students On Climate Change (SOCC) initiative to reach out to a broad audience, including college and university students, by employing social media as a tool and the UN as a platform for education to engage others in climate change discourse. Student delegates in this program work to connect with a diverse audience through shared values, ultimately engaging and motivating others in a common purpose of climate change education and advocacy. Campaign strategizing efforts constantly evolve and improve in this mission, as more students bring their insights and expertise to the SOCC campaign. As student delegates prepare for and attend the UN Climate Talks in Lima, Peru, we work at our home institutions and abroad strategizing outreach efforts to show how the scientific realities
of climate change translate into real-world consequences, affecting the lived experiences of men and women across the globe.

CHED 1680

Geopolitical effects of climate change in the Arctic

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Dealing with the effects of climate change is one of the greatest challenges that our governments, and the younger generations of today, will face in the coming years. A number of adverse impacts will have an effect on the lives of each and every one of us and some will have significant geopolitical consequences. One place where this is particularly evident is the arctic. I attended the 2014 United Nations Framework Convention on Climate Change 20th Conference of Parties in Lima, Peru as a student representing the American Chemical Society. My focus was climate impacts in the arctic and geopolitical consequences. With the polar ice cap melting at an alarming rate, there are a number of important issues that will need to be dealt with. The Arctic Council, comprised of the United States, Canada, Russia, Finland, Norway, Sweden, Iceland, and Denmark, will engage in intense negotiations in the coming years. An estimated 25–30% of the world’s undiscovered natural gas, 15% of the world’s undiscovered oil reserves, and large deposits of diamonds and other minerals, are believed to be offshore in the arctic. This, in addition to the possibility of being able to pass ships through the Northwest Passage, will no doubt create a number of geopolitical issues in the coming years. As a result of this, nations in the arctic are beginning to bolster their military and make territorial claims to the arctic in an effort to make claim to these resources. The possibility of a future conflict in the arctic cannot be overlooked.

CHED 1681

How climate change will exacerbate the food, energy, and water nexus

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As a global society, we are at a precipice of great change. With increased scientific research and interdisciplinary collaboration, we are beginning to understand the holistic ramifications that climate change will have on all people across the globe. One new platform of understanding is the relationship between our energy, food and water resources. Each is inextricably linked to the other, and all will be threatened by changes in world climate. I attended the 2014 United Nations Framework Convention on Climate Change 20th Conference of Parties in Lima, Peru as a student delegate representing the American Chemical Society. I focused on the new security threats that will come to
fruition as climate change stresses our water resources and food production. In this presentation I will explore the current relationship between energy, water and food resources and how changes in climate (and a growing population) will intensify the pressure on these systems. Specifically, I will talk about climate smart agricultural innovations being utilized and how sustainable agriculture can be employed as a tool to control carbon emissions.

CHED 1682

Future stance on climate change

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Climate change is a global issue. It has been caused by past actions, but affects the present and future wellbeing of every human on the planet. Because of this, the question arises as to how upcoming generations plan on tackling this issue. As a young adult, I attended the 2014 United Nations Framework Convention on Climate Change 20\textsuperscript{th} Conference of Parties in Lima, Peru in order to gain more knowledge about what progress is being made. My presentation looks at movements, policies, and technologies that are currently available and how this compares and contrasts to what younger populations are doing and hope to see done. Specifically, I will focus on how younger populations are moving forward and inciting change. Broad coalitions of youth are attempting to influence climate negotiations. Around the globe, youth are engaged in grass-root efforts and outreach programs within their communities.

CHED 1683

Framing the chemistry curriculum: Year 1

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The goal of this project is to develop a sustainable two-semester chemistry course sequence at Nebraska Indian Community College (NICC) in collaboration with nearby Little Priest Tribal College that can be disseminated to other tribal colleges. During the first year, a Joint Advisory Board consisting of members from the community was assembled and they met to identify community topics. Soon afterward, a Case Study group of faculty and students was assembled to connect the community topics to scientifically measurable parameters. The connections were used to create the first lab manual. The idea is for students to learn how to connect topics of interest to the community by way of partnerships that involve community leaders, college faculty, college students and community outreach. The resulting materials and practices could
be applicable to all educators seeking to increase participation of underrepresented STEM groups. The course is being offered for the first time during the second year.

The project consists of a cycle of four parts: Advisory Board; Case Study Group; Two-Semester Chemistry Sequence; and Faculty Workshop to disseminate.

CHED 1684

49erTeach: Building capacity for teachers of chemistry and physics through NSF’s Noyce teacher scholarship program

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Increasing attention is being given to the high demand for high school science teachers who hold appropriate credentials. UNC Charlotte has joined the efforts to meet this demand through the Robert Noyce Teacher Scholarship Program, which supports students pursuing chemistry or physics licensure at the secondary school level. We aim to support 12 Noyce Scholars in a four-year period, a 200% increase over the current teacher certification graduates in chemistry or physics.

The 49erTeach program is based on the collaborative efforts of faculty from Liberal Arts and Sciences with expertise in chemistry and physics, along with science and math education experts from the College of Education. A partnership between science educators and science faculty led to the redesign of introductory chemistry and physics
courses, and is being expanded to include chemistry and physics teacher candidates as peer leaders in these courses. Noyce Scholars and potential applicants are given additional opportunities to gain experience in classroom management and curriculum planning issues.

This presentation will discuss recruitment efforts; academic and professional mentoring of the Noyce Scholars while they are in the 49erTeach program; and induction plans for the first three years of their teaching career.

CHED 1685

Denver Metro Chem Scholars, an NSF S-STEM program at a large urban PUI

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The first 18 months of the Denver Metro Chem Scholars (DMCS) Program, an NSF S-STEM project (DUE 1259336) will be discussed. Included will be a brief description of the crafting of the grant application and various issues encountered with that process. Program documents will be presented, in order to give an overview of how the scholars (sophomore and junior chemistry majors) were recruited and selected, and the benefits the scholars have received and will continue to receive through their senior year. We will also discuss how the program is being evaluated. The Student Success passport will be highlighted and issues pertinent to an urban commuter campus with non-traditional students will be addressed. We will also discuss the the issues of implementing a program at a state-funded PUI in transition from a teaching mission to a teaching and research mission.

CHED 1686

NSF programs that support undergraduate education

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Lock Haven University’s Nanoscience Scholars II program has provided scholarships and academic support to science students pursuing a BS in any science discipline, with either a major in Applied Physics or Chemistry, a minor in Nanotechnology, or an Associate of Applied Science in Nanotechnology degree. The program was funded by the Department of Undergraduate Education as an S-STEM grant. The program uses nanoscale science and nanotechnology, exciting fields at the interface between disciplines, to attract and engage new students. It builds on an existing NSF sponsored S-STEM program that has supported 4 cohorts of nanoscience scholars to date. The grant supports two important goals: (1) It has enabled us to thoroughly evaluate whether our strategy of focusing on interdisciplinary nanotechnology, intensive support through our Global Honors Program and our Nano Club science learning community, and
increasingly independent research opportunities is an effective and replicable means to encourage more students to pursue education and careers in science and to help them succeed and graduate and (2) by enabling us to support a total of 4 additional cohorts of students for four years each, create sufficient 'critical mass' in terms of successful students and graduates over a long enough duration to institutionalize and sustain the program without external funding.

In terms of outcomes the project has been quite successful. We have recruited numerous students to our program demonstrating greater success in attracting and retaining women and first-generation college students than other underserved populations. We've engaged students in undergraduate research experiences at our institution and helped them participate in summer REU programs. Our students have made numerous presentations of their research at national conferences. Our students have been successful in gaining employment in industry and acceptance to top graduate programs across the country. We are currently working on curricular revisions to increase the institutionalization of the program and increase the diversity of majors on our campus who are including nanoscale science in their educational and scholarly work.

Our contribution to the symposium will focus on what we have learned, obstacles faced and achievements to date.

CHED 1687

Implementing and assessing the efficacy of open access ChemWiki textbook resource

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The ChemWiki is the primary and most developed component in the University of California, Davis Hyperlibrary project with six other pseudo-independently operating and interconnected "STEMWikis" that focus on developing and disseminating viable online post-secondary textbook alternatives within a central integrated environment. The Hyperlibrary is a "crowd-sourced" project that is developed by a consortium of students and faculty across multiple campuses and countries. Development entails collecting, integrating, vetting, and building open-access content within a unified and hyperlinked infrastructure. Preliminary results of a data-driven quantitative three-quarter pilot to test the efficacy of the ChemWiki are positive. The effectiveness of the ChemWiki was assessed during the spring quarter of 2014 in the third quarter general chemistry course at UCD. The experimental class \((n = 478)\) used the ChemWiki as its primary resource, while the control class \((n = 448)\) used the standard textbook for the general chemistry sequence. Both classes were taught back-to-back by the same instructor (Larsen) with
the same set of teaching assistants and assessment protocols. Both classes used the same exams designed to measure the overall learning gain of the students in both classes, which were also confirmed with pre/post exam comparisons. The results showed that the normalized learning gains for both classes were not statistically different when accounting for student demographics. The Colorado Learning Attitudes about Science Survey (CLASS) chemistry survey was employed at the beginning and end of the quarter to determine if either class's beliefs about chemistry changed based on the primary resource they used; results from the survey showed that both classes were not statistically different. A weekly time-on-task survey was developed to monitor the hours spent working on the material outside of the classroom. The student reported data showed that the average student in the experimental class spent ~0.4 more hours a week studying.

(Left) Daily traffic for student usage of Chem 2C Wikitext (3rd quarter Gen. Chem. at UC Davis). Spikes originate from students “cramming” before exams. (Right) Integration Scheme of Hyperlibrary

**CHED 1688**

**Impact of technology on chemistry instruction**

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During the period of time from Sputnik to the present, phenomenal technological advances have impacted the way chemistry instruction is delivered by instructors, how chemistry is learned by students, and the manner in which student performance is assessed. These advances were made possible by the availability of relatively inexpensive, high-speed, large-capacity computers. Computer chips have taken us from print media to a digital environment that chemical educators have just begun to exploit.
Students who once came to class with textbook, notebook, and slide-rule in hand to watch a lecture written in chalk on a blackboard with an occasional overhead projector image, now come with laptop computers, ipads and smart phones in a more interactive classroom environment in which chemistry is taught on smart boards and instructors interact with students using mobile devices. In the past written homework might have been periodically graded in a day or so. Today students are doing on-line homework using sophisticated programs that give students immediate feedback that addresses student misconceptions and assigns grades to the homework assignments. Formative assessment of student work that used to wait for the first written exam now occurs daily. These homework programs are now becoming adaptive with each student following a different learning path that is based on continuous assessment of student mastery. In the future adaptive learning will enable instructors to more successfully deliver chemistry instruction to remedial students as well as students with enhanced backgrounds.

However, these technology-driven advances have created new problems. Information that was once gleaned in minutes from the Handbook of Chemistry and Physics or hours of library research is now found in seconds on the worldwide web. But, compared to refereed journals, faulty information more frequently finds its way to websites. Without guidance students are not discerning users of information they find on the web. Ethical issues involving placing proprietary information on web sites and plagiarism have become more frequent. Also, technology-driven social media can serve as a positive peer-education tool or merely a distraction.

This presentation outlines the history of the impact of technology on chemical education, the promise technology holds for the future, and the problems technology has created.

CHED 1689

Laboratory instruction: Less verification, more discovery

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Most chemistry educators consider laboratory instruction to be an essential component of chemistry education. They believe that hands-on experimentation provides a unique opportunity for students to gain a deeper understanding of chemistry, as well as enabling authentic assessment of their chemistry knowledge. Students’ attitudes, interests, and perceptions are all influenced by their laboratory experiences. Skills to be gained, concepts to be mastered, and understanding the nature of the scientific enterprise are often cited as some objectives of the laboratory’s role. Many different approaches have been proposed, implemented, and evaluated for students of all ages. This paper will explore some of the changes in laboratory instruction that have occurred during the last half-century, including research on the intent and effectiveness of the transition from verification activities to student-designed experiments. Misconceptions
about the design and role of the modern teaching laboratory curricula are also addressed.

CHED 1690

Evolution of undergraduate research as a critical component in the education of chemistry students

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An emerging, and still developing, theme has been the inclusion of a research experience as a central component of an undergraduate chemistry curriculum. Over a half century ago undergraduate research between a faculty mentor and undergraduate students could be found on islands of exceptional activity that were primarily located on private liberal arts colleges. In the following decades undergraduate research evolved beyond the small college environment to include some or all of the following: 1. Addition of a “cap-stone” undergraduate research experience as a requirement for graduation. 2. Revision of “cook-book” laboratory experiments into “research focused” experiments. 3. Inclusion of semesters long research project into traditional laboratories. 4. Movement of undergraduate research experiences to early in the four-year curriculum. These four are not an exhaustive list but chemistry faculty have been leaders in these, and other, revisions that are now impacting many disciplines on college campuses. This presentation will detail the evolution of undergraduate research as a critical component in the education of undergraduate chemistry students and the influence of chemist on the dissemination to other disciplines.

CHED 1691

Standards and expectations

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The launching of Sputnik in 1957 renewed interest in K-12 science education, but it wasn't until the 1990s that the standards movement gained traction. Before the standards era newly hired teachers were often handed a single text as the only resource to guide their instruction. Standards provide a framework defining the science that is important for all students to know, understand, and be able to do, but they do not define curriculum. That is a task reserved for states and local school districts. The first science standards document, National Science Education Standards, was published in 1996 and led to the unveiling of the Next Generation Science Standards in 2013. Both also emphasize a change in the way science is taught. Later most states created their own set of standards loosely based on the national ones. One goal is to graduate a greater number of scientifically literate students. This paper will consider the following questions. 1. What were the expectations of the scientists and educators who authored
the standards documents? 2. What are the intended and unintended consequences of using standards to guide curriculum and instruction? 3. How will chemistry education at the tertiary level change to accommodate a student who has successfully completed a K-12 standards based science curriculum?

CHED 1692

Trajectory of testing in chemistry education

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As a discipline, chemistry provides an unusual means for investigating how trends in testing influence and are influenced by educational reform developments. The existence of the ACS Exams Institute for the past 80 years has provided a platform for developing student testing enhancements, and as a result it now also serves as a source of artifacts for the trajectory of testing and assessment within chemistry education. This talk will look at some key changes in what chemistry students have been expected to know and do in the past 50 years. In addition, new opportunities for testing student knowledge that have emerged due to technology enhancements will be used to predict possible future pathways for testing and assessment in chemistry.

CHED 1693

Inquiry activities based on Simulations and Animations

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Inquiry in its modern form has been around since the 1950’s. It’s initial emphasis focused on hands-on laboratory investigations. Two NSF sponsored high school chemistry curriculum development projects, the Chemical Bond Approach (1959) and the Chemical Education Curriculum Study were early examples of inquiry instruction based on laboratory activities. A form of inquiry instruction, called the learning cycle approach, divides instruction into three phases; exploration, invention and application. The exploration phase relies on data collection in the laboratory, followed by group discussion to invent the critical concept from the data, and application activities to help deepen understanding of the concept. At about the same time as inquiry instruction was being emphasized, many forms of technology began to appear in the classroom along with activities that used the technology in instruction. However, early use of microcomputers in the classroom, when associated with the laboratory did not always support an inquiry approach. One of the weaknesses of inquiry instruction based on laboratory activities, which by their very nature presents information at the macroscopic level, was the difficulty of inventing particulate level concepts and explanations. With
dynamic particulate level simulations it became possible to investigate conceptual understanding at the particulate level. Written inquiry activities were built with these simulations to allow students to invent concepts based on a particulate level view.

CHED 1694

Developments in chemical education: Influences, successes, and failures in adaptations in other countries

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International and regional organizations such as UNESCO, ICSU, IUPAC and the European Commission have made many attempts to encourage new developments worldwide in chemical education over the last fifty years. Some have been huge in scope and endeavor, for example the UNESCO Pilot Project for Chemistry Teaching in Asia, produced modules which could be introduced into the curricula of countries stretching from Afghanistan to Korea. On a less grand scale, these organizations have promoted international cooperation through teacher workshops and small dedicated modules of work of contemporary significance.

The core activity of IUPAC has been in organizing biannual International Conferences on Chemical Education. Its first meetings were low key and the Conferences as we now know them, fashioned at Ljubljana in 1977, have become a focus of innovation worldwide and are shared by professional chemical educators and teachers. ICSU masermined the particularly influential Bangalore Conference, Science and Technology and Future Human Needs in 1985. The eight themes included Ethics, Industry and Technology, Health, the Environment, leading to a nine volume series of books.

Both the European Commission and NATO have also been fostering collaboration and chemical education has benefitted.

A second stream of work that had considerable influence are the large national projects of the 1960s and 1970s in the US and UK, for example CHEM Study, CBA and the Nuffield projects which were promoted in developing countries and more recently ChemCom, Chemistry in Context and the two Salters projects.

This paper will trace these influences on curricula and show that the keys to global influence are dedicated individuals and the problems that they need to overcome in implementing new strategies in many countries.

CHED 1695

Award Address (George C. Pimentel Award in Chemical Education sponsored by Cengage Learning and the ACS Division of Chemical Education). Challenges for the next generation
Chemistry education has made tremendous progress in the last half century, and more great things are surely on the way. However, most advances are also accompanied by associated retreats that must be managed. For example, tools for enabling students to visualize microscopic phenomena are incredibly good, and are constantly improving. The down side is that students receive great explanations for phenomena they are not likely to ever experience. Another example: Applying research findings from the cognitive sciences offers the promise of designing an optimal instructional protocol for every student. However, the relentless pressure to deliver instruction to more students for less money may make this level of individualization impossible. And yet another: The increasing availability of curricula for online instruction provides access to instruction that would otherwise be unavailable for many students. On the other hand, students in online courses do not benefit from the one-on-one guidance and counseling of real chemistry teachers, which may be essential for really learning a subject. Capitalizing on the positives while minimizing the effect of the negatives is indeed a daunting, but exciting, challenge for the next generation of chemistry educators.

CHED 1696

Rethinking homework: The impact of content, format, and process on physical chemistry learning outcomes

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While it is assumed that homework is an essential element of any physical chemistry course, does it matter the type of problem assigned, the frequency of assignments, whether or not it is completed online or paper, whether it is graded for completion or correctness? This presentation will describe a number of changes made to the way homework was assigned and administered in physical chemistry and the resulting impact on student learning outcomes. Using an online wiki platform, students created an electronic portfolio of “assessments” which they could easily modify, revise, and reflect on as the course progressed. Each assignment consisted of four questions that were explicitly mapped to a learning taxonomy comprised of four cognitive levels: recall, comprehension, analysis, and knowledge utilization. Results reveal that this online portfolio model of homework gave students a platform to provide meaningful analysis of their learning gains and successful mastery of course content.

CHED 1697

Preparing students for effective engagement in group problem solving

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In teaching physical chemistry, particularly the quantum mechanics sequence, students can become discouraged by the effort required to understand and work through challenging and complex mathematics in both laboratory and homework calculations. One way to support students is to dedicate a portion of the course to discussion and collaborative problem solving. When the assigned work is given in advance or the project is a laboratory, however, some students find it difficult to resist attempting to complete the entire assignment independently, even if a collaborative work session has been scheduled. This detracts from the problem-solving environment and work that was intended to be completed collaboratively can, instead, become overwhelming when attempted independently. I will discuss some successes and challenges of this approach along with methods for capturing student enthusiasm toward collaborative work.

CHED 1698

Influences of student discourse in overcoming barriers in physical chemistry

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In thermodynamics, students often struggle to explain concepts like work, heat capacity, enthalpy, entropy, and Gibbs Energy. Discourse analysis is one way to better understand how students reason through and develop an understanding of thermodynamics conceptually and mathematically. This project looks at different physical chemistry classrooms and the influences that having students engage in discourse can have on student understanding of thermodynamic concepts. Data were collected by recording and transcribing student and instructor interactions and conversations. These data were then analyzed using Toulmin’s Model of Argumentation to see how well students were able to articulate a scientific argument. These arguments were then analyzed using a rubric that looks at the scientific acceptability of the student generated arguments, and with an analytical approach that examined how well the students are able to translate between macro, sub-micro, and symbolic levels of representation. The transcripts were also analyzed using the Inquiry Oriented Discursive Moves framework to look at the influence of the instructor on student discourse, argumentation, and conceptual understanding. Analysis of the course materials using the levels of representation helped to identify which questions encouraged which representational level of conceptual thinking, and the extent to which they prompt meaningful collaborative discourses. This analysis has led to insights into how encouraging students to engage in discourse was able to help overcome common barriers found in physical chemistry.

CHED 1699
POGIL in the physical chemistry laboratory

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The NSF-funded POGIL-PCL project has implemented the principles of Process Oriented Guided Inquiry Learning (POGIL) in order to improve student learning in the physical chemistry laboratory (PCL) course. POGIL principles have been used to develop inquiry-based physical chemistry experiments that emphasize modeling of both macroscopic and microscopic chemical phenomena. The structure of these activities requires students to design, discuss, and refine experimental protocols. Students work in groups to explore data and with instructor guidance develop models to explain their data. The last phase of a lab activity is the development of conceptual understanding and application of that understanding. Most lab activities that have been developed require at least two lab periods to perform, however, we find that the development of student understanding during the lab periods is worth the extended time working on these experiments. Basic structural design and a brief overview of the experimental topics will be discussed.

CHED 1700

Quantum first physical chemistry at a regional liberal arts college

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For teaching purposes, the discipline of physical chemistry is generally broken up into four areas: thermodynamics, kinetics, quantum mechanics, and statistical mechanics. The traditional approach to a two-semester physical chemistry sequence is generally to teach thermodynamics during the first semester and quantum mechanics in the second semester. Statistical mechanics then follows quantum mechanics, with kinetics at the end of either semester, depending of the preference of the instructor. A number of years ago, the order of topics began to shift to a “quantum first” curriculum and as a result of number of new textbooks have been introduced. While this new approach has been adopted by faculty at a number of larger institutions, faculty at smaller colleges have been more hesitant. In this talk, I will present my results of teaching physical chemistry at a regional liberal arts college where I begin with quantum mechanics and spectroscopy (including the Boltzmann distribution) the first semester and continue with statistical mechanics, thermodynamics, and kinetics the second semester. This order makes more sense from a pedagogical standpoint in that the systems in quantum mechanics are limited, whereas systems in thermodynamics are more abstract and open-ended. The simpler systems increase student comprehension of the basic principles, despite the fact that the mathematics of quantum mechanics may be more
unfamiliar. Furthermore, I will provide evidence that suggests students retain information from the quantum semester more readily when topics are presented in this order, most likely due to the fact that certain ideas are encountered again in the statistical mechanics portion of the semester. At the end of the semester, the three areas of quantum mechanics, statistical mechanics, and thermodynamics may be integrated in the teaching of chemical kinetics.

CHED 1701

Learning by doing: Teaching physical chemistry using guided inquiry with frequent feedback

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A traditional two-semester physical chemistry course is taught using guided inquiry activities and collaborative learning teams (POGIL) coupled with online homework and “clickers” (personal responders). Perhaps counterintuitively, forgoing lecture for guided inquiry and team learning has proven to be vital to keeping students engaged as our class sizes have grown from 40-60 students up to 70-140 students. Regular practice and feedback via online homework (LON-CAPA, Learning Online Network - Computer Assisted Personalized Approach) and clickers give students multiple opportunities to apply the concepts they learn during class. Student results from ACS exam scores, semester exam scores, and journal discussions will be presented.

CHED 1702

Multistep synthesis of benzoyl peroxide for the second semester organic laboratory

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The three-step synthesis of benzoyl peroxide has been developed and implemented as a multistep, multi week laboratory at St. Catherine University. This target is of interest to students because of it use as bleaching agent for flour, an active component in acne medications, and as a polymerization initiator. This lab is completed over the first four weeks of second semester organic laboratory. First, bromobenzene is converted into benzoic acid using a Grignard reaction. Then benzoic acid is turned into benzoyl chloride using thionyl chloride. Finally benzoyl peroxide is synthesized by treating the benzoyl chloride with in situ created sodium hydrogen peroxide. All starting materials for each of these steps are commercially available in case a student’s reaction is unsuccessful. All products can be characterized using IR, NMR, and melting point analysis. This synthetic scheme is especially pertinent since all the required reaction mechanisms are taught during the second semester of organic instruction.
Where's the ketone: A laboratory showing the control of reaction intermediates in Grignard reactions with esters

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In most chemical reactions the intermediates or transition states largely control the outcome of the reactions. The described laboratory exercise is an hands-on/inquiry-based laboratory exercise that demonstrates this basic principle of chemistry that is often overlooked or ignored by students, but is critical for them to understand in order to accurately predict the outcome of chemical reactions they will study in a first year organic chemistry course.

Most students of Organic Chemistry have learned that the addition of two equivalents (2 equiv) of a Grignard salt (e.g. CH$_3$MgBr) to one equiv of an ester will produce 1 equiv of a tertiary alcohol that involves the formation of a ketone as an intermediate step. However, when students are asked to predict the outcome of a Grignard reaction when only 1 equiv of the Grignard salt is added to 1 equiv of the ester most will answer that 1 equiv of the ketone will be the final product. The correct answer is that ½ equiv of the tertiary alcohol and ½ equiv of unreacted ester will be the final products. The main reason that most students are unable to correctly predict the outcome of this reaction is because they do not take into account the control that the intermediate ketone has on the formation of the tertiary alcohol.

To demonstrate the control of the intermediate states in the reactions of esters with Grignard reagents, three related Grignard reactions are described which shows that the intermediate ketones determine the outcome of Grignard reactions with esters.

Carbocation rearrangements in the undergraduate laboratory: GC/MS and NMR deduction of products from electrophilic aromatic substitution in a discovery laboratory experiment

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We have developed electrophilic aromatic substitution reactions, some involving carbocation rearrangements, and have implemented them successfully in the undergraduate teaching laboratory. Our work is based on the known Friedel-Crafts alkylation of 1,4-dimethoxybenzene with $t$-butanol. We extended this reaction into an undergraduate discovery laboratory format in which faculty may choose from seven
alcohols that students transform into products. Students then solve the structures of their products using GC/MS, $^1$H NMR, and $^{13}$C NMR.

Two of our reactions involve a backbone rearrangement in the alkylation of 1,4-dimethoxybenzene: a [1,2]-hydride shift with 3-methyl-2-butanol ($R = H$) that students compare with 2-methyl-2-butanol and a [1,2]-methyl shift with 3,3-dimethyl-2-butanol ($R = \text{CH}_3$) that students compare with 2,3-dimethyl-2-butanol. Working in pairs, students with a matched set of alcohols generate the same product, adding an important level of problem-solving to this discovery-based experiment.

We further extended this method to include two more tertiary alcohols (3-methyl-3-pentanol and 3-ethyl-3-pentanol) and, importantly, eliminated tempting alcohols that, unfortunately, do not react under these conditions.

In summary, identical reaction conditions were used for all four alcohols such that students provided with 1,4-dimethoxybenzene and one of seven alcohols can participate in a discovery laboratory experiment that requires careful analysis of instrumental data (and not reaction conditions) to determine the identity and structure of their products.

CHED 1705

Importance of sampling: The first lab in the analytical chemistry class

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Analytical chemistry students are told from the very first day of class that sampling is the most important step in the process of analysis. Emphasis is placed on the fact that no amount of meticulous and scrupulous laboratory work can make up for a sample that is not representative of the lot. The usual example used is that of a boxcar of silver or iron ore that an analytical chemist has to assay for the percent of metal that can be extracted. Ore that is mined is never homogeneous and it is important to plan the sampling step so that a representative bulk sample is taken from the lot. Even after this importance is stressed, when a solid unknown is given to students in a sealed vial, most often it does not occur to them that settling might have caused some amount of separation of concomitants and analyte. As a result they take replicate samples beginning at the top of the vial, leading to poor accuracy and precision. This presentation will give details of a simple experiment that serves to reinforce the importance of effective sampling, using copper pennies. Students are required to determine the average density of copper, but arrive at an erroneous value depending on whether the samples consist of coins minted before or after 1982. Comparison of experimental results obtained by all the members of the class leads to the realization that knowledge of the kind of sample being analyzed is essential for proper sampling techniques.

CHED 1706
Organic chemistry and the native plants of the Sonoran Desert: A new model for the undergraduate laboratory

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The Physical Science Department at Mesa Community College (Mesa, Arizona) is developing a novel organic chemistry laboratory curriculum that uses the natural products found in local native plants such as jojoba and chia as a starting point for laboratory activities using guided inquiry. MCC chemistry faculty Timothy Minger, Valentina Nedelkova and John Zikopoulos have been designing and implementing laboratory activities for undergraduate students to extract, purify, and study organic molecules from desert plants. The project is funded in part by a grant from the National Science Foundation awarded in 2012 (“Organic Chemistry and Native Plants of the Sonoran Desert: A New Model for the Undergraduate Laboratory”, NSF grant 1140887). Project progress is being evaluated by M. Jean Young & Associates of Tucson using formative and summative assessments. Project objectives include isolating and identifying materials from native plants; providing hands-on training for students in key organic laboratory instrumentation for analysis and purification of plant materials; introducing students to variety of applications of the compounds found in plants, e.g., medicinal, agricultural and other contexts; and encouraging student participation in independent study outside the lab classes. Many of these native plants hold a traditional place of importance in Hispanic and Native American cultures and have medicinal and other applications. MCC students and others are getting hands-on experience with applying actual research methods to contemporary and relevant scientific topics. Over the last three years, students taking organic chemistry lab courses at MCC have worked with a variety of plants. For example, our students have extracted oil from the seeds of the jojoba plant and converted it to biodiesel using a transesterification reaction. They have also extracted and analyzed the oil from chia seeds, learning about fatty acids and triglycerides in the process.

CHED 1707

Safety for chemical demonstrations

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A recent safety alert was issued from the U.S. Chemical Safety Board called "Key Lessons for Preventing Incidents from Flammable Chemicals in Educational Demonstrations" (http://www.csb.gov/csb-releases-key-lessons-for-preventing-incidents-from-flammable-chemicals-in-educational-demonstrations-in-wake-of-several-serious-methanol-accidents-that-injured-children-and-adults/) The alert was based on three recent serious incidents in Nevada, Colorado, and Illinois where children were burned while observing laboratory demonstrations involving flammable liquid methanol. The Division of Chemical Education of the ACS, NSTA, and Flinn Scientific, Inc. have
published minimum safety guidelines for demonstrators which have been in place for many years. These guidelines do not, however, address a number of steps that demonstrators must take to insure safety to both the demonstrator and their audience. This paper will look at some practices that can lead to safer chemical demonstrations.

CHED 1708

Synthesis and the three-separate independent purification of 3-nitroacetanilide: An exercise in recrystallization, extraction and radial chromatography in the undergraduate organic chemistry labs

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One of the many challenges that students face in the first-year organic chemistry teaching lab is understanding the connection between the synthesis and the purification of organic molecules. To facilitate the students’ comprehension of this connection, I developed an experiment that enables students to successfully carry out a single-step synthesis that requires them to divide the resulting product into three separate defined portions and to utilize one of the three independent purification techniques specific to each sample. The purification techniques investigated were liquid-liquid extraction, recrystallization, and radial chromatography. The synthesis was carried out by combining 3-nitroaniline with acetic anhydride in a Erlenmeyer flask. The resulting 3-nitroacetanilide product was collected and divided into three defined samples. Each sample was either subjected to recrystallization (from water), extraction (from ethyl acetate and 10% HCl), or radial chromatography (utilizing previously reported protocols). The purified material from each technique was massed, a percent recovery was calculated, and both a melting point and a 300 $^1$H NMR were obtained. Based on the data that was gathered and analyzed, students hypothesized which technique provided the best acceptable yield and adequate purity of the synthesized anilide. The overall percent recoveries, physical data and spectral data analyzed were shown to be within acceptable parameters. In addition to presenting these results, this paper will also describe the methodology of this three-part independent purification of a synthesized sample of 3-nitroacetanilide.

CHED 1709

Teaching research in organic chemistry with a “guided-research” laboratory experience

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The integration of research into teaching laboratories has been slow despite the numerous pedagogical benefits. We report a new “guided-research” laboratory course herein. This semester-long laboratory allowed the students to cultivate multiple higher-
order cognitive skills necessary for research. For example, the students developed information literacy through searching and evaluating the primary literature. Students were actively engaged in decision-making at all levels (i.e. picking a procedure, implementing a procedure, optimizing a procedure, etc). The students were also taught how to evaluate their results utilizing modern spectroscopic methods. In addition to primary scientific skills, communication and teamwork were emphasized throughout this research project.

CHED 1710

Investigating enzyme assays

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Biochemistry laboratory at Lebanon Valley College currently is a single semester course experience that most students take in the spring of their junior or senior year. Following a series of 8 to 10 experiments that introduce students to essential protein methods (e.g. quantitation, purification, electrophoresis, etc.), multi-week research projects round out the remainder of the course. Students begin the course with a range of experiences: some students have been engaged in long-term student-faculty research projects, yet others have no laboratory experiences outside of their course work. With a combination of majors (i.e., biology, biochemistry & molecular biology, and chemistry) and planned career paths (i.e., employment at the technical level, graduate school or a professional program in one of the health sciences), students have a range of expectations for the course.

Research projects are used to engage this diverse group of students in a meaningful and productive experience. Lately, the central theme of these projects is the investigation of enzyme assays. Early in the course, students purify lactate dehydrogenase, so they are familiar with how to work with proteins, follow enzyme activity and do activity calculations. For their research project, students are asked to implement, design or modify an assay for an enzyme. They are assigned an enzyme or can choose from a diverse collection of enzymes such as amylase, lipase, horse radish peroxidase, Bromelain and pectin methyl esterase - enzymes are chosen for their availability at a local health food store or for their occurrence in common fruits and vegetables. Tasks can range from simply implementing and reproducibly using a method found in the literature, to designing a new activity assay. Students interact with the primary literature, propose a research plan, gather & prepare materials & reagents, implement their plan, demonstrate effective and reproducible methods, troubleshoot, use proper controls, document their work, and communicate their work effectively in a poster session.

Collectively, this type of project-based experimentation engages students with a broad range of knowledge & skills, while fostering the development of essential research & critical thinking skills. Further, the diversity of enzymes leads to a much broader exposure to topics and methods for the class as whole, than having all students investigate the same topic in a project setting.
CHED 1711

Introduction of the professional quote format and compound screening to project-based experiments in the biochemistry laboratory

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Writing within the subject area of chemistry is well established as an important way for students to hone communication skills, which educators as well as industry professionals see as key to success in the workplace. To enhance our students’ professional training, we have developed a professional quote format in collaboration with local industry, which is employed as the vehicle for experimental proposals in our first semester biochemistry laboratory. This laboratory is conducted in a cooperative learning guided-inquiry format where students work in teams and design their own protocols. After initial training in basic techniques, teams complete a two-part, multi-week project to purify and characterize the enzyme tyrosinase. Moreover, as part of the latter sub-project that focuses on kinetic characterization of the enzyme, teams examine the effects of various thiosemicarbazone compounds on enzyme activity. These compounds were produced in the organic chemistry laboratory the previous year; for some compounds tested, the inhibitory characteristics have not been published, providing students with a taste of an original research experience. This talk will discuss implementation of the professional quote format, student experiences, conceptual barriers, and project results.

CHED 1712

Design and implementation of a multi-method enzyme kinetics project for a junior-level studio laboratory

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In order to add a biochemistry component to a junior-level integrative studio laboratory for chemistry majors, a project on enzyme kinetics using multiple assay methods was developed. The project focuses on the proteolytic activity of caspase-3 and uses both colorimetric assays on a plate reader and calorimetric assays using isotherma titration calorimetry. The project is broken into four phases: 1) recombinant protein expression and purification from a bacterial system, 2) enzyme kinetics characterization using a colorimetric assay, 3) enzyme kinetics comparison using a calorimetric assay, and 4) investigation of enzyme kinetics on a potential natural substrate. As the project progresses, the students compare the two assay methods, evaluate the Michaelis constant and the substrate-binding constant results, and explore the enzyme kinetics of proteolysis on potential cellular substrates. The project design and implementation will be discussed along with ideas for incorporation in other courses and implementing a similar project with limited instrumentation.
CHED 1713

Green chemistry of biodiesel production

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Biodiesel as a renewable fuel has the potential to replace non-renewable fossil fuels and associated environmental pollution. The most commonly used method in biodiesel production is transesterification of virgin and used oil feedstock. The basic chemistry of this reaction is a highly efficient reaction. However, the biodiesel chemical reaction (transesterification) does not proceed spontaneously, which means excess reactants are required to move the reaction to completion. The biodiesel reaction efficiency can be improved by incorporating the green chemistry principles and process intensification effects. Green chemistry is the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances. Microwave based biodiesel synthesis can enhance the reaction efficiency due to higher product recovery, low by-product formation, and reduced energy consumption. In addition, a few green metrics such as E-factor, atom economy (utilization), mass intensity or mass productivity, and reaction mass efficiency can help design safer and highly efficient biodiesel synthesis. This presentation discusses the green chemistry principles for microwave enhanced biodiesel production in detail for the first time in the literature.

CHED 1714

Biorefinery: A molecular design platform for green surfactants and soft materials

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In future research, developing materials from renewable resources would be fascinating yet demanding practice, which will have a direct impact on industrial applications, and economically viable alternatives. This study presents a novel and emerging concept of generating new chemicals, intermediates and materials in a ‘Biorefinery’. Our continuous efforts in this area have led us to develop new amphiphiles and surfactants from industrial by-products, which upon self-assembly produced molecular materials including micelles, emulsions, lipid nanotubes, twisted/helical nanofibers, thickening agents (molecular gels) and liquid crystals. More recently, harnessing the availability of ‘chiral pool’ of carbohydrates and selectivity of enzymes catalysis, we have produced an array of amphiphilic molecules from simple sugars and sugar alcohols. Intriguingly, by combining biocatalysis, with principles of green and supramolecular chemistry, we have developed building blocks-to-assembled materials. These results will lead to efficient molecular design of supramolecular architectures and multifunctional soft materials from underutilized plant/crop-based renewable feedstock.
Greener synthesis of photochromic, fluorescent, and industrially important organic compounds for one- and two-semester organic chemistry laboratories

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CLICK (Color and Light to Improve Chemical Knowledge) is a recently funded NSF TUES grant designed to increase engagement in chemistry courses using activities centered around color and light. Synthesis experiments have been developed for organic chemistry that are rapid, environmentally friendly, and colorful. In addition, the compounds students synthesize are known to be useful industrially (e.g., in the pharmaceutical or electronics industry) or are close analogs. We will present two projects that have been class-tested (thiosemicarbazone and imine syntheses) and another currently under development (electroluminescent compound synthesis). The thiosemicarbazone (TSC) synthesis involves a greener synthesis of compounds known to inhibit the enzyme tyrosinase, the enzyme responsible for fruit and vegetable browning. In spring 2014, each student in a lab section synthesized a different TSC and analyzed it by NMR (1H, 13C, and DEPT) followed by a qualitative analysis of its reactions with different metal ions to form colorful complexes. The experiment was class-tested again in the fall 2015 one-semester organic laboratory. Here, pairs of students synthesized different TSCs, formed metal complexes, and qualitatively tested their compound on apples and potatoes for inhibitory activity on tyrosinase. Some of these compounds will be quantitatively analyzed in collaboration with biochemistry students. The imine synthesis is a rapid room-temperature synthesis of photochromic and/or fluorescent imines. Imines have a broad variety of applications, such as starting materials for prescription drugs and their use in O-LEDs. Each pair of students in the one-semester laboratory identified a different unknown aniline by IR and melting point, then performed a 1-5 minute room-temperature reaction with a common aldehyde. In addition, they evaluated the photochromic and/or fluorescent properties of their compounds.

Nickel-catalyzed Suzuki–Miyaura cross-coupling in a green alcohol solvent for an undergraduate organic chemistry laboratory

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This presentation will describe the development of a modern undergraduate organic chemistry laboratory experiment involving the Suzuki-Miyaura coupling. The laboratory procedure exposes students to a variety of contemporary topics in organic chemistry, including transition metal-catalyzed cross-couplings, non-precious metal catalysis,
green chemistry, and the importance of heterocycles in drug discovery. The experimental protocol uses commercially available reagents and should prove useful in both organic and inorganic instructional laboratories.

CHED 1717

Paper to plastics: An interdisciplinary outreach program in sustainable research

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An outreach program designed for high school aged girls and underrepresented minorities is described whose major scientific goal is to convert used office paper into the biodegradable polymer, poly(lactic acid). The month long summer program entitled “Paper to Plastics” is designed to incorporate elements of research into a real world application so as to inform students about issues in sustainability and to excite them about pursuing careers in science. Through a series of five steps, students are taught techniques commonly used in biochemistry, organic chemistry, and polymer chemistry such as fermentation, chirality, catalysis, and polymer synthesis to achieve their scientific objective. Along the way, students have the opportunity to interact with undergraduate and graduate students, and get to utilize state-of-the-art equipment that is available to research institutions. It is our experience that such exposure leads to increased enthusiasm for science and scientific discovery, but the Paper to Plastics program is modular so that all or some of the experiments can be carried out in most four-year colleges and many high school classrooms. These modules will be presented in detail, and analysis of short term and projected long-term efficacy of the program will be discussed.

CHED 1718

Hands-on, inquiry-based laboratory experiment for chemistry and engineering students comparing "green" and "nongreen" Noble metal nanoparticle synthesis methods

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Recently, nanoscience and nanotechnology have been at the forefront of scientific interest and investigation. Nanomaterials have numerous applications and the industry is predicted to contribute $2.5 trillion to the global economy by 2015. In an attempt to encourage interest in nanoscience in the minds of young students, which will become the next generation of environmentally conscientious scientists and engineers, this unique, laboratory activity focuses on both “green” and “nongreen” methods of the
synthesis of noble nanoparticles (NPs). In addition to focusing on the environmental aspects of synthesizing NPs, this activity incorporates a guided, inquiry-based exploration of alternative, environmentally-friendly fabrication methods of both gold and silver NPs. This hands-on activity involves implementing “green” reducing agents (e.g. tea extracts, coffee, honey and banana peel) to produce gold and silver NPs. This inquiry-based activity was developed according to the five essential factors of scientific inquiry accepted by the National Research Council. This activity was successfully used with science and engineering students at both the undergraduate and graduate levels. Students gained theoretical knowledge and hands-on experience with both conventional, non-green methods for the fabrication of colloidal gold and silver NPs. Participants in this session will participate in the synthesis of NPs using “green” fabrication techniques and compare results to traditional methods of NP fabrication. In addition, new laboratory skills, an increased interest in green nanochemistry and experience in creative and critical thinking are developed through this laboratory.

CHED 1719

Green chemistry principles illustrated through the synthesis of renewable triblock copolymers: an inquiry-based experiment

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Plastics are ubiquitous in our daily lives and represent both the past success of the chemical industry as well as one of the greatest challenges it now faces today. The buildup of these organic polymers and their negative effect on the environment and human health is an important and relevant topic to engage the diverse population of students that enroll in organic chemistry laboratory courses. This experiment illustrates how starting materials found in nature and used by the flavors and fragrance industry can be used in place of traditional fossil fuels and used to synthesize polymers with inherent biodegradable properties using green reaction conditions. In addition, the experiment exemplifies modern approaches to tuning the properties of thermoplastic elastomers through changing the structure of the midblock and exploring the weight percent of the end-block, providing an inquiry-based laboratory experience. The structures of the midblock and triblock copolymers can be probed through IR and NMR analyses with the latter also providing estimates of the overall number average molecular mass of the copolymer. This experiment has been successfully incorporated in the large university sophomore-level organic chemistry laboratory course and is adaptable to other polymer and related classes.
Decision-making based on evaluation of the benefits, costs, and risks associated with the use and production of chemicals

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To support sustainable development, chemistry students must learn to use scientific knowledge and practices to make informed decisions in authentic contexts. This often involves the consideration of sets of factors (social, economic, environmental, ethical) that are seldom analyzed and discussed in conventional chemistry classrooms. Dominant curricula at all educational levels focus on the elaboration of central concepts in the discipline without much substantive analysis of the benefits, costs, and risks associated with using chemical products or engaging in chemical practices. In the context of a framework for characterizing chemical thinking in terms of the development of reasoning involved in practicing chemistry, we are interested in identifying and characterizing levels of sophistication in benefits-costs-risks thinking in chemistry. Data were collected from chemistry undergraduate and graduate students, as well as professors, using an activity in which participants evaluated the consequences of using different fuels to power a car. Qualitative analysis elicited reasoning patterns that ranged from intuitive to mixed to normative to nuanced, with students mostly in mid-undergraduate years demonstrating a mixture of intuitive and normative chemical ways of thinking. Intuitive reasoning was governed primarily by affective impressions about the substances under evaluation. Consideration of compositional, structural, and energetic features of substances was observed with increased training in chemistry, with a tendency to mix particle-level explanations with intuitive assumptions. Normative thinking shifted toward proactive use of appropriate disciplinary knowledge, recognition of a need for more data about bulk properties particularly on large scales, and
consideration of pros, cons, and trade-offs. Nuanced thinkers additionally applied specific expertise in chemistry, consideration of the constraints of the problem, and integration of factors across local and global concerns. Implications will be discussed for ways to improve the undergraduate chemistry curriculum so that students gain proficiency in making productive judgments and informed decisions relying on chemistry knowledge.

CHED 1721

Development of a chemistry concept inventory online database

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A large body of misconceptions research has focused on what chemistry students do not know. However, the primary way of determining these misconceptions is to interview students which is impossible to do for most instructors. Because of this reason, concept inventories were developed to be able to measure students' misconceptions quickly using a primarily multiple choice assessment. There have been many concept inventories developed over the last 20 years but there is still a lack of use of these inventories outside of the chemistry education research community due to the lack of awareness and amount of time it takes to find them in the research literature. Therefore, an extensive review of the literature has been undertaken to collect all research-based chemistry concept inventories across all levels of instruction in order to organize them in a searchable online database that instructors will have access to. This presentation will focus on the development of the database in addition to an analysis of the concept inventories currently included in the database. The findings will help to inform researchers of what areas still need valid and reliable assessments and will aid instructors in providing access to and information related to using concept inventories in their courses.

CHED 1722

Student alternative conceptions of theory application during first year General Chemistry: Does anything really change?

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The analysis of what misconceptions are occurring with students is of importance from both the safety aspect and from science theory application. Students need to be able to apply scientific theory to laboratory work and be able to interpret science concepts to their own chemical safety considerations. The purpose of this research study was to identify common general chemistry students' misconceptions at a medium size public university and understanding how their misconceptions were generated or eliminated throughout the year. This project was done to understand and assist in understanding
what alternate conceptions about chemistry and laboratory theory applications were prevalent within chemistry classes and how these conceptions evolved throughout the general chemistry curricula. The goal of the questionnaire was to assess the typical student’s misconceptions about chemistry theory application within a chemistry laboratory class. The questionnaire was analyzed by identifying key words and concepts for the given situations posed to the students.

CHED 1723

Development of stereochemistry concept inventory using principles of effective test construction and results from national surveys

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The purpose of this study was to develop a concept inventory to assess students’ knowledge of stereochemical concepts. Different rigorous methods were employed to ensure quality of the assessment instrument. Two national surveys and were conducted to investigate which stereochemistry topics are important (N = 241) and to collect feedback on potential questions (N = 322). Items were mapped onto a blueprint and corresponding content validity indices were measured to warrant suitability of the instrument for classroom assessment. Several pilot tests were conducted at different institutions and psychometric quality of items was investigated followed by revisions of problematic items. Overall, the newly developed Stereochemistry Concept Inventory is a useful tool that can provide practitioners with information about abundance of different incorrect ideas that students have developed or provide insights on relative efficiency of intervention methods.

CHED 1724

Detecting incorrect ideas in stereochemistry

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Students possess a variety of incorrect ideas about stereochemistry topics. These incorrect ideas may prevent students from succeeding in an organic chemistry course and from recognizing different types of visualizations used in organic chemistry. Several methods were used to detect incorrect ideas: multiple-choice questions, open-ended questions, think-aloud protocols, and concept maps. A constant comparison method was used to analyze data from multiple sources. A detailed analysis of data yielded several genuine and spurious incorrect ideas which were characterized using Zoller’s classification scheme. An overview of different diagnostic methods along with their benefits and limitations will be discussed.
CHED 1725

Students' short and long term impressions, attitudes, perceived learning, and actual performance using two online homework systems: Embedded text vs. linked text

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Students in the first semester of a general chemistry course at a large southwestern university completed a 3-week homework assignment using Mindtap, a Cengage Learning product. Mindtap is an electronic product that has homework questions embedded in the text, such that students read a short section of text then answer a question set. Due to technical difficulties, students were moved to OWL version 1 (Online Web Learning from Cengage Learning) for their next homework sets. The OWL system has the homework questions with a link to the text in a separate window, rather than embedded. With OWL, they completed two 2-week homework assignments. A survey was given after the second OWL homework assignment was completed. The survey included Likert-scaled and open-response questions dealing with students perceived level of understanding using the different systems, how easy the systems were to use, and the advantages/disadvantages of each system. At the end of the second semester of general chemistry, the students were given another survey dealing with delayed attitudes towards the systems after using OWL for the second semester. The next semester one section of a general chemistry course used MindTap and one section used OWL for a full semester. Performance for each class was evaluated and compared to determine if one system helps students more than the other in terms of perceived and actual performance. This presentation will discuss the findings from a 300-person class for the quantitative and qualitative portions of the original survey, plus the delayed survey, and an evaluation of the full semester use of each system with recommendations for the future.

CHED 1726

Developing student-generated content in sapling learning

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A new online resource was developed as a tool for students to master the basic concepts in a first-semester organic chemistry course. Ten skill-based topics were identified as important to doing well in the course, and included arrow pushing, resonance, acid/base chemistry, stereochemistry, transition states, and electrophilic addition reactions. Each authored question provides specific feedback to the students
when they answer the question incorrectly. To develop this resource, students were selected to participate in a special course that tasked them with generating a set number of questions in the Sapling Learning interface. The content selection, format and peer review process (both internal and external) to generate over 600 questions in one year will be discussed.

CHED 1727

Form vs. function: A comparison of Lewis structure drawing tools and the cognitive loads they induce

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In recent years, the use of online homework and questioning systems has increased in popularity in the chemistry classroom. While such systems offer a number of advantages in comparison to more traditional pen-and-paper approaches, their impact on students’ cognitive load has remained largely unexplored. This research seeks to address this gap. Three groups of general chemistry students were asked to construct a series of Lewis structures: one group using pen-and-paper, the second using the beSocratic system, and the third using ChemDraw, an interface utilized by popular online homework systems. Changes in cognitive load were concurrently measured using changes in heart rate. This presentation will highlight the results of this study and focus on the cognitive load differences between the three different testing environments.

CHED 1728

How many tries are optimal for on-line homework?

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We have performed an Item Response Theory (IRT) analysis of the On-line Web Learning (OWL) system for two years of homework data. We analyzed approximately 31 million responses from nearly 69,000 students. Analysis of the IRT Total Information Curves shows that students have typically completed the important learning progression by the time they have submitted the homework three times. Total Information Curves show that on the first try usually the best students attempt the homework. On the second try, average students are attempting and completing the homework. By the third and subsequent tries only the poorer ability students are still attempting to do the homework. We will show how the analysis of this work was performed along with several Total Information Curves indicating how students respond to multiple tries on homework. We will attempt to explain the differences in student response attempts to question and mastery modes.
CHED 1729

Introduction to POGIL and The POGIL Project

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Process Oriented Guided Inquiry Learning (POGIL) is a student-centered approach to instruction based on research on how students learn best. In a POGIL classroom, students work in groups of 3 or 4 using specially-designed materials that guide them to develop concepts and that provide the context for the enhancement of important learning skills such as critical thinking, problem solving, and teamwork. The POGIL Project provides professional development for instructors at the secondary and post-secondary level to support teachers who are interested in facilitating this type of learning environment. This presentation will introduce the fundamental principles of POGIL, provide evidence of the effectiveness of the approach, and describe the opportunities provided by The POGIL Project.

CHED 1730

High school chemistry POGIL activities on a dollar store budget

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Many high school students struggle in an introductory high school chemistry course due to the abstract nature of the concepts. These POGIL activities have been created to introduce students to the fundamental concepts and allow them to formulate their own understandings while manipulating objects that have been purchased on a dollar store budget.

CHED 1731

Using knowledge surveys to assess student knowledge gains from POGIL activities

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Knowledge surveys ask students to rate how confident they are in being able to meet specific learning goals in a course. I have used knowledge surveys before and after POGIL activities in three courses: both semesters of general chemistry, first semester of physical chemistry, and in “The Art and Science of Brewing”, a non-majors course. Our general chemistry course uses a majority of published (Moog and Farrell) POGIL activities, supplemented by a few self-authored activities. In physical chemistry I have used activities currently being developed by Sheppard and Grushow, supplemented
with activities authored by Spencer, Moog, and Farrell. The activities in the brewing course are self-authored. I will discuss how the surveys are administered and the use of the results to improve facilitation or revise activities.

CHED 1732

Quantum, spectroscopy, bonding with POGIL in first semester physical chemistry

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Facilitating learning in physical chemistry courses can be challenging for many reasons. A major obstacle to student learning arises when instructors lack understanding of student preparation. Over the course of six semesters, I have developed, used and refined a series of POGIL-inspired activities focusing on quantum mechanics, spectroscopy, and bonding for a first semester physical chemistry course. Activities deployed in student groups of 2-3 are designed to comprise approximately half a 50-minute class period. Observing and interacting with students working on the groupwork activities provided this instructor ample opportunity to learn stumbling blocks for students. Design and refinement of activities as well as deeper understanding of material that proves difficult for students will comprise this presentation.

CHED 1733

POGIL on a large scale

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While POGIL is often seen in small group settings, and seems tailor-made for recitation sections, POGIL is possible in a room of 500 students. In this presentation, we will outline how UT Austin was able to transform the large section General Chemistry course from a lecture-based environment to a student-centered active learning environment based on POGIL principles without the added time and cost of discussion sections. Active learning at scale is possible because the direct teaching is accomplished outside of class via Canvas-based learning modules. Class time is then freed up for the active learning. Peer Learning Assistants, students who have passed the course and gone through an experiential learning environment, circulate in the room to work with students. Our Peer Learning Assistant (PLA) program was developed to specifically support the transformed sections of chemistry by creating a scalable administrative structure and curriculum that trains the peer learning assistants to serve as POGIL facilitators without adding to the overall cost of teaching general chemistry. The PLA curriculum includes chemistry content, professional behaviors, and facilitation techniques. In its fourth year, the active learning program has grown from a single
section of 500 students in the pilot year to serving 5 sections of 350 to 500 students each fall and spring. The accompanying PLA program has grown from six original undergraduates to 60 undergraduates enrolled in a PLA course (CH372C). Six faculty members continue to improve the curriculum and work together to foster an interactive classroom.

CHED 1734

Using POGIL in a large lecture setting: The benefits and the challenges

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Process Oriented Guided Inquiry (POGIL) was used to cover select chapters in a general chemistry sequence taught during a summer term for class sizes between 55 - 75 students. POGIL exercises were used mainly to allow students to develop critical thinking skills and to get more practice with challenging problems. Following a description of the structure of a typical POGIL lesson, the benefits and challenges are discussed. Benefits include increased class attendance, and a student centered environment. Challenges include the organizing lessons for a larger class size, classroom management, and student participation.

CHED 1735

Guided inquiry in chemistry: Teaching assistant training courses for undergraduates

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“Guided Inquiry in Chemistry” is a teaching assistant training course that introduces undergraduate students to the principles of guided inquiry, active learning, and collaborative learning in chemistry through practical, hands-on class work, discussions, and readings. Students in the course facilitate recitation sections using guided-inquiry, group-based activities. Each student develops a guided inquiry activity on an assigned general chemistry topic such as precipitation, energy, or equilibrium, and then presents a description of the activity orally to the class. Upon successful completion of this course, students may take the subsequent course “Chemistry Preceptorship,” continuing as teaching assistants for both laboratory and lecture courses. A primary objective of both courses is that students begin to reflect on how they learn. Examples of student reflections on teaching and learning will be presented.

CHED 1736

ETTA: Educational Training for Teaching Associates
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Educational Training for Teaching Associates (ETTA) is a program offered by the Center for Teaching and Learning to graduate students in the area of teaching, complementing discipline-specific efforts. Research shows TAs with training exhibit a significantly higher level of self-efficacy than those with no training (Prieto and Altmaier, 1994), as well as being more confident, comfortable in front of students, and overall more effective in the classroom. The keystone event of the ETTA is the Fall Conference. In its second year, the conference is an all-day event designed for all IUPUI graduate students who serve in any type of teaching-related role. 130 students attended the Fall 2014 conference, with 71 attendees from the School of Science, and 90 total from STEM disciplines. Session evaluations showed positive responses, and will be used to refine session offerings for next year’s conference. Lessons learned are transferable to chemistry TA training.

CHED 1737

Orientation and teacher training programs for graduate students

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At research universities graduate students provide important staffing for instructional laboratories. It is therefore necessary to insure that these graduate students are prepared for this new endeavor and for the rigors of graduate school. New graduate students at South Dakota State University are provided thorough training exercises to help them matriculate through the early years of graduate school and to build strong leadership skills needed by teaching assistants. Graduate students arrive on campus in early July to begin the training. The orientation program includes departmental and graduate school requirements discussions, graduate plan of study preparation and course explanations, safety and fire extinguisher training, ethics and human resources guidance, along with the opportunity to practice every freshman-level laboratory exercise. During the laboratory practice all new graduate students are expected to practice on numerous occasions laboratory “kickoffs”; these are 15 – 20 minute discussions or lectures that help the undergraduate successfully complete the lab exercise. Students are shown a variety of pedagogical models they could use to conduct these kickoffs. Some of these practice kickoffs are even conducted “live” with summer school undergraduate students. In addition, the new graduate students enroll in a 2 credit teaching class: Chemistry Instruction in Higher Education. This course provides the new graduate students with theoretical perspectives on teaching. Examples of theory discussed include constructive perspectives and group learning principles. Throughout the summer the course models a variety of teaching pedagogies so new graduate students can discuss the benefits and disadvantages of different teaching styles. Each student is expected to lead group sessions and to deliver a 15-
minute presentation of a general chemistry topic during a microteaching activity. The syllabus of this course will be discussed in detail. A survey taken by teaching assistants has solicited feedback as to what components of the course have been useful.

CHED 1738

Evaluation methods and findings for interdisciplinary graduate training programs at UBC

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Graduate students in chemical sciences at the University of British Columbia may apply to participate in one of several Collaborative Research and Training Experience (CREATE) programs made possible by funding from the Natural Sciences and Engineering Research Council of Canada. Each unique CREATE program provides training experiences designed to prepare students for their future careers. Our CREATE programs in atmospheric aerosols, sustainable synthesis, and quantum electronic science and technology are designed to add value to traditional graduate programs. Trainees supported by each program are drawn from diverse fields, facilitating the development of interdisciplinary research competencies. Trainees engage in activities designed to improve their teamwork and communication skills, project management ability, teaching ability, and business understanding. Trainees interact with each other, research collaborators, and industry partners at symposia, special training sessions, graduate courses, and research group rotations. Industrial internships provide additional practical experience and encourage graduate mobility. Each program is evaluated to assess the extent to which its goals are met; a formative evaluation approach is taken, with the findings used to make improvements to the programs. Specifically, the effectiveness of these programs in developing interdisciplinary knowledge, skills and attitudes in their trainees is being explored and enhanced using a range of methods, including interviews, questionnaires, competency-defining surveys (modified Delphi approach) and concept mapping activities. The outcomes of this work have so far resulted in (i) the development of several teaching and assessment tools applicable to interdisciplinary education, and (ii) the development of a range of best practices applicable to the preparation of graduate-level trainees for interdisciplinary careers, whether within academic research, industry, or beyond.

CHED 1739

Graduate teaching assistants’ potential benefits and professional development associated with teaching general chemistry laboratories
Graduate teaching assistants (GTAs) play a prominent role in chemistry laboratory instruction at large US universities. However, their role in laboratory instruction has often been overlooked in educational research. Moreover, consideration of chemistry GTAs has traditionally revolved around their abilities to perform their responsibilities in compliance with a well-established curriculum or in tune with a given instructional innovation. That is, an instrumentalist view of the role of GTAs has prevailed, and only rarely have they been considered actual partners in instruction or has attention been paid to the impact that teaching experiences may have on their professional development. Seldom has “TAing” been actively seen as integral part of chemistry graduate education, and often it seems to be reduced to a necessary evil to secure graduate researchers’ financial support. To address this, a research program was designed to investigate the effects that engagement in different laboratory instructional environments has on GTAs. This presentation will address published work that originated from this program and relates to graduate students’ experiences, gains and benefits, and the construction of their teaching assistant self-image. In addition, findings from a recent comparative, cross-case study of two GTAs in an inquiry laboratory will be presented. The latter exemplifies the effect that the learning environment may have on GTAs. Overall, findings suggest that appropriate teaching experiences may contribute towards better preparing GTAs for their journey in becoming scientists, specifically in relation to their epistemological development. Outcomes from this research program may assist laboratory instructors and coordinators in reconsidering GTA training and support in a new and different light.

CHED 1740

It takes a village: Transition from graduate student to practitioner

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A main goal of Ph.D. training in any field is, ostensibly, to help students become independent practitioners. Over the past several decades, however, much concern has been expressed about the effectiveness with which this transition is achieved. Most recently the report, “Advancing Graduate Education in the Chemical Sciences,” prepared by this organization’s Presidential Commission on Graduate Education in the Chemical Sciences raised important questions regarding the preparation of Ph.D. students for entry into the workforce. As part of our long-term interest to better understand through educational research how students develop into practicing chemists, we have gained significant insights from our studies of the experiences of
chemistry Ph.D. students. In this talk we will briefly describe some of this research and present factors that appear to catalyze the evolution of student into practitioner.

CHED 1741

Bringing chemical research into the undergraduate teaching lab: A graduate student perspective

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Bridging the gap between graduate research and introductory undergraduate teaching labs offers an opportunity for graduate students to develop pedagogical skills and for undergraduate students to have first-hand experience with research currently being conducted. Data analysis from contemporary research was adapted into an Excel training exercise, requiring undergraduate students to engage with the data by performing a series of analytical tasks guided by commentary from the researcher. The exercise allowed students to practice problem solving in the form of troubleshooting and to learn common data analysis techniques. After reading the primary article, students prepared questions for the graduate student author that were used as a starting point for an in-class discussion of the research findings, techniques, considerations, and future goals. The conversation between general chemistry students and the graduate student researcher was coupled with a tour of the research lab and served to humanize the researcher’s enterprise for the undergraduate students. This activity serves as a model for collaborations between researchers and teaching labs, and the feedback from undergraduate students supports further joint ventures between research and instructional laboratories.

CHED 1742

How my teaching role has impacted my graduate student experience

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Graduate students earn a PhD in chemistry based on the work they have done in the laboratory. The process of earning the degree is one steeped in tradition arising from its hierarchical development in the laboratory of Justus von Liebig. Yet the expectation is that graduates from PhD programs are expected to teach this chemical knowledge that they have gained through this research-based degree. How do these graduates develop their ability to teach? What experiences in the graduate program led to the construction of knowledge toward teaching? We will discuss three graduate student cases in which students have had the opportunity to be involved in leadership decisions in the course they taught. Each graduate student had the opportunity to teach in unique
undergraduate course situations. Several taught in a general chemistry lecture-style course for chemistry and biochemistry majors and honors students while others have taught in project-based laboratory courses for second-year chemistry and biochemistry majors. Through surveys and round-table discussions the graduate students answered questions as to how these teaching experiences helped construct their current vision of teaching chemistry and biochemistry. This presentation will describe the activities in which the graduate students participated and led the teaching activities. Additionally, the three case study participants will present in their own words how these experiences impacted their graduate student learning.

CHED 1743

Agent-based modeling as a tool for a discovery-based TLC experiment

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A discovery-based thin-layer chromatography (TLC) experiment has been developed for introductory organic chemistry laboratories utilizing agent-based modeling. During the first week of lab, students make use of an agent-based computer modeling program, Starlogo TNG, to determine the impact of altering the polarity of solute and solvent on TLC results. Students also utilize the program to model the separation of a mixed sample of solutes with varying polarity. During the second week, students work in the lab determining an unknown sample of two solutes via TLC analysis. Since incorporating this experiment in the organic chemistry curriculum, our assessment of the students shows excellent retention of the principles of TLC.

CHED 1744

Home-built instruments as group projects in instrumental analysis courses

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We present the use of arduino technology to create home-built instrumentation for chemical analysis in an instrumental analysis course. Students built a spectrophotometer with a motorized diffraction grating and data acquisition controlled by an arduino. Through the process of designing and building a spectrophotometer, a clear understanding and appreciation of signal transduction and the operation principle was obtained. We also present home-built instrumentation based on arduino technology for a one-credit course designed specifically for chemistry and electronics engineering technology majors to build instrumentation with basic electronics and programming skills. Our experience has shown that instrument construction provides students with a unique opportunity to explore signal transduction and principles of chemical analysis.
Implementation of cost-effective tablet technology for the development of electronic laboratory notebook skills and to promote active learning at the undergraduate level

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Electronic laboratory notebooks (ELN) have been a reality for nearly twenty years, though primarily in industry. However slow academia has been to adapt to the technology, the changeover now seems inevitable as tablet technology becomes more ubiquitous. The chemistry department at University of North Georgia has recently implemented an iPad loaner program in order to give undergraduate students experience with ELNs, a skill they will likely employ during their graduate or professional careers. The technology benefits students and faculty in both the lab and classroom setting. Student ELNs tend to include more detail, with pictures and recordings. Collaborations between student groups and faculty are facilitated through cloud storage using intuitive iPad apps with minimal or no cost. In the lecture setting, free electronic textbook options have been explored and students use iPads to record lecture notes and to work in-class example problems. The technology facilitates active learning by allowing students to share work publically in real-time with digital content mirroring. The benefits and challenges of implementation and student response to the technology will be presented.

Flipping the General Chemistry laboratory

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The concept of flipping the classroom has been infused throughout the science curriculum at a number of institutions. At this small liberal arts institution, flipping has been a part of General Chemistry lecture for the past 2 years with some success. Recently, the idea of flipping has become infused into the chemistry laboratory curriculum. Students often have difficulty with time management in lab while trying to learn new techniques, generate data, and carry out appropriate analyses. When a portion of their laboratory time is allocated for pre-lab lectures, this becomes a greater issue. Students don’t have time at the end of lab to process what they have done. This presentation will look at the implementation of the flipped model in the general chemistry laboratory. Students view videos related to the instrumental technique and data analysis prior to coming to the laboratory session. This method results in students arriving more prepared and having greater confidence in their abilities to perform the necessary techniques.
A significant issue facing many small chemistry departments is a lack of instrumentation for lab courses. While many labs in introductory courses do not require advanced equipment, traditionally high enrollment in these courses can exacerbate this problem for those experiments that do require some form of instrumentation. One such experiment common in freshman labs is a demonstration of Beer’s Law by graphing the absorption of a solution with an increasing concentration of a colored compound, CoCl₂, in our case. To quantify this measurement and track the absorbance, a colorimeter or spectrometer is needed, which would normally cost at least a few hundred dollars for an educational model.

Using a 3D printer, we were able to create a reliable and extremely portable colorimeter for under ten dollars (see figure with top removed for clarity). This cost-effective device relies on an LED for a light source, as well as another LED connected to a multimeter as a detector. The 3D printer was used to create a holder for these LEDs as well as a slot for a cuvette, while a resistor, banana socket, and several screws were the only other pieces used.

During the lab, instead of recording absorbance, students recorded the voltage produced by the detector LED. The students then calculated the percent transmission and then the absorbance. This seemingly unsophisticated arrangement turned out to be beneficial because it required the students to demonstrate a greater understanding of the concepts in the lab, as opposed to simply writing down numbers.
Designing and implementing effective virtual laboratory experiments in general chemistry

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Virtual experiments can serve as effective substitutes for laboratory experiments. Currently, general chemistry students are performing experiments in the virtual world of Second Life and showing equivalent or greater gains in attitude and knowledge compared to students performing similar experiments in the physical laboratory. Considerable resources and effort were necessary to successfully design and implement these virtual experiments. Addressing the feasibility and technical limitations of programming in Second Life as well as gaining support from students, instructors, staff and administrators have been major challenges. The project leaders will present their solutions, demonstrate the Second Life experiments being conducted and discuss the benefits of virtual experiments.

A student performs an experiment in Second Life. The student's avatar and the avatar of his lab partner are visible on the screen.

CHED 1749

Organic lab transformation

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The organic labs at St. Edward's University have been taken over by technology. Technologies that have been used to transform the student experience in the labs include Google forms, WordPress, Prezi, YouTube, GoPro, and Adobe Premiere Pro. The main objective of this transformation was to change the conversation during lab from "How do I do this?" to "Why am I doing this?".
The standard lab experience at St. Edward’s consisted of three parts: 1) pre-lab assignment 2) experiment 3) lab report. Traditionally the pre-lab assignment included reading the written protocol, answering questions pertaining to the lab, and was due the day of the lab. Students came into the lab with many questions about how to carry out the procedure they had read. Often it was when students wrote up the lab report that they finally realized the chemical principles that were happening during the experiment and these reports were due in class the week after a lab was performed.

This lab structure had two main issues. First, students were not coming to lab with sufficient preparation to undertake the technical aspects of the lab in a timely manner and thus often could devote no time to thinking about the chemical aspects of the experiment. Second, students only thought about the experiment twice a week and often were trying to think about two different experiments on the same day.

The new lab experience consists of students reading the written protocol and watching a short pre-lab video before lab. Students submit answers to pre-lab questions, which force them to read the protocol and watch the video, via a Google form that is due by midnight the night before the lab. Students then come to lab more technically prepared and more confident to perform the experiment. Now students are able to give more thought to the chemical principles that are happening during the experiment and more fully understand the lab as they do it. Then students write up the lab report, which is due one day before the next lab experiment is started. With this new structure, students are forced to think about one lab experiment on three separate occasions during the week. One objective with this new strategy is to not make more work for the students, but to ‘frontload’ the work in the pre-lab assignment so time spent on performing the experiment and writing the report decrease.

CHED 1750

Electronic grading of laboratory reports to account for variation in student data

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Electronic learning systems that reduce the time needed to grade and provide feedback to students have been growing in popularity. Their use in the laboratory has been hindered by the variation among collected student data and the effects of tolerance stacking throughout calculations. This presentation details a system that enables students to enter their actual data, and the system then calculates the necessary values to verify that students’ calculations were correctly performed. This allows for grading of students’ data analysis procedure rather than forcing excessive precision in obtaining starting materials. Discussion of this system’s implementation will include integration of pre- and post-lab work.

CHED 1751
Using QR codes and online videos in the undergraduate organic chemistry lab

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The inverted or flipped course has become an increasingly popular method of teaching in the past decade at both the college and high school levels. The classes involve the use of online lectures for student to review prior to class. In small undergraduate institutions where there are no graduate students or teaching assistants in laboratory classes it is often difficult to help students with instrumentation outside of the assigned lab hours. This problem is further compounded by having a short laboratory period (3 Hours and 10 minutes). This presentation describes the use of online lectures and QR codes to both increase class lab time by reducing the prelab preparation time and by providing instant instruction on how to operate the instruments and prepare samples. This method has been in both the organic I and organic II sophomore labs for the last year and a half. This method has given students more time in the laboratory, an ability to review the prelab instructions and methods for analysis as well as video directed instruction at the instruments.

CHED 1752

What makes an electron a valence electron? Introducing students to computational chemistry in the POGIL-PCL framework

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Undergraduates learn the diatomic molecular orbital diagram at three typical points: General Chemistry, Inorganic Chemistry, and Physical Chemistry. In general, they are well-trained at drawing and labeling it from memory and using it to determine the diatomic electron configuration, bond order, and bond strength relative to the related cations and anions. More probing questions reveal that surface knowledge of the MO diagram masks a fundamental lack of understanding about the nature of atomic and molecular orbitals. In this experiment, students are introduced to computational chemistry software while addressing misconceptions about atomic and molecular orbitals in the POGIL-PCL (POGIL for the Physical Chemistry Laboratory) framework. First, as a class, students generate the atomic orbital diagrams for the first and second row atoms to examine periodic behavior. Next, they cooperatively create a potential energy curve for Li₂. Finally, they generate quantitative MO diagrams for the first and second row diatomics. During the experiment, students rewrite the definition of valence electrons in three trips through a learning cycle. In the process, they discover the reasons for treating valence electrons separately from the core and the periodic behavior of the atomic and molecular orbital energies.

CHED 1753
Exploring the nature of hydrogen bonding using ab initio natural bond orbital calculations

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A project for students in an independent study class is described in which they explore applications of modern electronic structure methods and natural bond orbital methods to investigate the origin of hydrogen bonding for a variety of binary complexes. They perform computational investigation using density functional theory, B3LYP with aug-cc-pVTZ basis set to optimized each binary complex, followed by natural bond orbital analysis, which provides best single “natural Lewis structure” (NLS) representation of chosen wavefunction (Ψ). Our conclusion from this work finds charge transfer from a donor Lewis-type NBO (nB) to an acceptor non-Lewis-type NBO (σHA*) is the primary cause for H-bonding. We provide a variety of experimental and theoretical descriptors to support the conclusion, such as IR frequency shift (ΔνHA), H-bond penetration distance (ΔR_{B..H}), and donor-acceptor stabilization energy (ΔE^{(2)}). Assessment of this project will be discussed.

CHED 1754

Utilizing electronic structure calculations in undergraduate inorganic chemistry

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Electronic structure calculations have become so commonplace in modern chemical research that a basic understanding of their application to solving chemical problems is critical for undergraduate chemistry students. In no discipline is this truer than inorganic chemistry, where a wide range of the most important fundamental concepts lend themselves to study by computational methods. Presented here are a variety of laboratory exercises in which students apply density functional theory (DFT) to understanding important inorganic chemical principles, including symmetry, vibrational mode analysis, d-orbital splitting, and metal spin state. These exercises involve a combination of synthetic laboratory experiments, physical measurements, and DFT calculations that allow students to study important inorganic systems in an authentic fashion that mimics the way such problems are studied in real-world research environments.

CHED 1755

Web based computational job submission for the undergraduate laboratory

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We report on our efforts to provide a simple, easy to use, but powerful interface for undergraduate students to submit computational jobs. Typically a computational job is broken into three parts: preparing an input file, submitting the job to a local computer or remote server, and visualizing/analyzing the output. Commercial software typically incorporates all three of these tasks into an easy to use graphical experience. On the other hand, free computational software is just as powerful as commercial computational software, but is oftentimes more difficult for chemistry undergraduates to use. Students' lack of computer skills can then become a barrier to learning through computational experiments. In our experience the second task, job submission, is the toughest aspect for undergraduates to deal with. Many excellent front-end software packages have been created by others to aid with this step, but these submit jobs to a student's local machine and are specific to a given software package. Our free front-end web-based software allows students to submit jobs to a central server and we anticipate expanding it to allow submission to several free computational packages. This simplifies client installation, allows for central logging of student activity, and encourages students to submit jobs from anywhere without tying up their local resources for long calculations. This web-based interface is currently in use in our Senior Integrated Laboratory at Sonoma State University, where students calculate bond lengths, vibrational modes, and molecular orbitals of various molecules using the GAMESS (General Atomic and Molecular Electronic Structure System) ab initio quantum chemistry package (maintained by the Gordon research group at Iowa State University). We will report on common misconceptions and difficulties submitting jobs that have been observed during this lab.

CHED 1756

Quantum and computational chemistry: A difficult and necessary classroom union

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The Physical Chemistry curriculum needs to incorporate Computational Chemistry as an essential component. In an effort to accomplish this at Washington and Lee University, the traditional one term Quantum Chemistry course has been significantly modified to include lectures on ab initio, semi-empirical, and DFT calculations. These lecture are preceded by rigorous introduction to quantum atomic and molecular theory. The subsequent Computational Chemistry lectures are accompanied by assignments on WebMO that utilize the techniques discussed. This is a new course and the results of initial assessment will be presented, along with details of the organization and content of the class.

CHED 1757

Gaussian-based laboratory exercises in physical chemistry
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The laboratory component of the second-semester Physical Chemistry course at Susquehanna University incorporates a significant computational component. Four of the seven multi-week laboratory exercises are computational in nature. Students use the Gaussian program and Gaussview to calculate molecular properties and visualize concepts they are concurrently learning in lecture. Experiments include calculation of vibrational and rotational parameters based on the harmonic oscillator and rigid rotor models, respectively, visualization of bond vibrations and use of calculated spectra to assign experimentally-obtained infrared and Raman spectra, electronic spectroscopy and molecular orbital theory. Students learn the fundamentals of computational methods and basis sets, learn how to operate the program and extract results from both the visual interface and output (text) files. These exercises have helped students understand molecular properties that are difficult to obtain using experimental methods only.

CHED 1758

Computational chemistry in the physical chemistry course

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Concerns about limited access to computational facilities, the cost of software, and increasing the course material have inhibited the integration of computational chemistry in undergraduate physical chemistry courses. We have found that ab initio quantum chemical modeling exercises can be integrated into the quantum mechanics part of an undergraduate physical chemistry course with minor modifications to the course curriculum. Software that is inexpensive and available to individual students was used so that students could carry out calculations on their own schedule. This eliminates the need for an institutional computational facility. This approach was used over a two-year period, and assessments were carried out using end-of-course surveys. Students found the added computational material to be useful and not overly difficult. Tutorials provide by the software supplier were used to introduce student to calculations. As a result, students had very few problems carrying out calculations without further assistance. The survey results will be discussed in detail.

CHED 1759

15-year retrospective of computational chemistry in the undergraduate curriculum at The University of Tulsa

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In 2000 a new course, Molecular Modeling, was added to the undergraduate curriculum at The University of Tulsa. This presentation will describe the evolution of the course over the past 15 years as it traversed from being an elective for chemistry majors to a required course for both chemistry and biochemistry majors. A description of the course structure and assessment methods will be provided. In addition, a rather novel measure of the course’s success will be presented.

CHED 1760

Assessment of student knowledge and opinions of computational chemistry in a physical chemistry for engineer’s course

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For the past four semesters, computational chemistry has been part of the formal curriculum in the physical chemistry for engineer’s course at the University of Pittsburgh. The curriculum consisted of short lectures, worksheets and exercises, one in-class exam and a class project. Projects were completed with one other student and were given as oral presentations or written reports. In the four semesters of implementation, class sizes have ranged from 19 to 110 students. An end of semester survey was administered to the students to gain an understanding of their perceived value and opinions of including computational chemistry as part of the course curriculum. The curriculum and resources used as well as benefits and difficulties of implementation will be discussed. Student survey results as well as exam and presentation performance will be presented and discussed.

CHED 1761

Atomistic level computational chemistry for visualization and calculation in the undergraduate chemistry laboratory

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Visualizing 3-dimensional molecules is a skill that must be developed by students who pursue careers in chemistry, and that can frequently be challenging for undergraduate students. Atomistic level computational packages can be very helpful, providing the possibility of viewing a molecule from different points in space, representing atoms and bonds in several ways, and calculating potential energy surfaces that will determine the stability and reaction pathways for the molecules. Beyond the basic visualization, calculations performed computationally can enhance the understanding of experimental results for interactions of molecules with electromagnetic radiation, providing a vivid model for _uv-vis_, IR, NMR, and Raman spectra. The synergy of experiment and calculation can lead to a deeper understanding of the phenomena addressed. Here we will review the use of Spartan in the first semester undergraduate chemistry laboratory to visualize molecules, and some more advanced work using appropriate levels of
theory to calculate several spectra, as well as thermodynamic properties, in student-developed and led laboratories in the second semester chemistry laboratory. The challenges faced by the students and faculty will be reviewed, and some of the more successful projects, which have led to publications, will be discussed.

CHED 1762

Adapting green chemistry metrics for nanoparticle synthesis

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Many metrics such as atom economy, molar efficiency, E-factor, and reaction mass efficiency have been developed for evaluating the efficiency or greenness of chemical reactions. While some of these have been applied to evaluating the chemical synthesis of nanoparticles, these tools have not been optimized for the evaluation of nanoparticle synthetic methods. There are complications with evaluating nanoparticle syntheses using these metrics that are not encountered when evaluating common organic reactions. A critical evaluation is provide here of existing green chemistry metrics applied to a series of published gold nanoparticle preparations. Through this, we have established a list of best practices for the use of metrics in evaluating nanoparticle syntheses. In addition, we evaluated the role of composition uncertainty in nanoparticle synthesis and how this influences efficiency metrics. In particular, while mass based metrics, such as E-factor, are insensitive to composition uncertainty other metrics provide different results depending on what assumptions are made about the molecular composition of the nanoparticles. Through this analysis we conclude that better nanoparticle metrics are needed to more accurately compare synthetic routes.

CHED 1763

New shoots from old vines: Greening reactions in the organic chemistry laboratory

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Students apply green chemistry strategies in an attempt to improve an existing procedure from the primary literature. These projects involve a series of short assignments and faculty coaching that lead students to identify reactions with potential for green improvements. Students carry out both the original literature procedure as well as their “greener” conditions. Using modern instrumental techniques, students determine whether the green conditions are feasible improvements. In this setting, students learn about the theory of how green chemistry can improve synthesis and
temper that understanding with a practical experience in the application of these ideas. Typically students tend to focus on modest changes such as solvent or reagent changes. An overview of the project design, limitations, representative reactions, and grading schemes will be discussed. In addition, student success rates and results from attitudinal surveys will be presented.

CHED 1764

Case study: Green chemistry - theory and practice in an undergraduate laboratory

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The laboratory, a potentially dangerous work environment is one of the major places within an academic environment that requires the implementation of green chemistry principles, coupled with the fact that the undergraduate students of universities are generally involved in laboratory procedures which are not only hazardous, considering their health and safety but may also damage the environment. The purpose of this study is therefore to assess the theory and practice of Green chemistry in the application of chemical substances and laboratory procedures at the undergraduate laboratory of the Department of Pharmacognosy, Obafemi Awolowo University (OAU), Ile-Ife, Nigeria. This study will serve as a motivation for similar studies that would be carried out in other laboratories both within and outside the above mentioned institution and especially in third world countries where awareness about Green chemistry is still very low. The participants of this study were 200level and 300level students of 2013/2014 academic session and staff. Interviews and direct observation were used to evaluate the level of awareness and practice of Green chemistry in the undergraduate laboratory. The interview was used to evaluate the level of awareness about the concept and theory of green chemistry, while direct observation was used to assess the degree of implementation of green chemistry principles in the undergraduate laboratory, using the laboratory manual and practical classes. A total of 153 students and 12 staff participated in this study. Only 3% of the students and 34% of staff was discovered to have an idea of green chemistry, however none of them is aware about the 12 principles of green chemistry. From direct observation of the laboratory manual and practical classes, it was discovered that there was inadvertent practice and implementation of 2 out of the 12 principles of green chemistry during the use of the laboratory manual for practical classes. The results therefore show that the level of awareness about the theory and practice of green chemistry is still very low among students and staff of the undergraduate laboratory in which this study was carried out. The implication of this study is that it would create the need for awareness about the theory and practice of green chemistry among students and staff of undergraduate laboratories so as to reduce risk to health and safety of laboratory users and the environment.
CHED 1765

Educating general chemistry students about green chemistry through their laboratory experience

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There is growing need for educational materials to be developed that not only incorporates, but also teaches the principles of green chemistry. A significant time to introduce green chemistry is when science students are beginning their college chemistry training. The general chemistry laboratory provides an excellent opportunity to educate students on how to evaluate and minimize the environmental impact of their future endeavors. This research involved mentoring undergraduate students in creating educational laboratory materials that thoroughly explains and challenges students in the customary topics found in a general chemistry laboratory manual while teaching them how to utilize the principles of green chemistry.

CHED 1766

Need for green chemistry at the undergraduate level

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It is important that chemistry students at all levels, whether they intend to pursue career in chemistry or not, should be introduced to green chemistry to recognize the impact it can have on human health and environment. Students should have the knowledge of the twelve principles of green chemistry which they can apply to their work place after graduation for a safer, less toxic and a healthier environment. With this in mind, Gargi College is working closely with the Green Chemistry Network Centre and have done greening of some of the existing chemistry labs which use toxic chemicals and have replaced them with eco-friendly chemicals. One such experiment is the qualitative analysis of inorganic mixtures using the H₂S scheme. This green scheme eliminates the use of any sulphur containing compound in the analysis and is less toxic with fewer steps. Some other experiments are microwave preparation of copper phthalocyanin, solvent free synthesis of inorganic complexes e.g. Ni(HDMG)₂, nano particles of gold, and green and blue fluorescent complexes of aluminum used as OLED will be discussed. Greening of chemistry experiments provides an outstanding opportunity to positively influence the opinion of students about chemistry and encourage them to take an active part in shaping the future of chemistry in our society.

CHED 1767

Incorporation of green principals across a chemistry curriculum at a small liberal arts college
For many colleges with smaller chemistry programs offering a standalone course in green chemistry is not an option due to teaching loads and budgetary concerns. Incorporating green chemistry across an entire chemistry curriculum is a more suitable option at many of these smaller institutions. Mapping green principals across introductory and upper division courses aims to ensure complete coverage of principals and leaves an impression that all types of chemistry can be improved and enhanced through green practices. Multiple experiences in green chemistry over the course of a four year curriculum will also make green practice a higher priority when students analyze chemical problems. Saint Catherine University has taken steps to gradually ingrate green chemistry into all of its chemistry courses including senior seminar, research for credit, and chemistry courses for non-majors. This seminar will highlight the steps taken to gradually move a curriculum in this direction without making drastic changes to existing courses.

CHED 1768

Project GreenLab: A regional student-faculty collaboration in green chemistry curriculum development, research, and outreach education

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The Project GreenLab initiative is focused on Green Chemistry education, research and outreach, and is being developed and coordinated by faculty from Bridgewater State University (BSU) and regional community colleges. The overarching goal of Project GreenLab is to build regional professional expertise in green chemistry, and an educated workforce trained with the knowledge and skills to enter new career opportunities in green and sustainable chemistry. This presentation will provide an introduction to the GreenLab project, and outline our plans to engage students and faculty from BSU and the regional community colleges in Green Chemistry research and curriculum development, inspire K-12 students and educators, and provide outreach education to inform society about the role and impact of chemicals in our daily lives. Funding for Project GreenLab was provided by a BSU Presidential Fellowship award and the Center for the Advancement of STEM Education.

CHED 1769

Green chemical education in curriculum: Cracking siloed education
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*Green* chemical education is an inherently complex and a multidisciplinary endeavor. Over the course of the last ten years and during the push in the higher education community to address the Millennium Development Goals, there have been a number of efforts in the higher education community to integrate sustainability topics in a siloed manner (i.e. within a single discipline). It is proposed that established siloed education frameworks leads students to think that business as usual practices are acceptable, at same time undermining key education characteristics that are now being commonly accepted as critical to transformative outcomes which contribute to innovation. This talk will; 1) highlight complimentary skill sets that support the multidisciplinary field of sustainability sciences, 2) compliment these skills with applied research and discuss how outreach initiated with local community resulted in integrated education outcomes (primary and secondary), 3) will present some possible paths forward to support rigorous green chemical education, 4) a portion of this talk will also be devoted to higher education institutions that tout materials as central programtic focuses. This talk is not geared towards reductionist science but supports reductionist scientists that adopt systems and holistic education pedagogy. The discussion that this talk promotes is important because teaching 'softer' sciences (e.g. social responsibility, policy, etc.) and chemical safety in hard science education has not progressed as the fields of engineering-science practice-research have in a similar time frame. Overall, this research suggests that novel education and possibly even degrees could be required to promote *more-green* chemical education.

**CHED 1770**

**Acid-base topic in the context of a nursing chemistry course**

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The acid-base topic has been explored in many areas of chemistry due to the difficulty students encounter in the understanding of key concepts related to the topic. This study explores the topic in the context of a nursing chemistry course. Core findings were derived from semi-structured interviews with experts in the area of chemistry and nursing, a national survey of expert's opinion, and semi-structured interviews with students. A review and evaluation of the acid-base topic and representations used of several General, Organic, and Biological (GOB) chemistry textbooks and nursing textbooks were also considered. The results and the implications for teaching and assessment will be discussed.

**CHED 1771**
Comparative study of organic chemistry representations and students’ cognitive load

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Cognitive load plays an important role in the ability of learners to process information and convert it to long-term memory. There are many factors that can affect the amount of cognitive load on the learner, in turn hindering the formation of long-term, meaningful memory. Our research group has been working on strategies to measure changes in cognitive load and has developed a reliable and valid method using changes in heart rate. In the current study, undergraduate, organic chemistry students were asked to predict the product of reactions, the reactants of which were presented using two different representational motifs – Lewis structures and skeletal structures. This presentation will summarize the results of this study and focus specifically on how representational and structural details impact students’ cognitive load.

CHED 1772

Student understanding of glycolysis: Organic chemistry tasks in a biochemistry context

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The prerequisite system is based on the notion that learning in a prerequisite course is necessary for success in a latter course. In this study, we explored the impact student knowledge of reactions and reaction mechanisms from organic chemistry coursework impact understanding of the products and mechanisms in glycolysis. Students who had just completed a yearlong organic chemistry course and students who had completed both organic chemistry and biochemistry courses were asked to complete a series of tasks: predict the product, propose a reaction mechanism, and explain a sequence of reactions. Results indicate that students applied one-reason decision-making processes when solving the tasks. Suggestions will be offered on how to help students recognize appropriate cues when considering unfamiliar reactions and reaction mechanisms.

CHED 1773

Biochemistry instructors’ perceptions of their classroom use of analogies

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Biochemistry education relies heavily on students' abilities to conceptualize abstract cellular and molecular processes, mechanisms, and components. From a constructivist standpoint, students build their understandings of these abstract processes by connecting, expanding, or revising their prior conceptions and experiences. As such, biochemistry instructors often use analogies to teach difficult or hard-to-visualize topics to their classes by relating these target concepts to more commonplace analogs with which their students may already be familiar. For example, the binding of an enzyme to its substrate is often compared to a lock and a key; and ATP is frequently referred to as a cellular energy currency in discussions of metabolism and reaction coupling. Although the use of analogies in biochemistry classrooms is fairly common, the specific ways biochemistry instructors use analogies differ from instructor to instructor and class to class. In this presentation, we will discuss biochemistry instructors' perceptions of the use of analogies in their classroom instruction. Specifically, we will discuss (1) biochemistry instructors' objectives for using analogies, (2) their perceptions of the advantages of using analogies, and (3) their perceptions of the disadvantages of using analogies.

CHED 1774

Concept mapping: A learning strategy for teaching Instrumental Chemical Analysis course

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Abstract

Recently, the teaching models are changing towards the consideration of students as the main actors. In this context, this work presents concept mapping as a possible teaching tool for constituting a commitment to independent study and promoting the development of skills in students. This study was designed to investigate the effect of using concept maps as a technique in teaching and learning instrumental chemical analysis course. Thus, control and experimental groups were designed. The students of the control groups were not introduced to the concept maps and were taught with the conventional learning method only while those of the experimental groups were introduced to the concept maps. Short survey and face-to-face interviews were used to evaluate the students' response on concept map strategy, in addition to the quizzes. The results indicate that the performance of the experimental group was higher than the control group.

Key words: Concept maps, Learning strategy

Acknowledgement

The support by the Chemistry Department and King Fahd University of Petroleum and
Over two years students at all-levels (freshman through M.S.) of a chemistry program were surveyed and asked to self-report predictions of their score on their exams. While there has been limited work done in chemistry with respect to student exam predictions nothing has been done to study all-levels throughout an entire program. Students at all-levels exhibited the Dunning-Kruger effect where the students earning > 90% on an exam tended to underpredict while students earning < 50% tended to grossly overpredict their scores.

<table>
<thead>
<tr>
<th>Group of Students</th>
<th>N</th>
<th>Predicted Exam Grade (Mean)(%)</th>
<th>Actual Exam Grade (Mean)(%)</th>
<th>Difference of Means (%)</th>
<th>% of Students Overpredicting Exam Grade</th>
</tr>
</thead>
<tbody>
<tr>
<td>&gt; 90%</td>
<td>505</td>
<td>85.53</td>
<td>95.35</td>
<td>-9.81</td>
<td>7.7</td>
</tr>
<tr>
<td>80-89%</td>
<td>500</td>
<td>81.48</td>
<td>84.36</td>
<td>-2.87</td>
<td>43.4</td>
</tr>
<tr>
<td>70-79%</td>
<td>712</td>
<td>78.83</td>
<td>74.40</td>
<td>4.43</td>
<td>60.8</td>
</tr>
<tr>
<td>60-69%</td>
<td>503</td>
<td>76.17</td>
<td>64.58</td>
<td>11.60</td>
<td>89.5</td>
</tr>
<tr>
<td>50-59%</td>
<td>345</td>
<td>72.31</td>
<td>54.76</td>
<td>17.55</td>
<td>92.2</td>
</tr>
<tr>
<td>&lt; 50%</td>
<td>502</td>
<td>67.81</td>
<td>36.57</td>
<td>31.24</td>
<td>96.0</td>
</tr>
</tbody>
</table>

Figure 1. Self-Reported Mean (%) for All Chemistry Courses.

Current physical chemistry education literature mainly focuses on two areas: Student misunderstandings and success predictors. Although this research has the potential to inform physical chemistry reform, the curriculum and teaching have yet to be described.
A description of the curriculum adds to the current research on student performance and sets the stage for future research and reform. To describe the curriculum of physical chemistry, a qualitative study using interpretive description methods was done. Six instructors were interviewed about their goals, learning objectives, and values in teaching of thermodynamics. Before the interview, instructors were asked to choose two topics and to provide artifacts of their formative and summative assessment activities. These topics and assessment items were used in the interview to discuss specific student learning outcomes for topics in thermodynamics. Classroom observations, when possible, were done to capture another dimension of the enacted curriculum. To analyze the data, thematic analysis was used to determine common learning objectives in the stated curriculum. These learning objectives were then applied to the videos of classroom observations and classroom artifacts (e.g., homework, tests) to determine the extent of their presence in the enacted curriculum. Preliminary results will be presented. This novel research into the stated and enacted curriculum, emergent themes in physical chemistry instruction, and the use of interpretive description methods have critical implications for both research and teaching.

CHED 1777

Improving general chemistry students' inquiry skills and confidence with research-inspired experiments

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A study of research-inspired lab experiments over a two-year period demonstrates that this new type of lab curriculum substantially improves the self-confidence and abilities of students to perform tasks related to research, including designing procedures, carrying out their experiments, then analyzing results. Women and international students showed the most improvement in self-efficacy. Outcomes were at least as good as those observed for students performing an inquiry-based lab curriculum and frequently comparable to outcomes found for students performing authentic research experiments. The implementation of research-inspired experiments in a first semester general chemistry lab was assessed using a pre-/post-semester attitudinal survey, grades, periodic opinion surveys of the curriculum, and evaluation of student performance by research faculty. In a research-inspired lab curriculum, experiments are based on research projects conducted by scientists but do not require substantial collaboration with a researcher, as is required for authentic research experiments. Therefore, this type of experiment is easier to incorporate into a general chemistry lab curriculum.

CHED 1778

Current research on learning in the chemistry college laboratory
Chemists and chemical educators alike defend with fervor the role of the academic laboratory in learning chemistry and becoming chemically literate. In recent years, chemistry education has experienced a surge in interest in improving instruction in the academic laboratories. New laboratory manuals and innovative approaches have proliferated. Nonetheless, this interest has not adequately translated into substantial research to properly guide laboratory curricular reforms. Controversy abounds concerning the specific goals of laboratory instruction and benefits that students accrue from engaging in laboratory activities. However informative, evidence collected and findings obtained at pre-college level should not be assumed transferable to higher education. The Research on Learning in the Laboratory Symposium was initiated as a means to draw attention to the need for more research and to support those researchers already engaged in learning in the academic laboratory. To mark the occasion of the symposium’s fifth annual edition, this presentation reviews research published in the past five years on laboratory learning at tertiary level. It also briefly reviews the work presented in the symposium since 2011. This contribution may afford a better picture of the current state of the field and help identify strengths, gaps, and possible new directions.

CHED 1779

Incorporation of instructional videos to encourage students’ coordination of theory and evidence in the physical chemistry laboratory

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A series of instructional videos were designed for an upper-division physical chemistry laboratory course. For each experiment in the course, students are required to view three videos prior to attending lab: a brief overview on the theoretical aspects of the chemical system under consideration, a detailed experimental procedure video (professionally filmed), and a data analysis video detailing relevant computing aspects for students’ lab reports (e.g. spreadsheet manipulations, curve fitting). These videos have been designed upon Mayer and Moreno’s cognitive theory of multimedia learning framework with the aim to minimize cognitive load and focus students in on the relevant conceptual and experimental components highlighted in each of the videos.\(^1\) An important purpose of these videos is to free up time and space for students to focus on actively thinking about the connection between the chemical system under investigation (theory) and the means of probing the system (experiment). A mixed-methods study has been designed in order to determine whether or not the overall course structure enables students to coordinate theory and evidence. The data consist of students’ lab reports, students’ results on the VOSE (Views on Science and Education) questionnaire to establish personal epistemology, one-on-one student interviews, and video-recorded discourse of student groups in the laboratory.\(^2\) Data is being collected through the Fall
2014 semester and analysis will begin immediately thereafter.

References:

CHED 1780

Examining student analogical reasoning in introductory chemistry laboratory

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We have been developing ways to engage students in analogical reasoning during laboratory investigations. One strategy has been to create a three-phase learning cycle called **CORE** (Chemical Observations, Representations, Experimentation) which involves (phase 1) guiding students through chemical observations and consideration of open-ended questions, (phase 2) exploring a structured analogy to build representations, and (phase 3) designing and conducting experimentation in response to a scientific question to foster more open inquiry. We have examined the extent that students have the capacity to understand analogy and appreciate the limits of analogical models after an introductory CORE experiment. We have also looked at learning gains using a bridging analogy in labs covering conservation of mass and limiting reactants. The talk will report on data involving student capacity for using analogy in lab, the extent that students make macroscopic and/or submicroscopic analogical connections, and normalized learning gains associated with CORE experimentation using a bridging analogy.

CHED 1781

Perceptions of students and teaching assistants regarding a project-based undergraduate laboratory

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The chemistry laboratory is considered an essential component of chemistry education of undergraduates. The benefits of laboratory instruction for students include: 1) increasing cognitive skills, 2) enhancing practical skills, and 3) increasing interest and attitude towards chemistry. However, recent reviews of the laboratory curriculum have questioned the usefulness of laboratory experiences to students’ chemistry education. There is a need for diverse and quality studies that investigate impact of chemistry labs
on student outcomes. Given the high cost of laboratory instruction, examination of student and teaching assistant (TA) perspectives of learning outcomes from different styles of laboratory instruction is of keen interest to the chemistry education community.

In the first phase of our study, we are investigating the perceptions of students and teaching assistants regarding a project-based (guided-inquiry) undergraduate chemistry laboratory. A phenomenographic approach was used to examine student and TA experiences in the course. Therefore, we conducted pre- and post-course semi-structured interviews with 18 students enrolled in a project-based organic chemistry laboratory course. We also interviewed teaching assistants about their perceptions of the laboratory course and of the undergraduate laboratory, in general. Around a framework of meaningful learning, we identified skill outcomes, affective outcomes, knowledge outcomes and learned abilities that students and TAs describe for this laboratory. In addition, we compared the perspectives of undergraduate students to that of the TAs. The emerging themes from these interviews will be presented and discussed.

CHED 1782

Reform in general chemistry laboratory instruction: How do students experience change between an expository laboratory and a cooperative project-based laboratory?

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Educational researchers have called attention to the contradiction between the ideal objectives of the academic science laboratory experience and its actual design by practitioners. In college chemistry, this awareness has resulted in a surge in research aimed at gathering evidence to support the implementation of appropriate laboratory instructional methods. Up until recently, this research was dominated by quantitative approaches that focused on performance criteria and compared groups of students in different learning environments. Students’ lived experiences have been typically neglected and, maybe for practical reasons, more so their informed opinions about learning environments. This study investigates the experience of a group of students exposed to two substantially different instructional environments in their General Chemistry Laboratory Program sequence. During their first semester, students participated in an expository program that used weekly verification experiences, traditional assessment, weekly reports, etc. For their second semester they were assigned to the pilot implementation of a cooperative, problem-based approach that had been designed by a group knowledgeable in instructional design and educational research. Eleven students were interviewed individually after their completion of the General Chemistry program. A phenomenological approach was used for the reduction, analysis, and interpretation of data. This presentation discusses preliminary results.
First-Year Research Experience (FYRE) program: A gateway to undergraduate research and enhanced STEM development at the University of Oklahoma

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The First-Year Research Experience (FYRE) program promotes STEM undergraduate research at the University of Oklahoma (OU) through allowing first-year students to conduct semester-long, mentored primary research internships. The design of the FYRE program gives talented STEM-oriented students an immersive and perspective-building experience in research at the beginning of their college career. The FYRE students are expected to perform 10-12 hours of research per week in a laboratory matched to their scientific interests and to attend the bi-weekly FYRE Colloquia meetings. The FYRE Colloquia sessions allow the student to bond as a STEM learning community and to interact with STEM-research professionals, in order to gain perspective of research-oriented career paths. The 2015 FYRE semester will include 70 FYRE students performing research with 28 different OU research groups, spread over several academic departments. The evolution of FYRE to a campus-wide STEM research vehicle now allows first-year students from many different majors, including non-science majors, to gain valuable experience in laboratory research. A general-interest FYRE project designed as a gateway to laboratory research for non-science majors is the “Molecular Gastronomy of Coffee” project. This project emphasizes the application of molecular techniques to elucidate the chemical composition of flavor and is ideal in introducing freshmen students to bench-centered research. This project allows students as a group to investigate flavor aspects of coffee as a function of the storage time of roasted coffee beans, the degree of roast and brewing conditions. Technically, students learn extraction techniques and chemical identification using gas chromatography-mass spectrometry (GC-MS). Last year, the 6 students participating in this project were able to identify and quantitate variations in around forty diverse flavor components in coffee from different kinds of coffee beans. The students also designed and conducted research to test individual hypotheses related to the study of coffee. The retention of these students in STEM related studies will be followed. This project demonstrates a scalable program to engage students in meaningful research that can readily incorporate independent inquiry.

Guiding a senior undergraduate in chemical education and computational chemistry research

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During the 2014-2015 academic year, I have guided a talented undergraduate in a two-track research project. The student’s research focused on computational chemistry: both performing relevant calculations and developing educational tools for upper level physical chemistry courses. The one-on-one mentoring model has allowed me to help the student develop the skills and content knowledge necessary to achieve his goals and be a successful researcher. This mentoring model along with some results from the student’s research will be described.

CHED 1785

PRISM: CSUSB strengthening the scientific workforce

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The PRISM (Proactive Recruiting in Introductory Science and Engineering) project at CSUSB seeks to increase the number of well-prepared STEM graduates from our Hispanic Serving/Minority Institution. Vital partnerships between faculty in chemistry/biochemistry, computer science, geology, mathematics, and physics provide significant early research experiences for promising freshmen and sophomores that illustrate the central role of mathematics in all scientific endeavors. PRISM also provides scholars with preparation prior to, and active mentoring after their initial research experience. Two different Mentors in chemistry/biochemistry have supervised 26 students pursuing two different early research experiences, over the first four years of the program. Details about the two chemistry/biochemistry research projects, student successes during and following the PRISM research period in our department, and progress of the entire multidisciplinary project will be shared.

CHED 1786

Integrating undergraduate research with teaching and learning: Unanticipated opportunities to broaden participation

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The scientific community has voiced concerns about the lack of pedagogical training provided to graduate students, who, in general, have traditionally walked into undergraduate laboratory courses with no prior teaching experience. Many institutions have taken action to develop teaching assistant (TA) training programs for incoming graduate students, which they must attend before taking charge of their teaching duties. But is this the right time to start TA training? Is the preparation and experience as a TA sufficient to prepare a future professor? Based on studies indicating that early involvement in a community of practice results in early identification as a practitioner and deeper engagement with the practice, we decided to test whether starting informal
but targeted pedagogical training at the undergraduate level, simultaneously with engagement in undergraduate research, would have positive results. We developed a program whereby students conducted research in their mentors’ laboratories during one full academic year and designed lecture or laboratory modules based on their research topic and research results. The undergraduate fellows presented their modules in courses/labs taught by their mentors. Their teaching effectiveness and the module content were evaluated by students attending the courses. Our approach and outcomes based on specific program objectives will be presented along with an unexpected result and a prime opportunity: renewed enthusiasm of faculty mentors to develop new curriculum. When asked if they were interested in developing a general chemistry laboratory course that integrated their own research while fulfilling the learning objectives of the course, they agreed, proposed content for the course and proceeded to develop it. One pilot course in chemistry is being implemented for the first time at our university this academic year. Preliminary results of course implementation will also be presented.

CHED 1787

Freshman research immersion: Transforming freshman into researchers

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A central feature of the national initiative to transform undergraduate STEM education is that students have authentic research experiences earlier in their college years. Binghamton University has recently implemented a Freshman Research Immersion (FRI) program with three pilot research streams: Biofilms, Neuroscience, and Smart Energy. As preparation for research, students take a Research Methods course in their freshman fall semester. Thereafter, students conduct real research on specific problems pertaining to their chosen stream in their spring semester. Finally, during the fall of their sophomore year, students spend an entire semester continuing the authentic research from their freshman year. Throughout the FRI program, students receive course credit toward their degree. Each research stream has a dedicated lab, newly renovated and well equipped for carrying out leading research within that particular stream. Overseeing the daily work of students and teaching assistants within each research stream are research educators, who are PhD-trained within the specified stream. Here will discuss the overall program and specifically, the Smart Energy research stream provides students with interdisciplinary research experience in chemistry, physics and materials science. Students learn how to apply conceptual and technical knowledge to energy related real-world problems and research questions that span the areas of electrically conducting polymers, thin films, solar cells and LED’s, electrochemistry and batteries, semiconductor device physics and stoichiometry and disorder in metal oxides. Overall, our FRI program is unique because faculty research teams oversee each stream and
we emphasize interdisciplinary research, the way to address the biggest world problems.

CHED 1788

Research-based analytical chemistry laboratory: Incorporation of students' self-designed projects into curriculum

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In a typical chemistry instrumentation laboratory, students learn analytical techniques through a well-developed procedure. Such a widely used approach does not engage students in a creative endeavor. To intrinsically motivate students’ desire to learn and improve their problem-solving skills, students’ self-designed analytical projects are developed in the course of Advanced Chemical Methods for junior and senior undergraduates at SUNY College at Old Westbury. In addition to a series of manual-based laboratories held on a regular basis, students also do a literature search to formulate their own ideas that are tested using appropriate analytical instruments. By participating in self-designed projects, students independently go through the key components of analytical chemistry: from literature survey, problem identification, experimental design, sample preparation, measurements, results and discussion to conclusion, in a self-inquiry-based learning environment. Assessment of written reports and students’ self-evaluations indicate successful implementation of the projects and students’ progress toward goals mentioned above. This project provides students a research-based chemistry laboratory for self-inquiry-driven learning and independent thinking.

CHED 1789

Increasing reach: Dealing with resource limitations and scalability issues by bringing collaborative research into the teaching laboratory

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While numerous studies have shown the strong, positive pedagogic value of undergraduate research, limits on laboratory space, faculty time and other resources often place constraints on the ability to provide this experience to a large number of students. In order to at least partially address these interrelated set of problems, I have evolved the laboratory component of our Inorganic Chemistry course (taken by all chemistry majors as well as many minors) from a traditional "cookbook" experience to a collaborative research model. In this approach, students work collaboratively with each other and with the instructor on open ended projects drawn from the instructor's research agenda. This collaborative approach, which includes sharing of experimental tasks, pooling of data, and authentic writing and presentation experiences, mimics a
research laboratory environment and the dynamics of a research group while allowing for authentic reproducibility and authentication of data. In this presentation, I will outline the evolution of the laboratory curriculum in this course and discuss lessons learned along the way.

CHED 1790

Components of a research-rich undergraduate chemistry curriculum

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Many people recognize that participation in research is often one of the best learning experiences for undergraduate students. Students benefit by completing a research-rich curriculum. A research-rich curriculum has two general components to it. The first is that it provides time for undergraduate students to participate in research and get credit for that participation. Many chemistry departments now require or provide opportunities for undergraduate students to participate in research. Faculty members must embrace undergraduates as collaborators and engage students in summer projects. The second, and equally important component, is that the skills needed to succeed in a research project are developed throughout the curriculum. The general features of how one can design a curriculum to support research, as well as specific research-supportive components of the curriculum within my own courses and within the chemistry department at Bates College, will be described.

CHED 1791

Nanotechnology experiments for inorganic chemistry laboratory

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This presentation will highlight nanotechnology experiments in a junior level inorganic chemistry course and share suggestions for adoption at other institutions. The laboratory exercises include the synthesis of CdSe nanoparticles, magnetic ferrofluids, and mesoporous materials. An overview of the experiments, pertinent literature, and assessments will be presented. The synthesis of these materials does not require special equipment beyond what would be found in an upper level chemistry laboratory. The characterization includes general techniques such as UV-Vis and specialized techniques such as nitrogen physisorption. The mesoporous materials experiment may be of special interest to many, as it incorporates polymer chemistry topics.

CHED 1792

Synthesis and exploration of Au nanoparticles in an open-ended junior-level capstone lab
This one-semester capstone laboratory experience highlights nanoparticle systems by introducing students to the different parameters that affect the synthesis of nanoparticles and their characterization. Investigation into the size of the nanoparticle via UV-Vis spectroscopy, the stability of the nanoparticles via zeta-potential studies, in addition to investigating the binding between nanoparticles and substrates via isothermal titration calorimetry (ITC) occurs in multiple phases. For this laboratory exploration, students need to implement research-group-style of teamwork and organization to progress towards the goals of the entire project.

CHED 1793

Harnessing the power of partnerships and technology in nanoscience education

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The purpose of the NSF-funded NanoExperiences was to develop and evaluate an out of school time (OST) program combining academic learning in emerging STEM content with additional supports setting high expectations, building background knowledge, and motivating students to prepare high school Career and Technical Education (CTE) students for postsecondary learning and credentials leading to participation in the STEM workforce. To move toward accomplishing these goals, we involved local industries and academia in school visitations and also had students visit the local industries. Selected students were provided with internships at some of the local industrial and academic sites. The academic link provided hands-on experiences for the students using portable AFM and STM systems, either during class time or after school NanoExperiences meetings. Based on the evaluation report from the pilot test, most students found the Atomic Force Microscope (AFM) the most interesting part of NanoSurvey, and other students reported that learning about the “size of nano” was interesting. While students generally enjoyed all three components, the pilot data indicates that students were most impacted by the Nano@Work portion of the NanoExperiences. The students who were able to participate in the business partner experiences reported that “it was an important experience and provided them with a valuable view of how nanotechnology is being developed in the Denver region.” In this session, you will learn about how key partnerships were established and nurtured, a new online tool to guide students through job shadow experiences, and how portable AFM and STM experiences can be used to educate and motivate secondary students.

CHED 1794
Debating societal impacts of nanotechnology through role playing

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Students in an introductory nanotechnology course play the roles of characters facing ethical dilemmas in realistic but fictitious stories. Each story requires participants to consider the benefits and costs of using nanotechnology to solve problems that affect the individual characters and their community. Topics include increased video monitoring for campus safety, RFID chips in products to monitor shopping habits, and creating student jobs in a local high tech company with possible negative effects on the environment. Students research their roles prior to the debate and write a position paper outlining their character’s view and the student’s personal view. Audience members express their opinions of the issues also. Student feedback, their changes in attitude about nanotechnology, and the ethical frameworks employed by students will be presented.

CHED 1795

Synthesis and comparative study of ZnO/Au, ZnO/Ag, MgO/Au, and MgO/Ag core-shell nanoparticles with their functionalization with antibiotics

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Core-shell nanoparticles are significant due to their highly functional applications in modifying antibiotic properties. This work focuses on the development of a simple strategy to produce ZnO/Au, ZnO/Ag, MgO/Au and MgO/Ag core-shell nanoparticles. For the gold shell formation we used HAuCl₄·3H₂O and AgNO₃ for the silver shell formation. Optical properties and characterization of the core-shell was performed by using UV-Vis absorption Spectroscopy and Diffracted Light Scattering (DLS). The size of the ZnO nanoparticles was 35nm, and the core-shell obtained was 270nm for ZnO/Au and 285nm for ZnO/Ag. The size of the MgO nanoparticles was 68nm, and the core-shell obtained was 261nm for MgO/Au and 278nm for the MgO/Ag. Vancomycin and Penicillin antibiotics were used for interaction with core-shell nanoparticles. UV-Vis analysis showed new peaks formation between 275nm to 300nm. Subsequent additions of 20µl up to 180µl total of antibiotics had an increase uptake. Red shift in the 275 nm band absorption occurred for 200-420µl additions; where the peak became sharpened. DLS analysis showed a good polydispersity index indicating uniformity of the sample.

CHED 1796

Investigating the antimicrobial properties of silver nanoparticles with respect to Desulfovibrio genus bacteria
This paper will demonstrate the synthesis of highly mono-dispersed silver nanoparticles in aqueous phase and attempt to quantify the magnitude of the antimicrobial effects of said particles. We show that synthesizing the nanoparticles from a precursor of silver hydroxide has advantages over the more commonly used method of synthesizing directly from silver nitrate, particularly the ability to create a mono-dispersed particle with controlled sizes that are considerably larger than those reported from other synthesis techniques. The precursor molecules are created using sodium hydroxide to provide a reaction pathway for silver hydroxide species to form from aqueous silver nitrate. The resulting silver hydroxide is subsequently reduced with sodium acrylate which also acts simultaneously as a capping agent for the aggregating nanoparticles. We characterize the resulting particles through the use of ultraviolet-visible spectroscopy (UV-Vis), X-Ray diffraction (XRD), and transmission electron microscopy (TEM); particles may also be sent to other facilities for more detailed characterization using high-resolution transmission electron microscopy (HRTEM). The current results from characterization suggest that the synthesized particles are relatively mono-dispersed and preliminary data suggests a controlled size of approximately 20 nm. Desulfovibrio bacterial growth inhibition assays using these particles will be performed with a 1249 modified Baars’ medium for sulfate reducers; this phase of the experiment has yet to be completed but preliminary particle characterization data suggests a morphology that has been shown by other researchers to possess strong antimicrobial properties.

CHED 1797

Computational chemistry should start in high school

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The computational sciences as a method of doing science is now well-established, just as are observational, experimental, and theoretical methods. Just as high school students learn and do chemistry at the lab bench, so should they learn the technologies, techniques, and tools of computational chemistry "in silico". At the North Carolina School of Science and Mathematics (NCSSM), a state supported residential school for students with a strong interest in those disciplines, we offer a full semester course in computational chemistry, using tools like Gaussian and MOPAC with the WebMO interface. In this course, students learn foundational mathematics, run calculations on a wide variety of chemical systems, and otherwise get a full program instruction in computational chemistry. The course concludes with the students proposing and implementing a small research problem in computational chemistry, with results communicated using the Journal of Computational Chemistry format.
Computational chemistry throughout the curriculum

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The Chemistry Department at Lock Haven University has been steadily increasing the use of molecular visualization and computation throughout its curriculum. Molecular visualization and computation is used to explore and enhance student understanding of topics such as molecular polarity, electronic structure, the relationship between VSEPR and molecular orbital models, and the origin and interpretation of infrared spectra. Examples from multiple levels of the curriculum will be presented, from non-major, liberal arts courses as well as general and organic chemistry using a variety of software including Jmol, WebMO, and Chem3D Ultra.

Additionally, an upper level elective course for chemistry, biology, and biology/chemistry students, "Introduction to computational chemistry", has been added to our rotation. This course explores a range of computational techniques via a connected set of activities focused on predicting the heat of formation of various compounds. Leveraging a concept the students are comfortable with and have used in previous courses has been a successful design decision for this upper level course.

CHED 1799

Computational modelling across the curriculum: General, organic and physical chemistry

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Chemical modeling is an important branch of chemistry that is critical to the prediction and interpretation of experimental results. As such, we have incorporated computational modeling across the curriculum with experiments in General Chemistry I, Organic Chemistry I Laboratory, and Physical Chemistry. In general chemistry the students explore periodic trends in bond length and bond angles for small molecules using ab initio calculations. In organic chemistry, the students calculate the energy difference between the axial and equatorial orientation of increasingly branched alkyl groups, and observe the overall trend. They also generate a conformational analysis diagram for different molecules and compare these calculations to that presented in class. In
physical chemistry students learn the basic terminology associated with modern ab initio calculations and compute various properties associated with common physical chemistry laboratory experiments, such as the vibrational frequency of HCl, and the enthalpy of formation of benzoic acid. In addition, physical chemistry students conduct a group project that incorporates both experimental and computational work, and present their final product in the form of a poster.

CHED 1800

Computational chemistry in an undergraduate curriculum: Strategies for deliverable skills

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Computational chemistry in an integral part of a modern undergraduate chemistry curriculum, providing tools and resources for students to better understand concepts learned in lecture and complementing benchtop experiments. By the end of their undergraduate education, students should be able to build molecules in one of the common computational programs, determine the type of calculation to perform, choose an appropriate level of theory and basis set, and obtain useful chemical information from their calculation. One approach would be to offer computational chemistry as an elective, but not all students would take the course, and as chemistry becomes increasingly interdisciplinary, all chemistry majors would benefit from having more computational chemistry. At Stevenson University, computational chemistry has been incorporated into all four years of the undergraduate curriculum, beginning with the first semester of general chemistry up through physical and inorganic chemistry. This approach was chosen for two reasons: 1) Students need to practice techniques multiple times to master those skills and 2) One or two activities are insufficient to expose students to enough theories, basis sets, and types of problems for them to have a strong foundation in computational chemistry. Currently there are thirteen experiments, spread throughout the curriculum, that use computational chemistry in some form. Some are standalone experiments; others use computational chemistry as a compliment to a benchtop experiment. The activities have been designed to build upon skills leaned in earlier activities and to fit into the broader goals of the computational curriculum.

CHED 1801

Examples of instructional units in computation and modeling for the undergraduate chemistry curriculum

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We have been working on inquiry based computational activities for the undergraduate chemistry curricula and group laboratory investigations that utilize 3-D visualization. Our goal is to develop a series of modules incorporating computational chemistry and modeling for use through the chemistry curriculum. These modules focus on core concepts and are intentionally designed to successively build in complexity. The modules are interactive, encouraging active inquiry and team based problem solving. Our initial efforts have focused on activities for the organic and inorganic courses. This presentation will focus on the development and implementation of activities that address polymer stereoregularity and solid state structures, as well as a discussion how to incorporate research data and examine more open ended questions of structure and activity using the skills developed in earlier activities.

CHED 1802

20 years of computational chemistry at a public regional university: Thoughts and experiences

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Over the past twenty years, we have incorporated computational molecular modeling into the organic chemistry curriculum through the use of exercises that students complete individually outside of class time. The challenges have always been the availability of appropriate exercises and the accessibility of computational software. Recently, we have been working to make these activities inquiry based and have included group laboratory investigations that utilize 3-D visualization. Students have responded to these with overwhelming enthusiasm and, more importantly, with a much clearer understanding of the problem posed and the answer obtained. This presentation will include an overview of our experiences, materials available, thoughts on where and how to incorporate computational activities into the curriculum, and student attitudes toward the activities.

CHED 1803

Computational chemistry: Practical issues in leveraging the Cloud

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The wide availability of computational chemistry software is bringing molecular modeling into the classroom more and more. However, any non-trivial calculations require high performance computing (HPC) platforms, which are costly to purchase and maintain. Cloud computing vendors, such as Amazon and Google, tout their HPC platforms as alternatives to in-house data centers with a variety of benefits including costs savings.
and (theoretically) infinitely expandable capacity. Our research shows that, under certain circumstances, these claims hold merit (see Figure); certain categories of computations -- in the right environment -- are less costly to complete using cloud computers and can take significantly less time. However, there are practical issues that must be faced by instructors in setting up a virtual computational chemistry lab "in the cloud." Such issues include software installation, provisioning of computing resources, management of student logins, etc. This presentation will provide empirical data for deciding when computational chemistry in the cloud makes financial sense and will discuss techniques for managing the practical issues involved.

![Graph showing EOM-CCSD/d-aug-cc-pVDZ costs](image)

**CHED 1804**

**PSI4Education: Computational chemistry labs using free software**

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Computational chemistry is an increasingly important part of modern research, and, yet, it is often not part of the typical undergraduate or graduate curriculum. Fortunately, the availability of free software like PSI4 and WebMO lowers the barrier to introducing computational chemistry laboratory modules. The PSI4Education project is a consortium of individuals who create, use, and share laboratory exercises across the disciplines of chemistry utilizing only free software. The current usage, implementation, and success of the existing labs will be discussed along with mention of installation for the requisite free programs PSI4 and WebMO as well as an appeal for additional collaboration, usage, and contribution.

CHED 1805

Challenges and rewards of the computational chemistry undergraduate thesis project

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Experiences associated with students completing an undergraduate computational chemistry research project will be discussed. While many components of the undergraduate thesis process are common to all projects, there are unique challenges and benefits particular to those thesis projects that are computational in nature. Some of the primary challenges include introducing computational chemistry in the laboratory curriculum, developing appropriate computational skills throughout all levels in the curriculum, generating interest in computational projects among students, finding appropriate computational resources and communicating results to colleagues. Some of the benefits include increased flexibility and lower overall financial cost compared to experimental projects. Aspects of the curriculum that support the introduction and development of computational skills will be presented. Outcomes from a variety of projects that use ab initio software packages and those that involve Monte Carlo modeling will be compared. In addition, strategies for introducing students to computational techniques and mentoring them in their projects will be presented. The assessment of undergraduate projects and the unique challenges associated with computational projects in this regard will also be discussed.

CHED 1806

NCSI workshops are ready to help train faculty to use computational chemistry in the classroom
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The National Computational Science Institute (NCSI) offers a variety of workshops that teach faculty members new skills in computational science. Faculty participants then use these skills to enhance the courses they teach and to perhaps develop new courses. The week-long chemistry workshops have focused on molecular modeling, visualization, and simulation using free or low-cost software. The effectiveness of these workshops will be presented using data from pre- and post-workshop surveys. Longer range assessment is based on the classroom materials that participants have developed for their courses, new courses that have been created, presentations by faculty at professional meetings, and peer-reviewed articles that have been submitted. Other methods to measure the impact of future workshops will also be discussed.

CHED 1807

**Building connections in biology and chemistry courses in the second year curriculum**

**Stephen R. Sieck**, sieckste@grinnell.edu. Grinnell College, Grinnell, Iowa, United States

Over the course of the past decade faculty members of both the biology and chemistry departments of Grinnell College have been intentionally building connections between the organic chemistry and biology course students take. A majority (>80%) of students enrolled in organic chemistry are also co-enrolled in a 200 level biology course called Molecules, Cells, and Organisms during their second year. In attempt to showcase the interdisciplinary nature of these sciences we have developed a number of shared resources, problem sets, conceptual modules, and exam questions that are appropriate for use in both the Organic Chemistry and Molecules, Cells, and Organisms courses. Many of the activities are specifically directed at helping students develop skills that enable them to address complex problems requiring multi-disciplinary approaches, and working in a community. We will discuss how we have designed, coordinated, and evaluate the enhancements to the curriculum we have implemented of the last ten years. In particular, we will discuss how we have developed and continue to maintain interdepartmental collaborations to make these activities possible.

CHED 1808

**Chemical analysis of paint: Development of multidisciplinary class sessions for chemistry and art students**
The development of multidisciplinary class sessions to teach chemistry and art students about the chemical analysis of paint will be presented. Students performed spectrophotometry experiments to understand color theory with mixing of watercolor paints. X-ray diffraction (XRD) of cadmium yellow and cadmium red pigments was used to teach about structural identification and tuning of colors via solid solutions. In this example, students learned about the selenium replacement of sulfur to form cadmium red from cadmium yellow. Additionally, XRD was used to demonstrate how oil and acrylic-based paints are often pigmented with organic dyes and have a similar base materials such as calcite ($\text{CaCO}_3$). Attenuated total reflectance-Fourier transform infrared spectroscopy was utilized to analyze paint binders and distinguish between egg-based and oil-based mediums. Other experiments for paint analysis will also be presented. We found that teaming art and chemistry students together for this project was a great benefit to each group of students. The chemistry students enjoyed using instrumentation to analyze materials that were unique to them, while helping art majors learn about the chemical composition of their paints.

CHED 1809

Interdisciplinary experimental approach for undergraduate chemistry students

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Nowadays interdisciplinary teaching and research are strong and important aspects requested for solving complex issues. In this context, individual disciplines are not adequately equipped to address all facets of a multifaceted problem. An interdisciplinary approach in courses and programs may help in facilitating or enhancing the transfer of higher-order cognitive skills (HOCS) such as: critical thinking, problem solving, decision making and laboratory practice. We presente a systematic integration of three undergraduate chemistry courses: Chemistry of Natural Products (CNP), Organic Chemistry Laboratory 2 (OCL2), and Analytical Chemistry Laboratory 1 (ACL1). By choosing a central topic we prepared a series of activities focused in interdisciplinary interaction and the development of students’ HOCS.

Three working groups were formed, each of which had one CNP student, two ACL1 students and four OCL2 students. The CNP students (mentors) were responsible for their groups, since they were the most advanced students. Specific activities were carried out around the common topic previously chosen, which was: acid-base indicators. Specific tasks were assigned: isolation and characterization of natural dyes, synthesis and characterization of phenolphthalein and application of both the natural and synthetic indicators in the titration of natural juices derived from regional fruits. The
students showed great interest and willingness to work in groups. The work dynamics was enriching provided the opportunity to confront different areas of knowledge. Throughout the experimental work, the three groups worked in harmony, integrating the isolation, synthesis, structural characterization and analytical application around a central topic in Chemistry. When students of different semesters interacted, those more advanced had to explain more clearly the concepts learned, and at the same time the newer students handled basic concepts more clearly and helped in the discussion of the results. This strategy potentiated collaborative learning, critical thought and problem solving, in short. The application of this multidisciplinary work strategy dealing with a central topic in Chemistry from the perspective of different areas, strengthened collaboration among teachers and made it possible for the students to learn in a significant way, it favors collaborative learning and generates an holistic view of Chemistry.

CHED 1810

Flipped classroom for large organic chemistry class

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After implementing clicker questions and online homework for a year in my large organic chemistry class of 200 students, I flipped the classroom. Students watch short video clips and take notes before they come to class. There is no formal lecture in class. Students do clicker problems and other in-class activities with ample time to ask questions and discuss different approaches to solve problems. Online homework is another way for them to get immediate feedback. As a result, students will be exposed to the same concept at least four to five times during their study, and they can study at any time and any place they feel comfortable with. The flipped classroom works very well for my large organic chemistry class.

CHED 1811

Half flipped: Using videos and online quizzes to maximize in class problem solving time

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A hybrid approach to the traditional lecture format and the newer flipped classroom pedagogy has been launched in the Organic Chemistry I and II lecture sequences as well as our Intermediate Organic Chemistry Course, which is a one semester short course. Short video lectures ranging from five to twelve minutes have been utilized to provide more in class time to work with students on problem solving skills. Each chapter includes two to five short videos, accompanied by an online quiz to be taken before class begins. The students may use their notes, the book, or the video to take the quiz,
but must work alone. This arrangement is designed to allow for roughly twenty five minutes of lecture and twenty five minutes (or more) of problem solving time for each class period. Preliminary results, including class participation, challenges, grade distribution and student feedback regarding the “half-flipped” model will be discussed.

CHED 1812

Flipping general chemistry to improve student success

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At Shippensburg University the DFW rate for General Chemistry I and II has averaged near 55% for the past 5 years. As a department we are attempting to address the issue. One approach has been to flip (or invert) my sections of General Chemistry I and II. In the traditional lecture format, students often lacked problem solving skills and were frequently unprepared for the class period (i.e. they did not read the textbook). Now video lectures are posted online that cover both chemistry concepts and problem solving strategies. Students are expected to bring notes from the video lectures to class, and class time is devoted to developing problem solving skills. While in class students work in small groups and typically use their notes to aid them on the in-class assignments. Students actively discuss the best approach to a problem and typically work together through difficult concepts. Several foreseeable outcomes have been observed such as the ability for students to review lecture material as much as they desire, an increase in student preparedness for class periods, the ability for the instructor to provide “real-time” feedback to the students, and an increase in student problem solving ability. In addition, other unexpected outcomes have been observed such as an increase student efficiency when taking exams, opportunities to write exams with more in-depth problems, and students wishing to view the General Chemistry II video lectures when taking the course with a different professor. In the flipped class sections, student grades have dramatically improved during the past two years (15% increase in the average score), and the DFW rates have fallen to 14%. This session will provide an overview of the flipped program at Shippensburg University and provide information on how to invert a class, technology options, best practices, and potential problems.

CHED 1813

Unit Conversion Literacy Project: A partnership model for driving curricular change

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Medication administration errors, especially incorrect dosage, are prevalent in the public health professions. Although the causes of such errors are debated, there is compelling precedent that dosage errors arise from difficulty conceptualizing and/or performing the
required calculation, and that such errors increase when the medication is administered as a solution (i.e. injection, IV drip or flow). Various web sites, such as rxlist.com or drugs.com, provide extensive dosage and administration data for many drug and nutrient solutions. A review of these data suggests that calculating a correct dosage is fundamentally a general chemistry problem; more specifically, a unit conversion problem that relies on a few fundamental concepts common to both secondary and post-secondary general chemistry curricula. To assess proficiency in these areas, we developed a series of “real world” dosage problems around unit conversions that were given to junior and senior NIU students in our Health and Human Sciences (HHS) and Liberal Arts and Sciences (LAS) Colleges. All students had some level of general chemistry on their transcripts. A greater than 50% incorrect response rate was observed across all disciplines examined due to errors that replicated those reported in the public health sector. Median error rates were statistically correlated with the general chemistry background of the student (i.e. general chemistry for non-science vs. science majors). These outcomes suggest that unit conversion literacy, arguably one of the most important conceptual areas of general chemistry, is not emphasized across programs of study for which general chemistry is a pre-requisite. An IRB protocol number was obtained (HS14-0130) to launch a more formal study of this issue by establishing interdisciplinary partners that are willing to create an integrated curricular model across programs and levels (secondary and post-secondary) for articulating unit conversion skills essential in the public health sector. The data, partnership model, and curricular integration framework will be presented.

CHED 1814

Engaging science students and the public through science-themed art

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This presentation will review one way in which chemistry teachers and other science educators can engage their students, and the public, through the visual arts. As the principal example, a series of oil paintings illustrating the history of organic chemistry was prepared and used in both classroom and art gallery settings. In the classroom, the paintings function as an image bank for portraits of notable chemists, significant molecules, reactions schemes, and a number of chemical diagrams, names, and formulae. The paintings also function well in lecture as motivational items with which to begin a lecture or to provide some historical context in a visually rich way. Both in and out of the classroom, these paintings can serve as access points for viewer reflection and departure points for discussions on the complex interactions of history, science, psychology, and culture. Anecdotal evidence indicates that this approach is particularly valuable for engaging the public in conversations about chemistry, science, and society.
A portrait of Charles Gerhardt and August Laurent, two French organic chemists of the mid-19th century. Their “Type Theory” revolutionized organic chemistry and made it possible for chemists to begin making predictions about chemical reactions based on the structure, or type, of compound involved.
Emil Fischer was a pioneering chemist who performed remarkable work on the synthesis and structure of carbohydrates. His ultimate triumph in this research, the so-called “Proof of Glucose”, won him wide praise and the Nobel Prize in 1902.

CHED 1815

Sophomore organic chemistry to synthesize that?

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Heterocyclic compounds are often given little treatment in the two-semester sophomore-level course. They are mentioned in the discussion of aromaticity and the use of N-heterocycles as organic bases. Many compounds exhibiting biological activity or prepared as potential drug candidates are heterocycles. Several of the synthetic routes to these compounds involve reaction types that are typically covered in the sophomore course. In this presentation, examples of reactions and reaction types familiar to undergraduates will be applied to the preparation of heterocyclic systems. This approach allows instructors to demonstrate the application of course material to solving real world synthesis problems and emphasizes basics or mechanistic organic chemistry.

CHED 1816

Capstone experience for the sophomore organic chemistry sequence emphasizing written and oral expression

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Students in second-semester organic chemistry participate in small-group, semester-long projects that utilize knowledge from the entire year-long sequence. Target molecules are chosen in consultation with the professor and students are asked to present background information and a multi-step synthesis leading to the target. A written paper, Powerpoint presentation, and scientific poster are required elements. Students gain experience in these three major forms of scientific dissemination, as well as bibliographic software, chemical drawing software, and scientific databases.

CHED 1817

Exploring DNA and protein structures with PyMOL

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A series of laboratory exercises using the open source molecular visualization software PyMOL were developed for students to investigate the structure of DNA and proteins in a two-semester biochemistry course. The \textit{in silico} labs have been developed and carried out during the past four years, and replace traditional wet labs twice each semester. The students are typically highly engaged in the PyMOL exercises, and report a deeper understanding of the structure-function relationships of the molecules studied. Several exercises incorporate reading and interpreting portions of the primary literature associated with these structures. The first PyMOL exercise serves as the initial introduction of the 3-dimensional structure of DNA for the course. The exercise focuses on the structure of a B-type DNA dodecamer (PDB ID 1BNA), and contrasts the structure with one containing a Watson-Crick mispair (PDB ID 1D80). The second PyMOL exercise introduces students to the primary, secondary, tertiary and quaternary structure of proteins using a recent structure of hemagglutinin from the 2009 H1N1 influenza virus (PDB ID 3LGZ). The third exercise explores transport of iron, via the siderophore enterobactin, through the $\beta$-barrel integral membrane protein, FepA, in \textit{E. coli} (PDB ID 1FEP). Finally, the fourth exercise explores the unit cell and crystal packing of Hen Egg White Lysozyme (PDB ID 1LPI), which prepares students to grow protein crystals of lysozyme the subsequent week in lab. Throughout the four exercises students improve their ability to manipulate, measure, and explore the crystal structures, and become familiar with availability of crystal structures the Protein Data Bank.

CHED 1818

Teaching general chemistry in context using the ChemConnections Activity Workbook

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What causes climate change? How does acid rain affect the environment? What is the food vs. fuel debate? This session will discuss how the ChemConnections Activity Workbook can be used to infuse thematic programing into the general chemistry curriculum. Composed of 59 classroom-tested activities and laboratories written in the context of societal and environmental issues, the ChemConnections Activity Workbook provides instructors a flexible platform to create thematic programing that not only reinforces general chemistry content, but also allows students to directly see how chemistry relates to the environment, technology, and nutrition. Additionally, the activities are designed with attention to student learning styles and pedagogy, allowing instructors to engage students through a range of activity types including data analysis, laboratory, guided inquiry, and discovery. Examples of thematic programing will be provided on such topics as climate change and renewable energy.

CHED 1819
Demonstrating the intelligence capabilities of the Q-electronic tutor

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With high growth in e-learning technologies Instructors at schools and universities are asked to add more duties to their teaching efforts. With the flood of information and operational activities e-learning demands from instructors a head start over students. On this regard, the Q-Electronic tutor with advanced ITS capabilities can moderate instructor’s effort while at the same time makes student and machine interaction an exciting experience. Problems from selected topics in General Chemistry will be processed using MS Visual Studio Express programming platform to demonstrate the intelligence capabilities of the Q-Electronic Tutor programs.

CHED 1820

Polycraft: Utilizing online gaming to enable next generation polymer chemistry education

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The United States is, sadly, falling behind the rest of the world in math and science education. In order to combat this trend, innovative methodologies must be sought to supplement or replace traditional classroom experiences. These experiences often frustrate or disengage students; however, students are often easily engaged through games. Indeed, child psychologists tell us that infants and young children learn the most about their world through play. Therefore, the introduction of academic concepts and subjects into games is an effectual way to expand a student’s understanding and learning.

Today, many students, from middle school to college, engage in the online world of Minecraft (almost 17,000,000 copies sold worldwide). Minecraft enables the player to create a virtual 3D world out of blocks and reshapе their world at will. This presents an excellent opportunity to incorporate the concepts of chemistry (including polymer and materials chemistry) into this world and teach students. To this end we have developed a mod for Minecraft called Polycraft.

Essentially, Polycraft incorporates the ideas of organic and polymer chemistry into the world of Minecraft enabling players to gather raw minerals (for catalysts) as well as crude oil, refine that oil, crack it, use the different streams to make monomers, use those monomers to make polymers, form those polymers into materials and use those materials to make things in the game.
Figure 1. A screenshot from Polycraft. Distillation and refinery instruments are shown against the walls of the building.

CHED 1821

Teaching and learning with a tablet

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Two methods are currently being employed at Kean University to use tablets to teach. Dr. Matthew Mongelli uses an Android based tablet as enhanced PowerPoint for General Chemistry and Analytical Chemistry Classes and Dr. Heather Stokes-Huby uses an iPad as a board replacement in her Organic Chemistry classroom. Drs. Mongelli and Stokes-Huby are going to give an overview of how they are using a tablet in the classroom and what they have learned from setting up tablet teaching classrooms. This will include apps that are useful and student feedback on the methods being used.

CHED 1822

Incorporating peer-review homework assignments into a large enrollment freshman chemistry course

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Homework assignments serve to provide students with additional practice aimed at promoting problem solving abilities. In general chemistry, a common theme is assigning homework using online homework-management systems. Such systems can promote a richer understanding by allowing students to pinpoint deficiencies from immediate feedback, but students' strategies are not specifically analyzed as with traditional paper-based assignments. Furthermore, online systems are often limited in the types of
responses that can be accepted and graded. At Stanford, we have taken a different approach for homework by creating a system that provides a quick turnaround while providing flexibility in the construction of the homework, as well as, providing students feedback regarding their problem solving approaches. Homework is administered through a cycle, which always consists of weekly peer-reviewed feedback. The peer-review component has two purposes: (1.) provide the students completing homework with detailed explanations of the correctness of their approach, and (2.) provide peer-reviewers an opportunity to review other problem solving strategies. By reviewing other students’ strategies, peer reviewers gain greater insight into problem solving. This presentation will discuss the design of peer-review homework, the implementation, and the results obtained in a large-enrollment class. This presentation will outline the process we utilized and the feedback we have received from students.

CHED 1823

Student designed organic laboratories as an alternative research project

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Student-centered research projects at the undergraduate level are excellent exercises to help students gain real experiences in developing experiments and solving problems in the laboratory before entering the real world. Teaching laboratory development can provide an alternative method for gaining these experiences in a form that may be more attractive to students seeking non-traditional career paths. Furthermore, the design of labs in concert with students helps to directly identify methods to actively engage student learning. Presented is a discussion of a student-designed laboratory procedure carried out as part of a senior capstone experience under faculty supervision. The development, implementation, and analysis of the project will be highlighted, along with key issues that arose during the process.

CHED 1824

Designing accessible interactive chemistry simulations for all students – including students with disabilities

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Currently, a significant disparity exists between science achievement by students with and without disabilities. Students with disabilities often have reduced opportunities for experimental learning – a foundational component of high-quality science education, while teachers can find adapting science materials to students’ needs challenging. Calls for increased student success in science have resulted in recent innovations, such as interactive science simulations, but to date much of the progress in science education
has not been made accessible to students with disabilities.

Recently, the PhET Interactive Simulations project (http://phet.colorado.edu) has begun the process of designing inclusive features for our new suite of HTML5 simulations. With 130+ mathematics and science simulations, including over 30 chemistry simulations – the PhET project aims to ensure that all students have access to these open educational resources. Inclusive features include: keyboard navigation, increased support for adaptive technologies, textual descriptions, and sonification. These features will allow students to engage with the simulations in multiple modes, with visual, sonic, and textual representations available along with expanded options for input and output methods (keyboard, screen readers, etc.). These inclusive features have the potential of increasing the effectiveness of simulations for all students, including those with disabilities. In this presentation, we share our progress in inclusively designed PhET simulations, prototype inclusive features, and show examples from preliminary student interviews of inclusive simulation use.

CHED 1825

Perceptions of competency for male and female chemistry majors: Does he receive more credit?

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Since the 1980’s, women earning Ph.D.’s in chemistry has grown from 25% to 37%. However, these numbers are not reflected in the number of women who hold Associate and Full professor positions. There are many explanations for this: from women’s choices, job flexibility and family responsibility, to discrimination. And while family responsibilities and women’s choices do play a role, those issues may be influenced by subtle forms of discrimination. In many STEM fields, women may find the deck is stacked against them. Previous studies have found that women must show more intelligence and competency for equal recognition. If they make a mistake, they will pay a greater penalty. To assess if these perceptions are true among today’s undergraduate students, two videos were produced using a male and female chemistry major in which they performed a simple solubility experiment. In one video, the male appears more competent and the female takes a follower role. In the other video, the script and behavior of each student is reversed. Videos of these experiments were shown to students across campus followed by a brief survey assessing perceptions of their competency, intelligence and capability in the field. Statistical analyses were used to examine differences in the benefit men receive when performing well compared to women and the penalty women pay when performing poorly compared to men.

CHED 1826

**Guided inquiry laboratory experiment water analysis and hands-on experience for K-12 students in the Advancing Mathematics and Science Skills Program**
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A selected guided inquiry laboratory experiment (GILE) involving a water quality analysis as a part of Department of Chemistry and North Carolina A&T State University Summer Advancing Mathematics and Science Skills Program (AMASS) program was conducted for K-12 students in order to motivate K-12 students in STEM. The overarching goal of the AMASS program is to increase the production of high achieving students who will pursue careers and increase diversity in the STEM workforce. The AMASS program also served as an avenue to train and to provide hands-on experiences in Biology, Chemistry and Physics. In the Chemistry component, students were trained on laboratory safety, the use of common laboratory apparatus, analytical techniques, and instrumentation for the K-12 students. Mini-seminars on general global water resource distributions, water utility, water quality parameters (chemical and biological), and water contamination were presented to the participants to create global water resources conservation awareness prior to laboratory activity. The students subsequently worked in groups to determine the water quality parameters, including the water pH, conductivity, water resistance, suspended solids, and total dissolved solids of a tap and lake water in Greensboro metropolis. Each team gave a post-laboratory data analysis and discussion of the results of their water analysis. A post-laboratory discussion and survey questionnaire was administered to the participants to evaluate their experiences in water analysis. The outcome of the discussions and the result of the analysis of survey questionnaire revealed that most participants found this hands-on GILE water analysis to be motivating and exciting. The result of the water quality analysis and the students’ experience in the Chemistry component of the AMASS program will be presented.

CHED 1827

Collaboration between historically black colleges and universities and local school districts to promote K–12 science education, North Carolina, USA

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A continued decline in the global ranking of U.S. students in science, reading, and mathematics is very troubling and is a wakeup call for concerted efforts by all major education stakeholders to strengthen K-12 science education. Studies have also demonstrated distinct advantages of active learning and the use of hands-on experience pedagogies for promoting student learning and critical thinking skills. However, the utility of active learning pedagogy and hands-on learning experiences in science education and provision of professional development programs for K-12
science educators is very limited in many K-12 school districts. Herein, the outcome of a collaboration between two Historically Black College Universities (HBCUs), North Carolina A&T State University Department of Chemistry and Winston-Salem State University Center for Mathematics, Science, and Technology Education, to offer an Active Learning Professional Development Program (ALPDP) workshop for targeted K-12 science educators in school districts in the state of North Carolina, USA is reported. A guided-inquiry-laboratory experiment (GILE) involving the determination of iron (Fe) content of selected vitamin food supplements using a UV-visible spectrophotometer was also conducted for the participants to provide hands-on experiences for science educators in the use of modern analytical techniques and instrumentation. The results of the determined Fe (mg) favorably compared with the actual Fe (mg) in the food supplements as demonstrated by the low relative errors of the sample analysis. Results of the workshop questionnaire analysis indicated that the majority (85%) of the participants believed that some aspects of the active learning pedagogy, demonstrations, and hands-on laboratory experiences gained from the workshop can be modified, adapted, incorporated, and implemented in their K-12 science education curriculum. Also, all of the participants (100%) found this workshop beneficial to their professional development. The experience gained in this workshop also motivated the participants to participate in future K-12 science educators’ professional development program workshops. The collaboration between the STEM faculty members from the HBCUs has also led to the provision of other necessary resources and facilities for local school districts in order to promote science education.

CHED 1828

Quantitative approach to the study of the effectiveness of using the Dual Credit General Chemistry I Program at Missouri Western State University as a recruiting tool

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The Dual Credit General Chemistry I course at Missouri Western State University has delivered a rigorous experience to well over 2000 high school students in northwest and north central Missouri for over 14 years. The enrollment is now averaging about 200 students per year, with more dual credit students than on-campus students completing the course in a given academic year. The year-long course is facilitated by trained high school teachers at the high school, while the MWSU faculty course coordinator serves as the instructor of record. The coordinator visits each classroom in the fall and in the spring, and students complete four laboratory exercises during two lab visits per year (of the fourteen total in the course). Delivery of the course is an important means of outreach by MWSU to the high schools, and an important recruiting tool for the department and university. Our current study is one piece of a multi-faceted approach to gather data on the effectiveness of the course through student and teacher surveys and collection of institutional data. In this presentation, we will discuss the results of our
recent institutional data collection efforts, addressing the matriculation rate to MWSU of General Chemistry I dual credit students, their persistence to graduation, which majors they are selecting, and a comparison of their success relative to that of on-campus students in on-campus chemistry courses through their second year. We will also compare the success of students in the dual credit General Chemistry I course relative to the on-campus course, based on course grade. We will then present our conclusions on how a deeper understanding of this data will assist us in planning for the future of the course and in improving our strategy for recruitment of high-ability students to MWSU.

CHED 1829

Electrolytic reactions of reagent precursors for preparation and standardization of commonly used reagents in an undergraduate laboratory

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A guide for instructors and laboratory assistants for preparing some common aqueous reagents used in an undergraduate laboratory will be presented. Dilute reagents consisting of $\text{H}^+(aq)$, $\text{I}_3^-(aq)$, $\text{Ce}^{4+}(aq)$, and $\text{Ag}^+(aq)$ were prepared by electrolytic oxidation of respective precursors. Electrolysis was promptly stopped when potassium hydrogen phthalate (KHP) was completely neutralized by $\text{OH}^-(aq)$ resulting from an electrolytic reduction of water in the cathode compartment. The amount of reagent produced at the anode was determined from the mass of KHP added to the cathode compartment. The concentration of reagents produced at the anode was independently confirmed by a volumetric titration. The electrolysis cell was directly powered by 18 V DC power supply eliminating the requirement of a coulometer.

CHED 1830

Towards increasing student engagement in the general chemistry laboratory with environmental research

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There has been a push in higher education to integrate research experiences into the undergraduate curriculum. Literature suggests that inclusion of authentic research activities in undergraduate STEM courses results in increases in understanding of content, retention in the field, and improved attitudes, critical-thinking skills, and self-efficacy. We have developed a collaborative network between three institutions in order to study the effects of embedded environmental research activities in biology and chemistry courses at several levels. This presentation focuses on a new research-
based lab for general chemistry recently implemented at Central Michigan University. Our group has developed a laboratory activity for general chemistry that introduces students to concepts in the context of current environmental research on the socio-scientific issue of hydraulic fracturing. The environmental research project seeks to evaluate the impacts of hydraulic fracturing and monitor the health of local water supplies over time. Students engage in cognitively-demanding processes such as experimental design, making judgments about data reliability, and construction of scientific arguments and explanations. Students collect and analyze data to contribute to an on-going database of water and soil quality in the local community. The activity was piloted at Central Michigan University in Summer 2014 with a group of 48 students, and then implemented full-scale with approximately 660 students in Fall 2014. Student impacts were assessed by administering surveys in a pre-test/post-test, control/experimental design. Preliminary observations and results on student impacts from the implementations this year will be discussed in this oral presentation.

CHED 1831

Utilizing 3D printing to create demonstrative models for freshman chemistry courses

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Representing complex chemical structures and phenomena is a challenge that has plagued chemistry teachers for years. Drawing chemical structures on a board and using molecular model kits can serve students well in the first half of first-semester chemistry, but visual representations get more difficult with polar bonds, valence electrons, and hybridization. Textbooks have gotten better at explaining these concepts with bright colorful pictures and diagrams, but these are still just two-dimensional representations of three-dimensional objects.

To better elucidate these concepts, undergraduate students in a general chemistry course assisted in the creation of several 3D models representing chemical principles. First, several models of polar and nonpolar molecules were made to demonstrate the differences in electron densities. The figure below shows a simple example of a diatomic nonpolar molecule like Cl₂ compared to a binary polar compound such as HCl. Second, the concept of valence and core electrons was demonstrated with s and p orbitals that could fit in each other, similar to nesting dolls. Finally, models of hybridized and unhybridized compounds were created to show how the electron density shifts when atoms are involved in different types of chemical bonds.

Due to the low-cost and ease of design, a great variety of models were used in the lecture class to demonstrate these sometimes unclear concepts.
CHED 1832

Integrative and exploratory junior-level studio laboratory for student-centered learning and scientific growth

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At Mercer University, we observed a skills gap in students beginning their senior-level original research projects. While these students were well prepared for most laboratory techniques, they often lacked necessary research process skills. In particular, they struggled with integrating concepts from courses and previous experiences for application to their project. They also required growth in reading and applying relevant peer-reviewed literature to their research. Finally, development of the informal oral and written communication of a deeper understanding of their work was needed. To address these issues curricularly, we designed a collaborative in-depth junior-level studio laboratory that supplants the typical junior-level course laboratories. The course requires students (in cohorts) to design a project based upon a guiding publication supplied by the faculty. The year-long course sequence allows for three major projects from different chemistry sub-disciplines, yet still covers the skills, techniques, and content desired by the faculty. General design, implementation, and assessment results will be discussed within the context of transferability and implementation at other institutions.

CHED 1833

Solution concentration uncertainty: An experiment to illustrate the concepts of precision and propagation of error through measurement of the molar extinction coefficient of Cu(NH$_3$)$_4$Cl$_2$

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The precision of scientific apparatus has direct implication on the accuracy of the measured results. This can be characterized by propagation of error and statistics. An experiment to measure the molar extinction coefficient of a compound was developed to illustrate this effect. Students were instructed to make two sets of solutions, one set
using volumetric flasks and pipets and the other set using only beakers. The students calculated the uncertainty in the concentration measures by propagating the error due to the tolerances of the glassware. The series of measured absorbances for each set was used to calculate the extinction coefficient of copper(II) ammonium chloride, Cu(NH$_3$)$_4$Cl$_2$, and its uncertainty. Cu(NH$_3$)$_4$Cl$_2$ was used due to the ready availability of copper (II) chloride in the laboratory. The use of CuCl$_2$ led to some issues which will be discussed and alternative materials will be suggested. Students were able to clearly see the effects of glassware tolerance on their results.

CHED 1834

Laboratory experiment: Carbonates and the ideal gas law

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A General Chemistry laboratory experiment has been developed that uses the ideal gas law to determine the molar mass of an unknown carbonate by allowing the carbonate to react with an aqueous 1 M HCl solution to produce CO$_2$ gas. The volume, temperature and pressure of the evolved CO$_2$ gas are measured. Good choices for the unknown carbonate are the environmentally friendly compounds NaHCO$_3$, CaCO$_3$ and K$_2$CO$_3$, which have a suitable range of molar masses. This experiment uses commonly available reagents and equipment and produces non-hazardous waste. Only very small quantities of reagents are used. This experiment produces a non-toxic gas (CO$_2$) and so does not require the use of a fume hood. The experiment illustrates the ideal gas law, conversions involving temperature, volume and pressure and Dalton’s Law of Partial Pressures. In this experiment, two trials can easily be performed in one laboratory period.

CHED 1835

Open source drug discovery with undergraduates and high school students

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In 2011, the Todd lab and the Medicines for Malaria Venture launched the Open Source Malaria (OSM)$^1$ project and embarked on the world’s first open source drug discovery venture. The aim of the project is to find a small molecule that is effective for the treatment of malaria, the difference being that everything is open, meaning that all the experiments are published in online electronic lab note books in real-time.$^2$ Additionally, all of the data are available and anyone can do anything they wish with the compounds, with the proviso that the project is cited.$^3$ One of the many advantages of this approach is that the barriers to participation are much lower than with traditional lab-based chemical research projects.
The unique features of the OSM project have enabled us to work within two areas of chemical education that are not typically associated with drug discovery; undergraduate teaching laboratories and high school practical classes.

Chemistry is an experimental science and the skills and understanding fostered through practical work is integral to student learning in this subject area. Traditionally, undergraduate teaching laboratories have focused on consolidating lecture material through carefully designed experiments and the introduction of techniques essential for research practices. However, many students are disengaged with laboratory teaching and fail to see the link between the practical and theoretical aspects of the course.

The dearth of provision for practical science in schools is also problematic. A recent report from the UK described that just 70% of high schools and 48% of primary schools have access to the ‘equipment and consumables’ required to teach practical science.4 Other reports from Australia have bemoaned a lack of training for teachers in the implementation of ‘inquiry based pedagogy’.5

The open nature of the OSM project means that anyone can take part and so we have expanded our team to include undergraduate and high school scientists. Here we describe our efforts to increase inquiry based learning and provision for exciting and informative practical science and attempts at alternative funding methods for such initiatives through crowdfunding.