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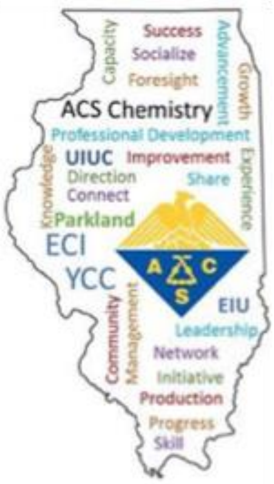
4TH ANNUAL
EAST CENTRAL ILLINOIS LOCAL SECTION
UNDERGRADUATE RESEARCH CONFERENCE

November 16, 2019

AWCCS UIUC



SACNAS
UIUC CHAPTER

ACS Student Chapter

NOBCChE℠
National Organization for the Professional Advancement of Black Chemists and Chemical Engineers

TABLE OF CONTENTS / INSTRUCTIONS

*found online at eciacs.org/conference

PRESENTERS – Please have your poster up five minutes before your session is supposed to begin and take them down promptly before the next session. You are expected to be present at your poster during the entire 50 minutes. Failure to do so will cause you to be disqualified from any awards.

JUDGES – Please pick up your folders at the registration booth when you sign-in and return them to the same place when finished.

AWARDS – Awards will be presented during the awards ceremony. If you are unable to attend the ceremony, you will be contacted through the e-mail you provided should you be chosen for an award.

SCHEDULE OF EVENTS

8:45 AM **REGISTRATION OPENS**

9:00 AM **NETWORKING BREAKFAST**

9:50 AM **OPENING REMARKS**

10:00 AM **ORAL SESSION I**

Erinn Dady (Chemical Ecology @ University of Illinois at Urbana-Champaign)
Soil Fertility and Arbuscular Mycorrhizal Colonization: Does it Impact Herbivore Induced Plant Volatiles in Tomato?

Katherine G. O'Malley (Hydrogeology @ Purdue University)
Calculation of 4-He/222-Rn Spring Water Ages of Owens Valley Spring Systems

Christopher M. Hanneman (Organic @ University of Illinois at Urbana-Champaign)
Homogeneous, Anhydrous Cross-Coupling of Heterocycles Using a Beneficial Lewis Acid: Trimethyl Borate

Yuan Jia (Organic @ University of Illinois at Urbana-Champaign)
Architecture-Controlled Ring-Opening Polymerization for Dynamic Covalent Poly(disulfide)s

11:00 AM **POSTER SESSION I**

12:00 PM **LUNCH BREAK, WCC PANEL**

1:30 PM **ORAL SESSION II**

Ruiwen Xu (Chemical Biology @ University of Illinois at Urbana-Champaign)
Optimization of Photoacoustic Probes for Nitric Oxide Detection

Elizabeth A. Thayer (Chemical Biology @ Purdue University)
Lipidomic Profiling in Amyloid Beta-Treated BV2 Microglia

Philip A. Kocheril (Chemical Biology @ University of Illinois at Urbana-Champaign)
Computational Analysis of Potential Small Molecule Therapeutics for Myotonic Dystrophy Type 1

Peng-Jui Chen (Chemical Biology @ University of Illinois at Urbana-Champaign)
Uncovering Lipophilicity Rules for Small-Molecule Mediated Transmembrane Metal Transport

2:30 PM **POSTER SESSION II**

3:30 PM **KEYNOTE SPEAKER – Ms. Patricia Simpson**

Life After Undergrad: Careers in Chemistry and the Chemical Sciences

4:30 PM **AWARDS CEREMONY**

INDEX OF PRESENTERS

DRIVING AND PARKING MAP

Driving Recommendations

Traveling east on I-74 (from Bloomington, IL; Macomb, IL) or south on I-57 (from Chicago, IL; Gary, IN; Milwaukee, WI). From I-57, take exit 237A for I-74 E. Once on I-74, take exit 183 for Lincoln Ave. Turn right at the light and take Lincoln Ave south towards the UIUC campus.

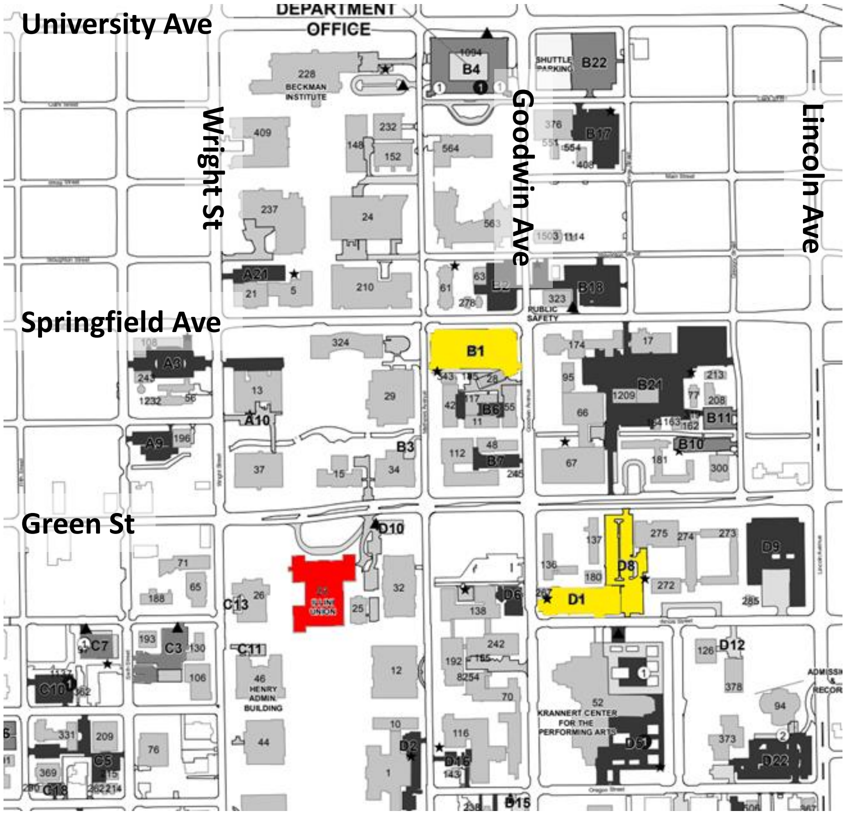
Traveling east on I-72 (from Decatur, IL; Jacksonville, IL, St. Louis, MO) or north on I-57 (from Charleston, IL). From I-57, take exist 235A for I-72 E. Once on I-72, continue onto University Ave towards the UIUC campus.

Traveling west on I-74 (West Lafayette, IN). From I-74, take exit 185 for IL-130. Continue straight as IL-130 becomes University Ave at the first stop light. Continue on University Ave towards the UIUC campus.

Parking Recommendations

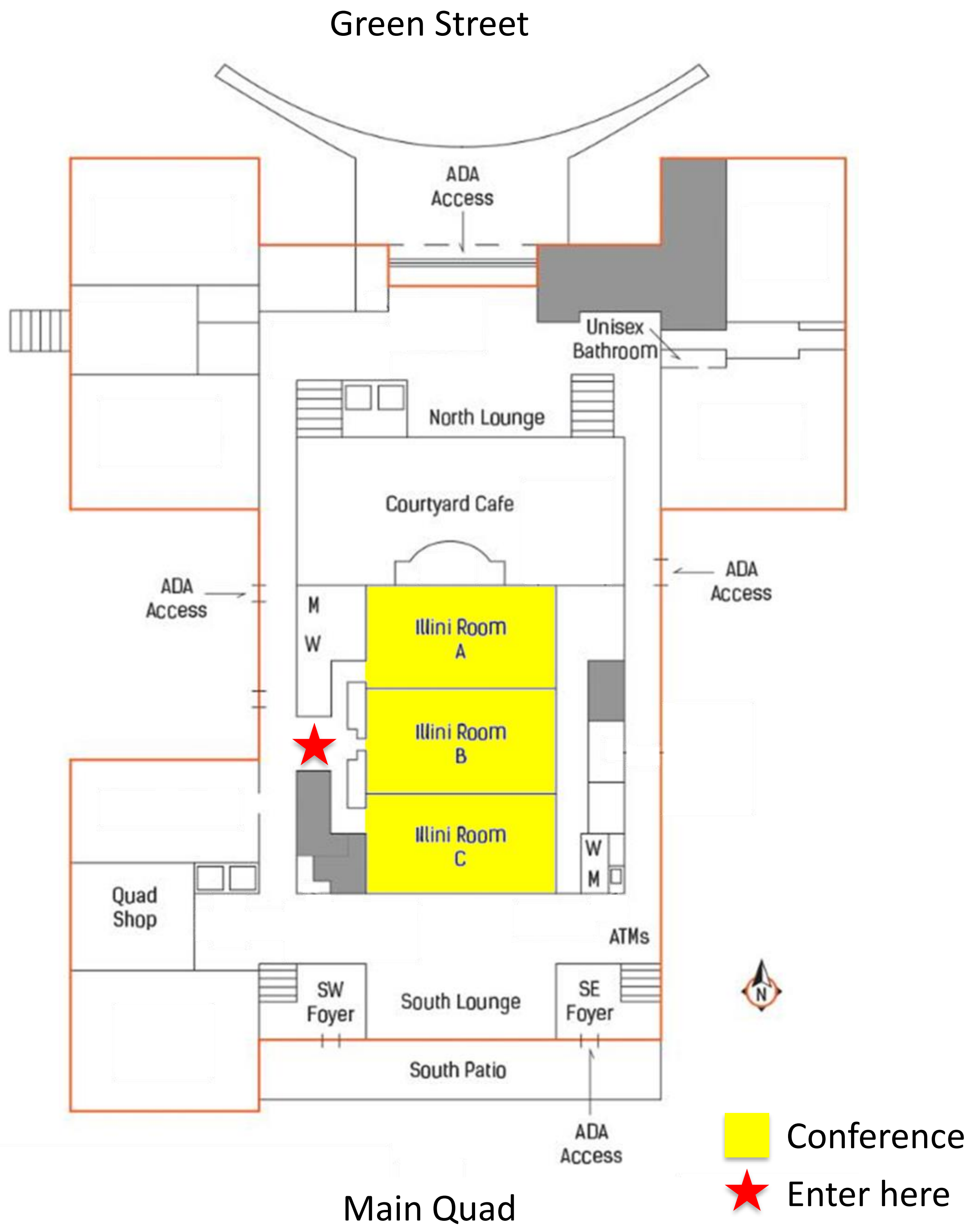
Excluding spaces individually marked by a blue sign, parking in UIUC lots is free on Saturdays. Many parking lots exist within a few blocks of the Illini Union (marked in red to the right). Smaller lots closer to the Illini Union can fill quickly depending on campus activities, but larger lots (marked in yellow to the right) should have plenty of space. For a full map, please visit the link below.

Notes: Metered street parking is typically controlled by the cities of Champaign and Urbana, both of which enforce meters on Saturday. Please read all posted signs carefully as policies may change without our knowledge.

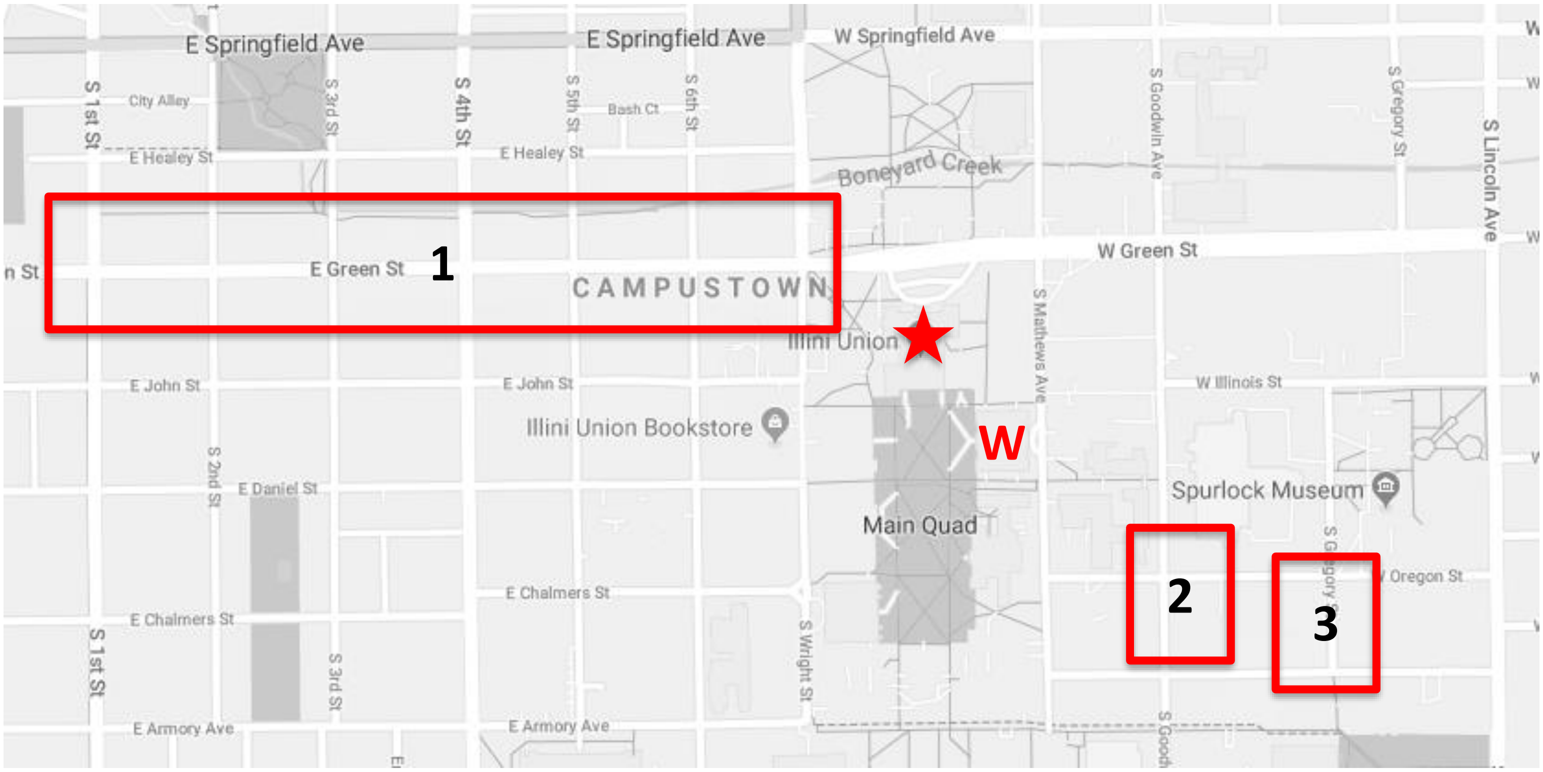


http://www.parking.illinois.edu/visitors/campus-maps/campus-parking-map

ILLINI UNION MAP



RESTAURANT MAP



Restaurant Recommendations

There are many restaurants in the area surrounding the Illini Union (red star above). Some key areas include Green St (1), the corner of Goodwin and Oregon (2), and Gregory St (3).

1. There are too many restaurants to name on Green St and the surrounding side streets, especially close to the Illini Union. American, Chinese, Indian, Italian, Korean, Mexican, and Thai, are just some of the cuisines available.
2. Interested in something more sit-down? The corner of Goodwin and Oregon features both Bread Company and Timpone's, common destinations for UIUC chemistry functions.
3. The stretch of Gregory St sandwiched between Oregon and Nevada is dense with options ranging from Cajun to sushi, from American diner to Korean.

Vegetarian or vegan? Unfortunately the exclusively vegan restaurant (The Red Herring) is closed on Saturdays. A number of the places along Green St have options, especially the Indian and Thai restaurants.

WCC Lunch Panel

If you registered for the graduate student panel discussion hosted by the UIUC Women Chemist Committee, lunch will be provided in Room 163 of Noyes Laboratory (the building marked by the W on the map above).

POSTER SESSION I: OVERVIEW

1. **Akua Biaa Adu** (Inorganic @ Illinois College)
   Synthesis of Indenyl Ruthenium Complexes with Target Ligands
2. **Ethan Aubuchon** (Organic @ Indiana University Northwest)
   Synthesis and Cu(I/II) Chelation of aza-thia[14]-ane Containing N-substituted Pendant Amino Phosphonic Acid Arms
3. **Sunday Bobori** (Inorganic @ Illinois College)
   Syntheses and Application of Nickel-Phosphorus Complexes with Chelating Ligands
4. **Nicholas M. Branson** (Organic @ Purdue University)
   Property Analysis of Adhesives from Walnut Juglone and Corn Zein Protein
5. **Douglas S. Chan** (Chemical Biology @ University of Illinois at Urbana-Champaign)
   Development of Probes for Photoacoustic Imaging of Tissue Hypoxia in Prostate Cancer
6. **Huguette Clemente, Max Garcia** (Biochemistry @ Saint Xavier University)
   Effects of Terpenoids on Protein Tyrosine Phosphatase 1β (PTP1β)
7. **Shyam Dedaniya** (Analytical @ Northeastern Illinois University)
   The Effect of Temperature on the Distribution of Chlorogenic Acid in Different Anatomical Parts of the Coffee Bean
8. **Duncan B. Eastin** (Organic @ Eastern Illinois University)
   Attempts at Synthesizing New Î²-Phenylcinnamaldehyde Semicarbazones
9. **Annie Fritz** (Bioinorganic Medicinal @ Northeastern Illinois University)
   Cytotoxicity and Crystal Structure of Arsenoplatin-1-Iodide Complex
10. **Lawrence Xi-Bin Fung** (Materials @ Purdue University)
    Synthesis and Characterization of Nontoxic Adhesives from Corn Zein Protein and Plant Phenolics
11. **Elizabeth Garcia, Karla Herandez-Garcia** (Analytical @ Alverno College)
    Colorimetric Determination of Pb2+ in the Kinnickinnic River Water
12. **Dalton L. Glasco** (Analytical @ Millikin University)
    Simple Method for Preparing Customizable Pyrolyzed Photoresin Carbon Electrodes Using 3D Printing
13. **Aidan M. Kelly** (Organic @ University of Illinois at Urbana-Champaign)
    Toward Democratization: Enabling Non-Expert Access to MIDA Boronate Synthesis
14. **Kate Kragness** (Organic @ Purdue University)
    FAP-targeted NIR Imaging of Cancer for Florescence Guided Surgery (FGS)
15. **Brittany N. Linn** (Inorganic @ Purdue University)
    Magnetocaloric effect (MCE) and Magnetic Properties of the Co doped Gadolinium Nickel Gallides (GdNi$_{3-x-y}$Co$_x$Ga$_y$)
16. **Matthew Martin** (Bioinorganic Medicinal @ Northeastern Illinois University)
    Synthesis, Characterization, and Anticancer Activity of Aresenoplatin-4
17. **Jonah Messinger** (Analytical @ National Renewable Energy Laboratory)
    Insights Into PV Device Performance and Composition Using Time-of-Flight Secondary Ion Mass Spectrometry
18. **Niya L. Mitchell** (Organic @ University of Illinois at Urbana-Champaign)
    Target-Guided Screening Method for Myotonic-Dystrophy Type 1 Inhibitors Using Small Molecules

POSTER SESSION I: OVERVIEW

19. **Makoy Overfelt** (Analytical @ Illinois State University)
    Ambient Mass Spectrometry of Agrochemicals in Soil Utilizing Paper Cone Spray Ionization Mass Spectrometry
20. **Andria Pace** (Organic @ University of Illinois at Urbana-Champaign)
    Pd(II)/SOX Catalyzed Allylic C-H Amination for the Synthesis of Naftifine Derivatives
21. **Sirikarn Phuangthong** (Inorganic @ Illinois College)
    Synthesis and Characterization of Imidazolium Ionic Liquids
22. **Isiah Ramos** (Chemical Biology @ Parkland College)
    Effects of Systemic Influenza Infection on Remyelination in an Animal Model
23. **Evan Reeves, Rachael Knieser** (Organic @ Purdue University)
    Role of Oxygen in the Formation of Indophenols upon Photolysis of Azidophenoxides
24. **Ayman Roslend** (Materials @ University of Illinois at Urbana-Champaign)
    Metal-Chelated Biliverdin Nanoparticles as Magnetic Resonance Imaging (MRI) Contrast Agents
25. **Karissa Scales** (Chemical Biology @ Western Illinois University)
    A Bioluminescent Calreticulin Reporter for Measurement of Immunogenic Cell Death in Pancreatic Cancer Cells
26. **Brittney Stelzl** (Analytical @ Alverno College)
    Determination and the Quantitative analysis of *E. Coli* in Milwaukee Rivers
27. **Boran Sun** (Materials @ University of Illinois at Urbana-Champaign)
    Self-assembly Behavior of Sequence-defined Pi-conjugated Oligopeptide
28. **Jun Zhi Tan** (Chemical Engineering @ University of Illinois at Urbana-Champaign)
    Solvent Effects on Alkene Epoxidations in Ti-zeolites
29. **Rachel W. Tham** (Chemical Engineering @ University of Illinois at Urbana-Champaign)
    Electrodepositing Switchable Photovoltaic Window Electron and Hole Transport Layers
30. **Ben Vaupen** (Organic @ Purdue University)
    Synthesis of Cyclopropene Derivatives for use as Ethylene Antagonists
31. **Brendan J. Wall, Mark F. Will** (Inorganic @ Illinois State University)
    Synthesis and Characterization of Ruthenium-Based Alzheimer's Disease Therapeutics
32. **Lindsey Weintraub** (Chemical Biology @ Western Illinois University)
    Antioxidant and Cytotoxic Activity of Acmella alba, Acmella oleracea, and Acmella calirrhiza
33. **Jael Wotsho** (Chemical Biology @ Western Illinois University)
    Lycopene in Grafted and Hydroponically Cultivated Heirloom Tomatoes
34. **Adam J. Youman** (Organic @ Illinois State University)
    Investigation of Electronic Parameters in Oxidopyrylium Based [5+2] Cycloadditions
35. **Patricia Zamora, Erika Olvera** (Inorganic @ Alverno College)
    Emerging Contaminants in the Kinnickinnic River - Metals
36. **Linzixuan (Rhoda) Zhang** (Chemical Engineering @ University of Illinois at Urbana-Champaign)
    A High-throughput MALDI-ToF MS-based Screening Method for Medium-chain Fatty Acid Detection

POSTER SESSION II: OVERVIEW

37. **Guadalupe Aguirre-Figueroa** (Chemical Biology @ University of Illinois at Urbana-Champaign)
Rational Design and Synthesis of a Red-Fluorescent Probe for Aldehyde Dehydrogenase 1A1
38. **Fatima Akili** (Organic @ University of Illinois at Chicago)
Chemoselective Differentiation of Bis(monoacylglycero)phosphate (BMP), Phosphatidylglycerol (PG)
39. **Ahmad H. Alfoudari, Charles R. Enlow** (Chemical Education @ Purdue University)
How to Create a GTA Manual - Investigation of Best Practices in GTA Training and Departmental Needs
40. **Anh M. Bui, Sara Y. Siddiqui** (Organic @ University of Illinois at Chicago)
Chiral Auxiliaries for Diastereoselective γ-Functionalizations of Carbonyl Substrates
41. **Sriyankari Chitti** (Organic @ University of Illinois at Urbana-Champaign)
Iterative Stereospecific Csp3-Csp3 Coupling Using Bifunctional Carbenoid-Boronate Building Blocks
42. **Phoebe C. Clowser, Jessica M. Holtz** (Analytical @ Illinois State University)
Environmental Ruggedness of a Portable MS System Coupled With Paper Spray Ionization During Field Operation
43. **Lilliana Dunterman** (Chemical Biology @ Western Illinois University)
Evaluating Biotransformation Efficiency of Oleic Acid to10-Hydrodroxystearic Acid by Two Secondary Alcohol Dehydrogenase Knockout Mutants of Nocardia cholesterolicum NRRL5767
44. **Jeffrey Dykstra** (Analytical @ Indiana University Northwest)
Unknown Nepetalactone Isomer Elucidated from Nepeta citriodora Extract
45. **Hannah L. Fino** (Physical @ Eastern Illinois University)
Implementing Extended Cross Correlation as a Tool to Identify Patterns in Microwave Spectra, and its Application to Fluoroethylene/Carbon Dioxide Clusters
46. **Matthew A. Frank** (Inorganic @ Milikin University)
The Search for New Solid-State Electrolytes: Investigating the Structural Properties of Substituted Li_5MO_4 or Li_6MO_4 Antifluorite Materials
47. **Kaylee D. Fuller-Svarz** (Organic @ Eastern Illinois University)
Preparing Imine Analogues of Cinnamaldehyde Semicarbazone to Explore Their Photochromicity
48. **Hoya Ihara** (Physical @ University of Illinois at Urbana-Champaign)
Polyurethane Hugoniot for Polymer-Bonded Explosives
49. **Hanning Jiang** (Analytical @ Purdue University)
2,6-Didehydropyridinium Cations Can React From An Excited Triplet State
50. **Rida Khan** (Organic @ University of Illinois at Chicago)
Synthesis of Chrysindin A and B via the Pauson-Khand Reaction
51. **Kailey Komnick** (Organic @ University of Illinois at Urbana-Champaign)
Structural-Activity Relationship Campaign Leads to a Novel Chain of Fusidic Acid with an Improved Resistance Profile
52. **Anna Larsen** (Biochemistry @ Western Illinois University)
Determination of Cell Binding Properties of a Novel Pancreatic Cancer Targeting Phage
53. **Brianna Lehr** (Inorganic @ Illinois State University)
Designing Novel Tunable Inorganic Pigments
54. **Alexis Magaña** (Materials @ *University of Illinois at Urbana-Champaign)*
Co-base catalyst in ORR

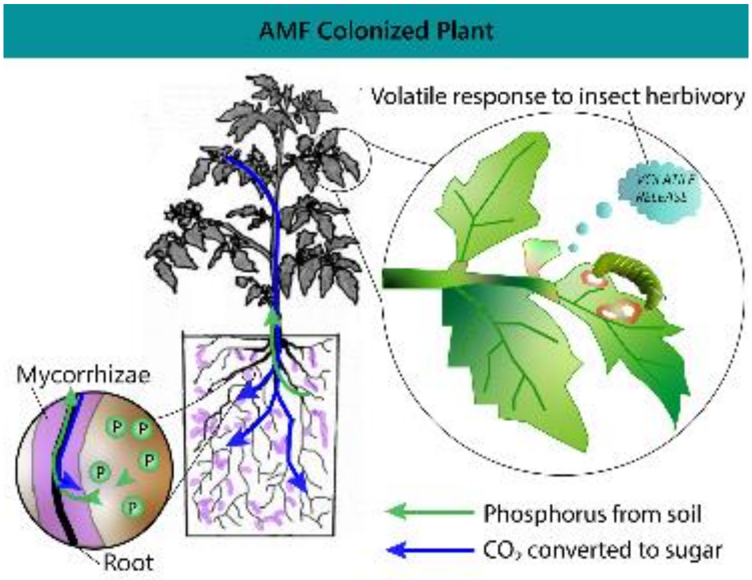
POSTER SESSION II: OVERVIEW

55. **Brittany Meyer** (Organic @ Purdue University)
    Targeting the Class II HMG-CoA Reductase Enzyme for the Development of Novel Antimicrobials
56. **Sarah Nowling** (Analytical @ Purdue University)
    Effects of Sample Storage and Handling on Jet Fuel Composition and Flash Point
57. **Ana Olvera, Erika Olvera** (Inorganic @ Alverno College)
    Emerging Contaminants in the Kinnickinnic River - Inorganic Anions and Pesticides
58. **Stephanie Ouchida** (Bioinorganic @ University of Illinois at Urbana-Champaign)
    Biosynthetic Models of Unique Structural Features in Cytochrome Oxidases Found in Pathogens
59. **Owen Ouyang** (Inorganic @ Washington University in St. Louis)
    Engineering an O2 transport protein into a CO2 reduction biocatalyst
60. **Nathan S. Purwanto** (Organic @ University of Illinois at Urbana-Champaign)
    Fast Mechanochromism of Regioisomeric Oxazines in Polymer Network
61. **Steven Ramirez** (Inorganic @ University of Illinois at Urbana-Champaign)
    Synthesis of Iridium and Rhodium Pincer Complexes to Catalyze Parahydrogen Induced Polarization (PHIP)
62. **Samantha Rokey** (Organic @ Illinois State University)
    Investigation of Polarization Effects on Intramolecular Oxidopyrylium-Alkene [5+2] Cycloadditions
63. **Alondra Sanchez** (Chemical Biology @ University of Illinois at Urbana-Champaign)
    The Structure-Activity Relationships of Enterococcal Cytolysin
64. **Naisong Shan** (Materials @ University of Illinois at Urbana-Champaign)
    Ion Exchange Reaction and its Influence on Network Ionic Polymer
65. **Daphne Shen** (Chemical Biology @ University of Illinois at Urbana-Champaign)
    High Pressure Freezing/Freeze Substitution Combined with Correlated Imaging Techniques for Investigating the Intracellular Lipid & Protein Distributions
66. **Kylie H. Smith** (Chemical Education @ Purdue University)
    Chemistry Laboratory Experiment: Molecular Interactions in Liquid Crystals
67. **Alex Solivais** (Analytical @ Indiana University Northwest)
    Quantification of Phytocannabinoids in CBD Products
68. **Justin Shing Him Wong** (Inorganic @ Purdue University)
    Magnetic properties of Co-doped Nickel Aluminides, DyNi3-x-yCoxAly
69. **Che Woodson** (Chemical Biology @ Western Illinois University)
    Phage Display Selection of a Hemagglutinin Targeting Peptide
70. **Chang Xia** (Analytical @ University of Illinois at Urbana-Champaign)
    Metal Substrates Modulation of Outer-Sphere Electron Transfer Kinetic on Single Layer Graphene
71. **Xuetao Zheng** (Materials @ University of Illinois at Urbana-Champaign)
    Synthesis of Polypeptides with Complex Architectures Through SIMPLE Strategy
72. **George Zurowski** (Inorganic @ Illinois State University)
    Exploring the Structure-Property Relationship in Oxyfluoride Pigments

Soil Fertility and Arbuscular Mycorrhizal Colonization: Does it Impact Herbivore Induced Plant Volatiles in Tomato?

Erinn Dady and Esther Ngumbi
University of Illinois at Urbana-Champaign

Arbuscular mycorrhizae fungi (AMF) are naturally occurring, beneficial fungi that grow in mutualism with many plants by colonizing their roots. Associations between host plants and AMF may enhance plant defense responses, including production of volatile organic compounds (VOCs). Emitted VOCs are a far-reaching plastic response to the challenges faced by plants' immobility. VOCs play important roles in the direct and indirect defenses of plants. Previous studies show the outcomes of AMF-tomato plant mutualism vary depending on fertilization and insect herbivory. This study was conducted to evaluate how mycorrhizal colonization in tomato plants influences volatile production under contrasting soil fertility. Using a model system consisting of two tomato genotypes (plant) and *Manduca sexta* (as herbivore), we tested the hypothesis that under conditions of nutrient limitation, mycorrhizal fungi mutualism will enhance plant defenses and alter the production of VOCs. We used solid phase microextraction to collect volatiles. The VOCs were identified using gas chromatography mass spectrometry (GC-MS). Results showed that soil fertility and mycorrhizal colonization affected the emissions of herbivore-induced VOCs in tomato.

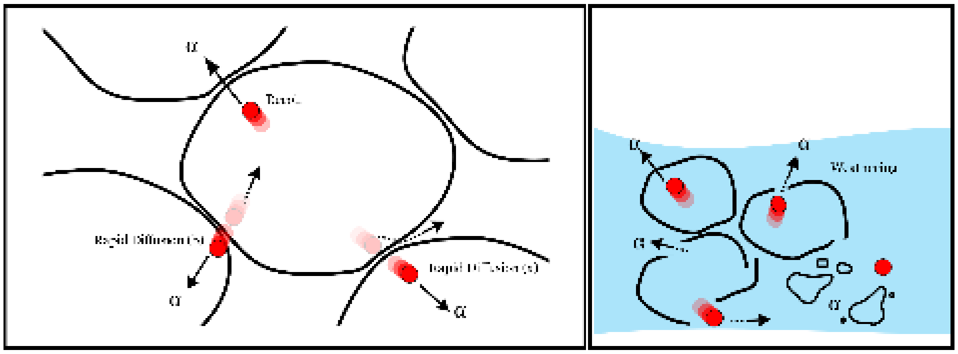


ORAL SESSION I: SPEAKER 2

Calculation of 4-He/222-Rn Spring Water Ages of Owens Valley Spring Systems

Katherine G. O'Malley, Marty D. Frisbee, and Zachary P. Meyers
Purdue University

This study demonstrates the use of 4He/222Rn ratio to estimate the age range of several springs within Owen's valley in California and Nevada to better understand the flow paths groundwater takes before emerging in a spring. With these observations, the hope was to further understand the what makes a spring resilient and resistance to changing climate conditions. By using 4He and 222Rn concentrations, the ages of 19 springs were calculated, 13 of these spring's mean age matched the age range estimated by 14C dating methods. Demonstrating an alternative method to age dating groundwater.



Homogeneous, Anhydrous Cross-Coupling of Heterocycles Using a Beneficial Lewis Acid: Trimethyl Borate

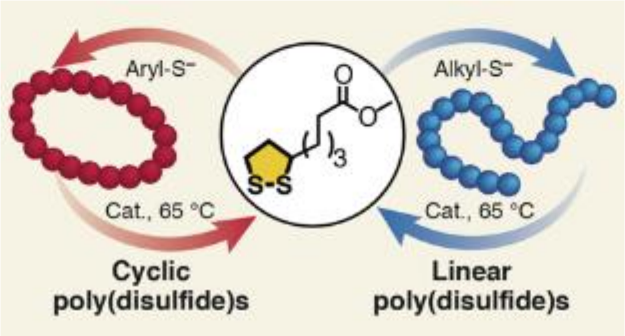
Christopher M. Hanneman, Connor P. Delaney, and Scott E. Denmark
University of Illinois at Urbana-Champaign

Heterocyclic boron nucleophiles are a problematic motif for the Suzuki-Miyaura reaction because of: (1) instability of boronic acids in protic solvents and (2) reaction inhibition by basic nitrogen heterocycles. Herein, we report a new method for the Suzuki-Miyaura cross-coupling of heterocyclic boronic esters. This new advance utilizes potassium trimethyl silanolate as a soluble base and trimethyl borate as a beneficial Lewis acid. The Lewis acid is employed to prevent coordination of the heterocycle to the catalyst and to inhibit the protodeboronation pathway. Moreover, potassium trimethyl silanolate acts as a soluble base enabling the use of ethereal, aprotic solvents. This new method facilitates a rapid cross-coupling of a wide array of heterocycles in high yield.

Architecture-Controlled Ring-Opening Polymerization for Dynamic Covalent Poly(disulfide)s

Yuan Jia, Yun Liu, Qiong Wu, and Jeffrey S. Moore
University of Illinois at Urbana-Champaign

The disulfide (S-S) bonds are well-studied dynamic covalent bonds and are widely present in biology, chemistry, materials science and energy. Poly(disulfide)s with dynamic covalent bonds have been applied in many areas, such as cellular delivery of drugs, self-healing material, and Li-S batteries. Methods to control the synthesis of different architectures of poly(disulfide)s remain absent. Here, we exploit a new scheme of anionic ring-opening polymerization which allows the controlled synthesis of cyclic or linear poly(disulfide)s.1 Aryl thiol initiators were used to shift the ring-chain equilibrium to yield cyclic polymers while alkyl thiols favor linear ones. We achieved high molar mass polymers (630 kDa) with a low polydispersity of 1.3 and demonstrated catalytic depolymerization to recycle monomers. This work provides a new avenue to create dynamic covalent polymers with controlled geometry and length, allowing a better characterization of structure-property relationships to expand their materials potentials.

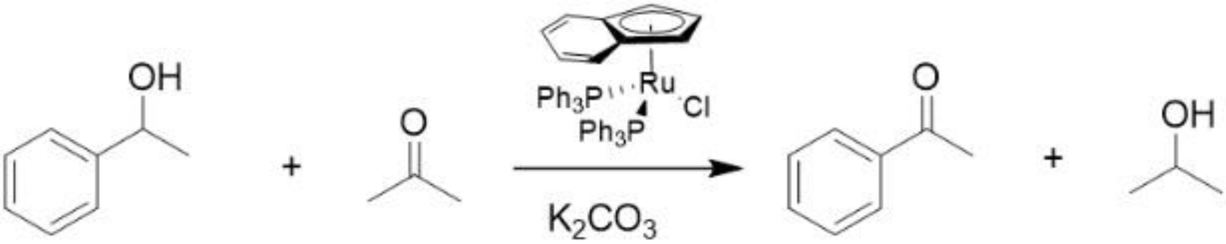


POSTER SESSION I: POSTER 1

Synthesis of Indenyl Ruthenium Complexes with Target Ligands

Akua Biaa Adu and Jocelyn Pineda Lanorio
Illinois College

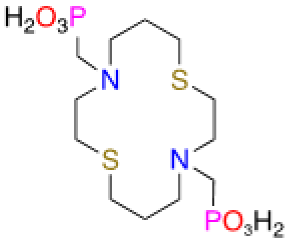
Ruthenium complexes have emerged as an attractive anticancer alternative to platinum metal due to their low toxicity, probable different mode of action, and diverse synthetic chemistry. The interest in indenyl (Ind) ligand originates from its resemblance to η^5-cyclopentadienyl Cp/Cp* ligands. Indenyl ruthenium (IndRu) complexes are known to exhibit reactivity and stereochemical features different from those of the corresponding Cp complexes, but evidence is still lacking or limited. This poster outlines the synthesis and characterization of a series of indenyl ruthenium complexes. Phosphites were also employed as ligand to some of the IndRu complexes synthesized. All prepared complexes were air and moisture stable. Furthermore, $IndRu(PPh_3)_2Cl$ was found to be an efficient catalyst in the oxidation reaction of 1-phenylalcohol and acetone with higher % conversion and turnover frequency (TOF) than the traditional Ru catalyst, $RuCl_2(PPh_3)_3$. Future work includes investigation of the catalytic efficiency of all the synthesized IndRu complexes in the chosen redox reaction, and investigation of their DNA-binding and/or antitumor activities.



Synthesis and Cu(I/II) Chelation of aza-thia[14]-ane Containing N-substituted Pendant Amino Phosphonic Acid Arms.

Ethan Aubuchon, Briana R. Schrage, Christopher J. Ziegler, Art van der Est, and Ian S. Taschner
Indiana University Northwest

Bifunctional mixed heteroatom ligand chelators make for powerful radiopharmaceuticals in positron emission tomography (PET). Herein, synthesis and characterization of N,N'-bisphosphonate pendent arms tethered to an aza-thia macrocycle is presented. Subjecting 1,8-dithia-4,11-diazacyclotetradecane to the Moedritzer-Irani hydrophosphorylation reaction afforded pendant arm macrocycle 1 in favorable yields. Further, a Kabachnik-Fields reaction was also implemented for reaction screening and optimization. The bifunctional heteroatom ligand was found to readily chelate copper(II) and undergo a retro-Moedritzer-Irani reaction in the presence of copper(I). Phosphonate macrocycle was subjected to a diffusion chamber to acquire an X-ray quality crystal. Physical properties such as pKa values and metal redox are presented along with the experimental details of each study.

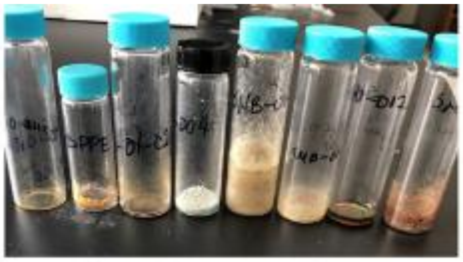


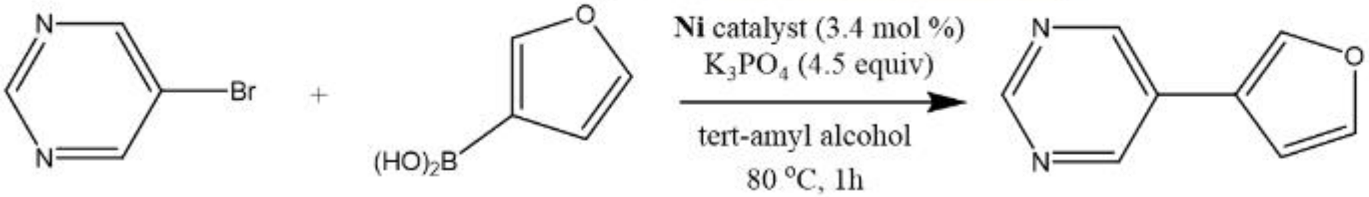
POSTER SESSION I: POSTER 3

Syntheses and Application of Nickel-Phosphorus Complexes with Chelating Ligands

Sunday Bobori and Jocelyn Pineda Lanorio
Illinois College

Suzuki-Miyaura coupling is a metal-catalyzed carbon-carbon bond reaction between organoboron and halide under basic conditions. Cross-coupling reactions are typically catalyzed by expensive palladium (Pd) catalyst. Thus, complementary approaches to achieve such coupling are highly sought after. One attractive alternative involves the use of nickel catalysts due to nickel being readily available, less toxic, and cheaper compared to Pd. Nickel catalysis can also be used to form linkages between two heterocyclic fragments producing important classes of compounds that serve as building blocks of pharmaceutical drugs such as antipsychotics, anti-leukemia, among others. A series of Ni-phosphorus complexes, $NiCl_2(DPPE)$, $NiCl_2(PPh_3)_2$, $NiCl_2(BINAP)$, $NiCl_2(P(OPh_3)_2)$, and $NiCl_2(P(OEt_3)_2)$, were successfully synthesized and characterized. Most of the prepared nickel complexes showed 100% efficiency as catalysts in the chosen Suzuki-Miyaura cross-coupling reaction. However, the Ni-phosphites did not show complete conversion of the cross-coupling reactants. It is recommended that investigation of the retrievability of the catalysts and determination of the exact action (*e.g.* % conversion; TOF calculation) of Ni-phosphite complexes in Suzuki-Miyaura reactions be done as future work.





Property Analysis of Adhesives from Walnut Juglone and Corn Zein Protein

Nicholas M. Branson, Lawrence X. Fung, and Gudrun Schmidt
Purdue University

Juglone is a phenolic component produced by most walnut tree species, among them the black walnut tree found in Indiana. The biological properties of this phenolic molecule include insecticidal, antimicrobial and antifungal effects that protect the tree from disease. When juglone is combined with corn zein protein, its antimicrobial properties may transfer to the blended polymer material. Here we investigate compositions of zein protein plus juglone for potential use as adhesive and packaging material. We use lap shear testing experiments and aluminum substrates to determine the adhesive strength of various zein-juglone formulations under different conditions. Adhesive versus cohesive failure is evaluated after the interface and the substrate are separated and the glue is retained or absent from the surfaces. Fourier transform infrared spectroscopy provides information about possible molecular interactions between zein and juglone during curing. Differential scanning calorimetry helps determine various thermal properties of zein-juglone mixtures, including glass transitions. We compare our results to the materials chemistry of other phenolic components to improve materials design.

Development of Probes for Photoacoustic Imaging of Tissue Hypoxia in Prostate Cancer

Douglas S. Chan, Hailey J. Knox, and Jefferson Chan
University of Illinois at Urbana-Champaign

Hypoxia occurs when tissue oxygen supply to rapidly growing tumors becomes inadequate to support physiological processes. This induces a series of changes in gene expression that play a role in tumor metastasis and treatment resistance. In particular, hypoxia has been directly correlated with tumor grade and clinical stage in prostate cancer. Therefore, identifying hypoxia in prostate tumors can guide treatment planning and predict patient responses. Previous work in our lab yielded the development of Hypoxia Probe 1 (HyP-1), a hypoxia-responsive small-molecule probe designed for hypoxia detection using photoacoustic (PA) imaging. PA imaging uses near-infrared light to induce the production of ultrasound signals, enabling acquisition of high-resolution images in deep tissue. Currently, we are focused on the development of a prostate cancer targeted hypoxia probe (HyP-PCa), which targets the prostate-specific membrane antigen overexpressed in almost all prostate cancers. The goal of our work is to combine HyP-PCa with modified clinical U.S. systems to enable PA imaging of prostate tumor hypoxia in order to determine tumor grade and clinical stage.

Effects of Terpenoids on Protein Tyrosine Phosphatase 1β (PTP1β)

Huguette Clemente, Max Garcia, and Sharada Buddha
Saint Xavier University

Protein tyrosine phosphatase-1β (PTP1β) is responsible for the negative regulation of insulin signaling and a therapeutic target for diabetes, cancer, and inflammation. Tremendous growth has been made in finding PTP1β inhibitors that comes from natural sources and exploring PTP1β regulatory mechanisms. The goal of our research is to see if thymoquinone, thymol, D-carvone, and carvacrol inhibit the enzyme protein tyrosine phosphatase-1β (PTP1β). Thymoquinone is a monoterpenoid and has been used as a drug for many things in recent history such as asthma, hypertension, diabetes, inflammation, cough, bronchitis, headache, eczema, fever, dizziness and influenza. Thymol is a monoterpenoid phenol and is an isomer of carvacrol, it is currently not used as a drug, as an antiseptic and is present in some essential oils. Carvacrol is a monoterpenoid phenol which also has not been used as a drug before and, is currently used in perfumes and foods for its strong oregano smell and taste. Carvone is a terpenoid that has D and L enantiomers which have very different reactivity. In our research, we are using the D enantiomer which has been used for digestive drugs in humans and animals. These PTP1β inhibitors may serve as a theoretical foundation for new concept drug discovery and design.

The Effect of Temperature on the Distribution of Chlorogenic Acid in Different Anatomical Parts of the Coffee Bean

Shyam Dedaniya and Chandana Meegoda
Northeastern Illinois University

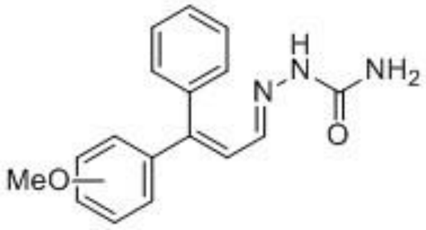
Pleasant aroma, good taste and brain stimulating activities have rendered coffee to become one of the most popular drinks in the world. Although there are more than hundred species of coffee being identified, Coffea arabica L. (commonly known as Arabica) and Coffea canephora Pierre (commonly known as Robusta) are the most popular and widely used in many parts of the world. Coffee beans are considered to be a rich source of Chlorogenic acids (CGA), which belong to a class of polyphenols with potential health benefits. Cross-sectioned green coffee beans were investigated using FT-Raman spectrometry contour mapping and the spatial distribution of chlorogenic acid across the bean endosperm was analyzed. Contour mappings show that the Chlorogenic acids were mostly located in the hard-external region of the endosperm, and a clear separation of borderline is visible. It was also observed that coffee Robusta has a higher CGA content in the internal region of endosperm. Slight heating of green coffee beans showed that the CGA migrates towards the upper region of the coffee bean and the CGA content in other areas of the coffee bean become lower as a result of heating.

POSTER SESSION I: POSTER 8

Attempts at Synthesizing New Î²-Phenylcinnamaldehyde Semicarbazones

Duncan B. Eastin and Edward M. Treadwell
Eastern Illinois University

Previously in this group, John M. Saathoff prepared and investigated the photochromicity of 24 different semicarbazones, and found that Î²-phenylcinnamaldehyde semicarbazone displayed significant reverse photochromatic properties. This project sought to prepare substituted Î²-phenylcinnamaldehyde semicarbazone to see how substituents off one of the rings affects the photochromatic properties. The preparation of Î²-(p-methoxyphenyl)cinnamaldehydes was attempted via a conjugate addition of 4-tolylmagnesium bromide, and a Mizoroki Heck addition of p-iodonitrobenzene, to p-methoxycinnamaldehyde. Additionally, a Pd-catalyzed double dehydrative Î²-arylation of propionaldehyde with p-iodoanisole was attempted. Lastly, both fluoride- and carbonate-assisted addition of calcium carbide to p-methylacetophenone to give an Î±-ethynyl alcohol, which would then undergo a Meyer-Schuster rearrangement. The results of these reactions, along with model reactions run alongside, will be discussed.



POSTER SESSION I: POSTER 9

Cytotoxicity and Crystal Structure of Arsenoplatin-1-Iodide Complex

Annie Fritz, Zohra Sattar Waxali, Wenan Qiang, Matthew Martin, Denana Miodragovic, and Thomas V. O'Halloran

Northeastern Illinois University

Arsenoplatins (AP) are a new class of anticancer compounds containing dual pharmacophore moieties from two inorganic, FDA approved anti-cancer drugs, cisplatin, [Pt(NH3)2Cl2] and arsenic trioxide, As2O3. Each of these two drugs induces apoptotic cell death but through different mechanisms: cisplatin targets nuclear DNA, whereas As2O3 targets zinc-finger proteins. Results of the NCI-60 (NCI: National Cancer Institute) human tumor cell line screen have shown that the first arsenoplatin compound synthesized [Pt(Î¼-NHC(CH3)O)2ClAs(OH)2], (AP-1), is more potent than As2O3 or cisplatin in the majority of cell lines tested. Furthermore, studies indicating increased anticancer activity of a cisplatin-iodide analog inspired us to synthesize an iodide complex (AP-5). Structural characterization of AP-5 has been determined by X-ray crystallography, elemental analysis, and NMR. The anti-cancer activity of AP-5 is tested in vitro against the triple negative breast MDA-MB-231 cancer cell line, an aggressive cancer currently lacking an effective method of treatment. The results of in vitro cytotoxicity assays have shown that AP-5 is even more cytotoxic than AP-1 or cisplatin. The effect of AP-1 and AP-5 on glutathione (GSH) level is investigated to understand the difference in the activity. The depletion of GSH is observed in cells treated with AP-5 but not with AP-1. The depletion of GSH sensitizes cancer cells to platinum drugs and could be a reason for the higher cytotoxicity of AP-5.

POSTER SESSION I: POSTER 10

Synthesis and Characterization of Nontoxic Adhesives from Corn Zein Protein and Plant Phenolics

Lawrence Xi-Bin Fung, Nicholas Branson, and Gudrun Schmidt
Purdue University

Corn zein protein is a nontoxic polymer often obtained as plant waste and biofuel byproduct. Tannic acid is a large polyphenolic molecule composed of condensed gallic acid units. Gallic acid, catechol and juglone are small phenolic molecules frequently found in plants. Large polyphenolic and small phenolic components can provide cohesive strength to polymers such as corn zein protein when used as cross-linking agent. This functionality is quite useful when designing nontoxic polymer glues and packaging materials. We use lap-shear testing experiments to determine the adhesive strength of various zein-phenolic compositions under different conditions. Fourier transform infrared (FTIR) spectroscopy provides certain molecular-level information regarding cross-linking reactions that may have taken place during curing of various adhesive compositions. We compare our results to the cross-linking chemistry of catechol in an attempt to elucidate the role of the phenolic component in making glue. Applications for glues made from corn protein and phenolics are most suitable for food and medical packaging. Other potential uses include denture adhesives, wound healing (â€œband aidsâ€) and applications that come in contact with skin.

POSTER SESSION I: POSTER 11

Colorimetric Determination of Pb2+ in the Kinnickinnic River Water

Elizabeth Garcia, Karla Herandez-Garcia, Joselin Rodriguez Santiago, Brittney Stelzl, and Jenna Coss
Alverno College

The focus of this investigative study was to determine the Pb2+ concentrations in three different locations along Milwaukee Kinnickinnic River. The water samples were collected from Wilson Park, Jackson Park, and Zablocki Park during the course of five weeks. In this study, a colorimetric method was used to create a series of dilutions were prepared to create the standard curve in order to interpolate the lead concentration of the river samples. Jackson Park had the highest average concentration of Pb2+ of 4.73ppm and Zablocki Park had the lowest average of 3.60ppm.

POSTER SESSION I: POSTER 12

Simple Method for Preparing Customizable Pyrolyzed Photoresin Carbon Electrodes Using 3D Printing

Dalton L. Glasco and Kyle N. Knust
Millikin University

In this research, an accessible fabrication procedure was developed to create pyrolyzed photoresin electrodes (PPE). A stereolithography 3D printer was used to pattern carbon containing photoresin on a quartz substrate. We then pyrolyzed the photoresin to prepare a carbon electrode with X and Y dimensions ranging from mm to a minimum feature size of approximately 200 Âµm as determined by optical microscopy. Stylus profilometery was used to determine PPE devices have an approximate step height of 600 nm. Atomic force microscopy was employed to examine the surface roughness of PPEs, which were found to have a rms roughness of approximately 25 nm. Cyclic voltammetry (CV) with hexamine ruthenium was performed to examine the electrochemical behavior of the PPEs, which were consistent with the Randles-Sevcik equation. The PPEs also demonstrated electrochemical characteristics similar to commercial glassy carbon electrodes.

Toward Democratization: Enabling Non-Expert Access to MIDA Boronate Synthesis

Aidan M. Kelly, Peng-Jui Chen, Daniel J. Blair, and Martin D. Burke
University of Illinois at Urbana-Champaign

Organic synthesis widely relies on customized routes for the synthesis of small molecules. Due to the high level of expertise required to design and execute a synthetic route, there is a synthetic bottleneck which limits the participation of non-specialists. Our group has previously created an automated synthesis platform that iteratively assembles N-methyliminodiacetic acid (MIDA) protected haloboronic acid building blocks via Suzuki-Miyaura cross coupling reactions. The ultimate objective of this platform is to prioritize discovery of new function by enabling non-experts to augment their own research; producing and testing molecules without expert consultation. There are over 10,000 commercially available boronic acids which have the potential to engage with this automated synthesizer, but current methods for converting them into MIDA boronate building blocks require specialized glassware and a background in synthetic organic chemistry. Seeking to broadly enable access to these building blocks we have devised a synthesis protocol for MIDA boronates which is analogous to the widely used and operationally simple nucleic acid isolation kits. The procedure utilizes the catch-and-release properties of the MIDA boronates to obtain pure products in high yields without the use of chromatography or rotary evaporation. By placing building block synthesis in the hands of non-experts we mark another important step towards empowering non-experts to harness the power of small molecules.

FAP-targeted NIR Imaging of Cancer for Florescence Guided Surgery (FGS)

Kate Kragness and Ramesh Mukkamala
Purdue University

According to the American Cancer Society in 2019, there will be an estimated 1,762,450 new cancer cases diagnosed. A typical post-diagnosis cancer treatment plan is surgery followed by radiation and/or chemotherapy. However, there are challenges when patients follow this standard treatment plan. First, it can be difficult to determine which tissues are cancerous; depending on the type of cancer and the size of the tumors. Second, if most of the cancer cannot be surgically removed, the odds of radiation or chemotherapy being successful are significantly lower. Some patients may have to go through multiple cycles of radiation or chemotherapy. Multiple treatments could compromise the health of patients and they may not be strong enough to continue their treatment plan depending on their stage of cancer. Fluorescence guided surgery (FGS) can solve the identification and localization of cancer tissues. Cancer cells express a protein called FAP (if this is an acronym, type it out, then put â€œFAPâ€in parentheses) that can be targeted by a (specialized/synthesized/custom) ligand with a florescence dye tag. The ligand will only bind to FAP and cause the cancer cells to glow under direct florescent light in surgery. FGS allows the surgeons to remove cancerous tissues from patients more thoroughly, which greatly improves their odds for a successful outcome.

Magnetocaloric effect (MCE) and Magnetic Properties of the Co doped Gadolinium Nickel Gallides ($GdNi_{3-x-y}Co_xGa_y$)

Brittany N. Linn, George Agbeworvi, and Corey M. Thompson
Purdue University

Magnetic refrigeration (MR) is a developing green technology with the potential to reduce the concentration of chlorofluorocarbons- an ozone reducing gas- in the atmosphere by utilizing the magnetocaloric effect (MCE) of metals. This cooling technique is more efficient than current gas cooling methods as MCE has properties related to the Carnot cycle. Gadolinium ions are most suited to MCE materials, having the largest number of unpaired spins and greatest magnetic moment. The aluminide, $GdNiAl_2$, is a well-known MCE material which shows giant MCE due to its high magnetic entropy change (16.0 J/kg K at 5 T) and low T_C (28 K) which makes it suitable for low-temperature MR. Nonetheless, nothing is known about the magnetic properties of the gallide, $GdNiGa_2$ analog. Here, we report on the tuning of the magnetic and the magnetocaloric properties of the $GdNiGa_2$ by the partial substitution of Ni or Ga by Co on the crystal lattice of the $GdNi_{3-x-y}Co_xGa_y$ compound with the aim of further understanding their structure-property relations. The structural and physical properties of these new compounds will be highlighted in this talk.

Synthesis, Characterization, and Anticancer Activity of Aresenoplatin-4

Matthew Martin, Zohra Sattar Waxali, Wenan Qiang, Annie Fritz, Denana Miodragovic, and Thomas V. O'Halloran

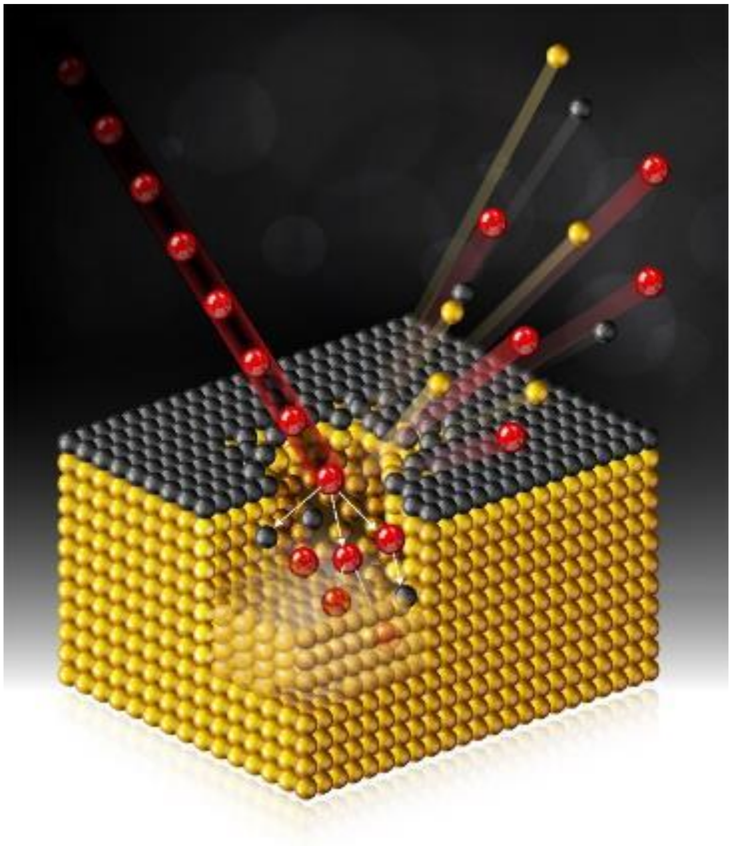
Northeastern Illinois University

The FDA approved anticancer drug, arsenic trioxide (As_2O_3), is highly efficient for treatment of acute promyelocytic leukemia, but due to its rapid renal clearance in the form of arsenous acid, $As(OH)_3$, it has been ineffective in the treatment of solid cancers. A new class of potent anticancer agents, that contain $As(OH)_2$ moiety bound to platinum(II) center, arsenoplatins $[Pt(\mu\text{-}NHC(R)O)_2XAs(OH)_2]$ ($R=CH_3$ or CH_3CH_2), X=Cl-, SCN-) have been synthesized. A high Pearson correlation coefficient (r = 0.96) was obtained while comparing anticancer activity of arsenoplatin-2 ($R = CH_3CH_2$, $X=Cl^-$; AP-2) to As_2O_3 in the NCI-60 screen, suggesting the two compounds act in a similar manner. This project aims to synthesize, characterize, and test the anticancer activity of an iodide analog of AP-2, labeled AP-4. X-ray, NMR, and elemental analysis have been completed to determine the structure and purity of this new compound. The cytotoxicity of AP-4 in the triple negative breast MDA-MB-231 cancer cell line has been evaluated by MTS cell proliferation assay. Interaction of AP-4 with the biologically important molecule glutathione (GSH) was assessed by fluorescent detection assay. GSH depletion has been shown to sensitize cancer cells that are resistant to platinum drugs. The effect of AP-4 concentrations on the GSH level is discussed. Based on current results, AP-2 and AP-4 may act as a delivery vehicle for As_2O_3, overcoming one of the primary limitations of As_2O_3 as a drug for solid cancers.

Insights Into PV Device Performance and Composition Using Time-of-Flight Secondary Ion Mass Spectrometry

Jonah Messinger, Fei Zhang, and Steve Harvey
National Renewable Energy Laboratory

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is a versatile ultra-high vacuum characterization technique widely employed in surface and interface analysis assays. TOF-SIMS analysis can obtain high-resolution surface spectrometry, imaging, depth profiling, and 3-D tomography. TOF-SIMS has excellent mass resolution spectrometry ($m/\Delta m > 9000$), lateral resolution capabilities on the order of 100nm, detection limits better than parts per million, and sub-nanometer depth resolution. The instrument can measure either positive or negative polarity secondary ion species and has adjustable primary ion beam energy and flux parameters that allow organic chemical information to be obtained. TOF-SIMS works by bombarding a sample at a surface with primary ions initiating a collision cascade in the sample, which ejects sample material as secondary ions. Secondary ions are then detected and characterized via time-of-flight analysis. TOF-SIMS is well-suited for surface and interfacial analysis of composition and species migration in thin-film solar cells, and in particular, organic-inorganic perovskite solar cells. My poster reports on my work this past summer at the National Renewable Energy Laboratory in the Interface and Surface Science group working on next-generation solar cells, both silicon-based and metal halide perovskite solar cells.



Target-Guided Screening Method for Myotonic-Dystrophy Type 1 Inhibitors Using Small Molecules

Niya L. Mitchell, Lauren D. Hagler, and Steven C. Zimmerman
University of Illinois at Urbana-Champaign

We want to find molecules that bind to DNA and inhibit the transcription of toxic RNA. We used Myotonic-Dystrophy Type 1 as a modeling system. I synthesized DNA-targeting small molecules with azide and alkyne functionalities for a target-guided screen against d(CTG)16. Groove-binding small molecules can undergo template-assisted click reactions and dimers containing these molecules inhibit transcription bidirectionally.

Ambient Mass Spectrometry of Agrochemicals in Soil Utilizing Paper Cone Spray Ionization Mass Spectrometry.

Makoy Overfelt, Shahnaz Mukta, and Cristopher C. Mulligan
Illinois State University

Various agrochemicals, such as pesticides and fertilizers, are regularly used to treat crops across the globe. These chemicals are used beneficially to protect and nourish a multitude of crops but can also have negative effects on the surrounding environments. Typical methods for identifying chemical contaminants in the environment consist of hyphenated mass spectrometry (MS) techniques; most commonly gas chromatography (GC) or liquid chromatography (LC) coupled MS. These techniques are highly reliable but require an inordinate amount of sample preparation and analyte processing. Paper Cone Spray Ionization (PCSI) can be coupled with portable MS systems to allow rapid on-site analysis of solid-phase material with virtually no prior sample preparation. PCSI involves using a dual-layer wax/filter paper cone to filter solid matrices from samples that would otherwise require extensive preparation. This technique allows both MS and MS/MS methods to be used to collect spectral data in-situ in a matter of minutes. The data obtained from the agrochemical samples in this experiment aligned closely with data obtained using traditional hyphenated MS methods in literature. This novel technique circumvents some of the tedious and time-consuming procedures present in previous techniques, and therefore has very promising potential applications in a variety of ambient situations.

Pd(II)/SOX Catalyzed Allylic C-H Amination for the Synthesis of Naftifine Derivatives

Andria Pace, Siraj Ali, Brenna Budaitis, and Jacob Garwin
University of Illinois at Urbana-Champaign

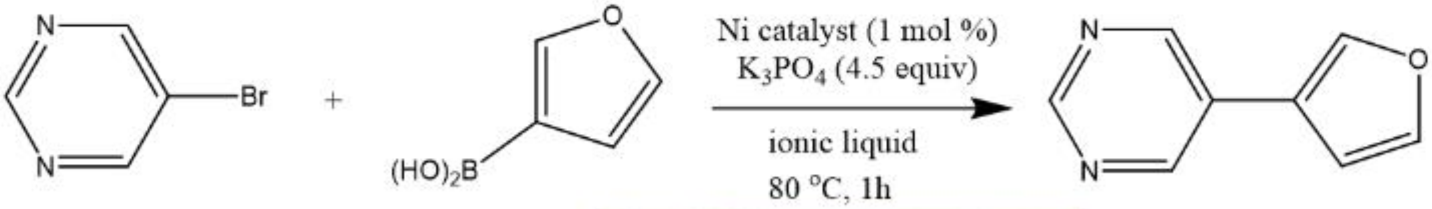
Tertiary amines are common motifs in numerous traditional and experimental therapeutics. Naftifine, a tertiary amine with antifungal properties, has recently been shown to exhibit anti-MRSA activity. An efficient route for derivatization would allow for a wide range of derivatives to be readily synthesized to be tested for further biological activity. C-H amination, which can directly install amine functionality into inert C-H bonds, has previously been limited to installing protected nitrogen sources, which requires deprotection and further manipulation to achieve the desired product. A method in which harsh deprotections or late-stage manipulations could be circumvented would therefore be ideal for the production of analogues for naftifine, thus allowing for a wide scope of derivatives to be produced efficiently. Herein we disclose such a method through a direct allylic C-H amination of transiently protected Lewis acid complexed amines via Pd(II)/ sulfoxide-oxazoline (Pd(II)/SOX) catalysis to synthesize naftifine and several key anti-MRSA derivatives.

POSTER SESSION I: POSTER 21

Synthesis and Characterization of Imidazolium Ionic Liquids

Sirikarn Phuangthong and Jocelyn Pineda Lanorio
Illinois College

Ionic liquid is defined as molten salt. Its properties such as being non-volatile, non-flammable, and non-combustible makes it a promising alternative for volatile organic solvents. There are currently several reactions that use ionic liquid as solvent. Furthermore, because of its high thermal stability and low solubility in water and polar organic solvents, ionic liquid can be recycled and reused, making it more environmentally friendly and promoting green chemistry. This poster describes the synthesis and characterization of a series of ionic liquids based off imidazole. Preliminary use of [bmim]Br ionic liquid in a Suzuki-Miyaura cross-coupling reaction proved to be successful, particularly when with polar $NiCl_2(PR_3)_2$ catalyst. Future work involves investigation of imidazolium ionic liquids as catalysts and optimization of conditions for their use as solvent and/or catalyst in Suzuki-Miyaura cross-coupling reactions.



Effects of Systemic Influenza Infection on Remyelination in an Animal Model

Isiah Ramos
Parkland College

Multiple Sclerosis (MS) is an autoimmune inflammatory disease of the central nervous system. MS is characterized by episodes of demyelination followed by partial remyelination. Cuprizone is a toxin that causes demyelination in specific regions of the C57BL/6 mouse brain, which remyelinate upon termination of cuprizone. Upper respiratory infections are known to exacerbate MS symptoms. We hypothesize that infection may impede remyelination, possibly due to a direct effect on oligodendrocyte maturation. If this is the case, we may find a reduced amount of mature oligodendrocytes and large amounts of oligodendrocyte precursor cells (OPCs) in areas of heavy demyelination in flu mice compared to controls. The aim of this study is to observe the impact of peripheral infection on remyelination in the corpus callosum, a known area of heavy demyelination in the cuprizone model.

Role of Oxygen in the Formation of Indophenols upon Photolysis of Azidophenoxides.

Evan Reeves, Rachael Knieser, and Paul G. Wenthold
Purdue University

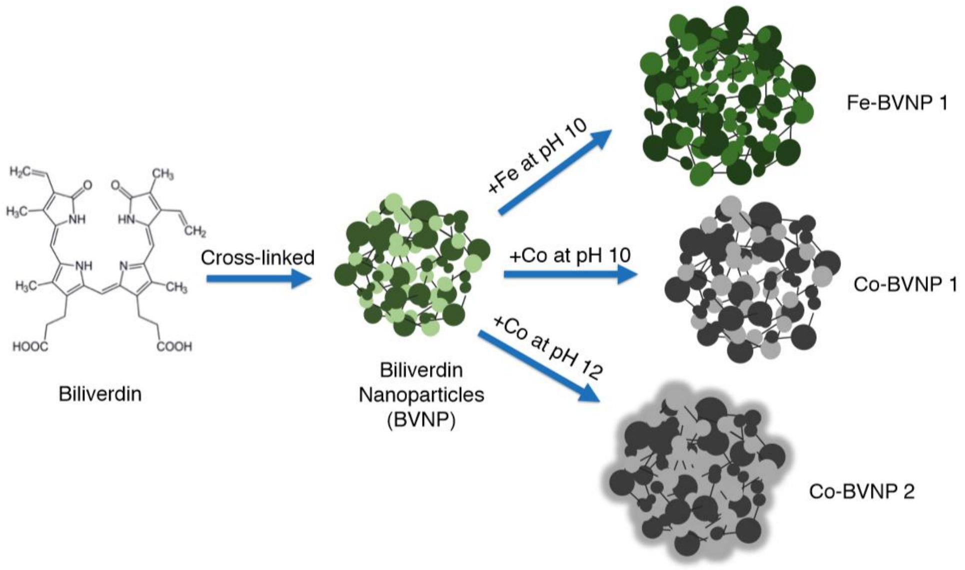
It has been found previously that indophenols can be formed by photolysis of p-azidophonoxide ions. The mechanism of the photolysis has been explored but remains not well understood. In this work, we have examined the mechanism of the reaction by using time-resolved electrospray ionization. Relative ion intensities of reactants and products were used to monitor and compare the indophenol formation over time. The role of oxygen in the photolysis mechanism was explored by running the reaction in solutions saturated with either oxygen or nitrogen. The results have shown that indophenol formation was increased in the oxygen saturated solutions and the nitrogen saturated solutions yielded indophenol formation consistent with the control, indicating that molecular oxygen participates in the reaction, suggesting a single-electron-transfer mechanism.

POSTER SESSION I: POSTER 24

Metal-Chelated Biliverdin Nanoparticles as Magnetic Resonance Imaging (MRI) Contrast Agents

Ayman Roslend, Parinaz Fathi, Fan Lam, and Dipanjan Pan
University of Illinois at Urbana-Champaign

Sentinel lymph node biopsies are commonly used to identify the extent and location of cancer metastases. Patients who undergo this procedure may be vulnerable to nerve damage, infection, and lymphedema. A non-invasive alternative to this current procedure that could potentially eliminate the risk of post-surgery complications is to utilize imageable nanoparticles. A recent study by our lab utilized biliverdin, an endogenous, metabolically biodegradable molecule produced in the liver, to create these nanoparticles. It was discovered that biliverdin nanoparticles (BVNPs) possess properties that are useful for photoacoustic imaging and fluorescence imaging. However, these imaging techniques are not commonly used in hospitals and clinics for medical imaging, obstructing the immediate clinical translation of BVNPs. This study focuses on the potential use of BVNPs as Magnetic Resonance Imaging (MRI) contrast agents, by which Co and Fe are chelated onto the tetrapyrroles in biliverdin, forming magnetized BVNPs that provide MRI contrast. In this work, we explored the role of synthesis conditions in the successful chelation of cobalt and iron atoms. Metal-chelated BVNPs were characterized using UV-Visible spectroscopy, fluorescence spectroscopy, transmission electron microscopy, inductively coupled plasma spectroscopy, and magnetic resonance imaging. We determined that the synthesis conditions and choice of metal had a direct impact on metal chelation and the resulting MRI contrast.



POSTER SESSION I: POSTER 25

A Bioluminescent Calreticulin Reporter for Measurement of Immunogenic Cell Death in Pancreatic Cancer Cells

Karissa Scales, Rebecca Bocian, April Franco, Eric Gurzell, and Mette Soendergaard
Western Illinois University

The five-year survival rate for pancreatic cancer patients is less than 7%, which emphasizes the need for more efficient treatments. Immunotherapy has proven to prolong the life of cancer patients, and in some instances long-term survival has been reported. Immunogenic cell death (ICD) is a type of programmed cell death for which translocation of calreticulin (CRT) to the plasma membrane is a hallmark event. Human CRT was tagged with the HiBit peptide sequence, which complexes with cell membrane impermeable LgBit to form a bioluminescent complex. In brief, polymerase chain reaction (PCR) was used to amplify the CRT gene. CRT was cloned into the HiBit plasmid using restriction enzyme digestion (SbfI and PspXI) and T4 DNA ligation. The ligation product was transformed into E. coli DH5Î±, isolated, and analyzed using gel electrophoresis and DNA Sanger sequencing. Results showed that the human CRT gene was successfully inserted into the HiBit plasmid. Next, the CRT-HiBit reporter was transfected into human pancreatic cancer cells (Mia-Paca-2). Cells were incubated with 1:6 CRT-HiBit DNA and TransIT LT1 transfection reagent (Mirus Bio, WI) in OptiMEMI for 30 minutes, and then allowed to grow at 37Â°C 5% CO2 for 48 h. Geneticin (2000 Î¼g/mL) was used to select transfected cells for 7 days. Transfected cells were propagated under 500 Î¼g/mL geneticin pressure. These cells will next be used to detect induction of ICD by compounds from natural compound and drug libraries.

Determination and the Quantitative analysis of *E. Coli* in Milwaukee Rivers

Brittney Stelzl, Elizabeth Garcia, Karla Herandez-Garcia, and Joselin Rodriguez Santiago
Alverno College

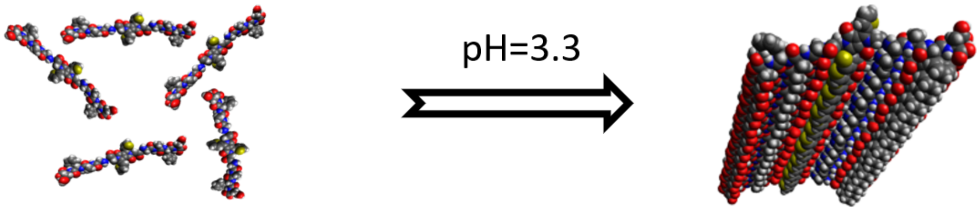
The focus of this investigation was to determine whether the water samples collected from three different locations of the Kinnikinic River, contained *Escherichia Coli* and how many colonies were present. The water samples were collected once a week from the following parks in the Milwaukee area: Wilson Park, Zablocki Park, and Jackson Park. Several procedures were used to confirm that *E. coli* was present in the water and a simple dilution method was used to determine the quantitative amount of *E. coli.* Jackson and Wilson Park had had the highest average concentration of E.coli at $10x10^7$ colonies. Zablocki had an average of $24x10^6$ colonies. The data was shared with the Milwaukee Riverkeepers.

POSTER SESSION I: POSTER 27

Self-assembly Behavior of Sequence-defined Pi-conjugated Oligopeptide

Boran Sun, Hao Yu, and Jeffrey S. Moore
University of Illinois at Urbana-Champaign

Supramolecular assembly is a powerful method to generate advanced materials with well-defined structures and emergent functionality. On the other hand, thiophene-diketopyrrolopyrrole (TT-DPP) is a donor-acceptor structure which is extensively used in high-performance industrial organic electronics. Here, we report the synthesis as well as pH-driven self-assembly behavior of π-conjugated oligopeptides built on a TT-DPP core. π-conjugated oligopeptide was synthesized by directly coupling single- or bi-functional TT-DPP conjugated core with sequence-defined oligopeptides. In this work, H-bonding between flanking peptides and π−π stacking between adjacent TT-DPP core interact synergistically to promote a programable control of self-assembly behavior. Controlled self-assembly upon lowering pH condition is characterized by UV-vis and fluorescence spectra. Our observation is attributed to a strong enthalpic H-bonding interaction under acidic conditions. With insight from Density Function Theory (DFT) calculations, we find that the electronic structure of TT-DPP conjugated core plays a key role in determining the self-assembly behavior. From a broad perspective, we envision this work will guide the design of next-generation organic semiconductor materials.



Solvent Effects on Alkene Epoxidations in Ti-zeolites

Jun Zhi Tan, Daniel T. Bregante, and David W. Flaherty
University of Illinois at Urbana-Champaign

Epoxides (e.g., propylene oxide; PO) are important precursors used within the plastics and pharmaceutical industries and are often produced using environmentally-harmful oxidants (e.g., chlorine). Currently, the hydrogen peroxide (H2O2)-PO process is one of the only industrial methods for epoxide production using a green oxidant (i.e., H2O2), which operates over titanium silicalite-1 catalyst in methanol (CH3OH) solvent. Rates for epoxidation vary by orders of magnitude when the solvent is substituted with acetonitrile (CH3CN) or when the catalyst is substituted with other Ti-silicates. The literature lacks governing design principles that identifies the optimum solvent and catalyst combination for epoxidation reactions. As such, understanding the role of solvents in stabilizing the reactive species responsible for epoxidation reactions is critical to the design of systems for other epoxidation reactions. Here, we analyze the reaction kinetics of 1-octene epoxidation on Ti-substituted zeolites in CH3CN and CH3OH. Turnover rates for epoxidation in Ti-BEA are lower by a factor of 10 in CH3OH than in CH3CN; however, this difference in turnover rates is not due to difference in mechanism or difference in identity and electronic properties of reactive intermediates, which are indistinguishable among all materials. The results show that the difference in turnover rates must reflect differences in the stabilization of reactive surface species mediated by the solvent molecules.

Electrodepositing Switchable Photovoltaic Window Electron and Hole Transport Layers

Rachel W. Tham[1], Kevin Prince[2,3], Anica Neumann[3], Caleb Boyd[3], and Lance Wheeler[3]
[1]*University of Illinois at Urbana-Champaign*
[2]*Colorado School of Mines*
[3]*National Renewable Energy Laboratory*

Vertical glass facade buildings, such as skyscrapers, have significant potential for generating electricity using solar window technologies, such as SwitchGlaze, a switchable photovoltaic window. This window contains a perovskite layer that absorbs visible and UV light. To commercialize this and other perovksite solar cells, it is essential to optimize a scalable production process, such as electrodeposition, which can controllably fabricate stable transport layers. This technique can then be used to fabricate back contact solar devices to decrease delamination occurrence and allow for more sunlight to directly interact with the perovskite and increase device efficiency. Nickel oxide (NiO_x) and tin oxide (SnO_2), are especially promising transport layers due to their high stability and electron mobility, respectively. Both can be fabricated at room temperature and are also suitable for window technology due to their high transparency. A three-electrode system was used to determine which electrolyte concentrations, electrodeposition times, current densities, and annealing times would electrodeposit transport layers that are the most uniform, thinnest, and have least surface roughness. This work was supported in part by the U.S. Department of Energy, Office of Science, Office of Workforce Development for Teachers and Scientists (WDTS) under the Science Undergraduate Laboratory Internships Program (SULI).

Synthesis of Cyclopropene Derivatives for use as Ethylene Antagonists

Ben Vaupen, Bin Zhang, and Mark Lipton
Purdue University

Ethylene is used by plants as a hormone to control many physiological processes throughout the lifetime of a plant, including seed germination, growth, and fruit ripening. Ethylene antagonists are used in the market for a wide variety of reasons; however, the most widely used compound, 1- methylcyclopropene, has several drawbacks. These include high volatility, low solubility in water, and high reactivity. The primary goal of this research is to functionalize cyclopropene compounds to be used for a broad range of market needs with fewer negative properties.

Synthesis and Characterization of Ruthenium-Based Alzheimer's Disease Therapeutics

Brendan J. Wall, Mark F. Will, and Michael I. Webb
Illinois State University

Amyloid-beta (Aβ) peptide aggregation is a primary characteristic of Alzheimer’s disease (AD), the most common neurodegenerative disorder. Aβ peptide aggregates have been observed to contain the redox-active metals, copper and zinc, which lead to the generation of reactive oxygen species which are damaging to nearby neural membranes, and is the basis for the development of AD. Given the affinity of Aβ peptide aggregates for metal ions present in the brain, metal-based therapeutics should offer an alternative target for Aβ, preventing aggregation and reactive oxygen species. The Ruthenium metal complex, imidazolium trans-tetrachloro(dimethylsulfoxide)imidazoleruthenium(III) (NAMI-A) has been studied for its effect on binding the Aβ peptide and have proven effects in preventing Aβ aggregation. However, questions regarding the relationship between the ligands around the Ruthenium metal center, and the complex’s activity need to be defined to advance development of Ruthenium-based AD therapeutics. We have prepared pyridine-based NAMI-A derivatives and have begun to characterize their interactions with Aβ. Preliminary data shows that there is association between our derivative complexes and the Aβ peptide, further evaluations of this interaction are ongoing and will be discussed.

POSTER SESSION I: POSTER 32

Antioxidant and Cytotoxic Activity of Acmella alba, Acmella oleracea, and Acmella calirrhiza

Lindsey Weintraub, Trisha Naftzger, Shelby Henning, and Mette Soendergaard
Western Illinois University

Plants of the genus Acmella are utilized as medicinal herbs. However, there is little research documenting cytotoxic and antioxidant properties of the plants. Acmella alba, Acmella oleracea, and Acmella calirrhiza were harvested, freeze dried and ground into a fine powder. For antioxidant assays, plant materials were extracted using 1% HCl in 90% aqueous methanol for 2 h. The supernatant was used in DPPH and Folin assays to determine the antioxidant capacity and phenolic content, respectively. Results showed that the antioxidant capacity of roots (Î¼mol/g dry weight) for all three plants was significantly lower compared to all other tissues. Similarly, the roots exhibited significantly lower phenolic content. The leaves contained the highest phenolic content for Acmella alba and Acmella oleracea, while for Acmella calirrhiza this was the case for the flowers. Interestingly, the flowers of Acmella calirrhiza is most commonly used for medicinal purposes. For cytotoxic analysis, plant materials was extracted thrice using methanol for 24 h. Extracts were evaporated at 50ÂºC, and dissolved in DMSO. Ovarian cancer (SKOV-3) cells were cultivated in McCoy's 5A with 10% FBS at 37Â°C, 5% CO2. Cells were then treated with 0.2 mg/mL extract, DMSO or 1 Î¼M paclitaxel for 24 h. Cell viability was determined using the tetrazolium dye assay. Interestingly, results showed that roots and flowers from Acmella calirrhiza significantly increased cell viability in ovarian cancer cells.

Lycopene in Grafted and Hydroponically Cultivated Heirloom Tomatoes

Jael Wotsho, Jamie Greathouse, Shelby Henning, and Mette Soendergaard
Western Illinois University

Heirloom tomato varieties are challenging to produce due to disease susceptibility and low yield. To overcome these difficulties, heirloom tomatoes may be grafted onto disease resistant rootstocks and be cultivated hydroponically. However, the effect of these cultivation methods on the lycopene content of heirloom tomatoes is unknown. Heirloom (Green Zebra and Black Krim) and standard (Big Beef) tomatoes were grafted onto wild type (WT) or disease resistant rootstocks (Arnold and Supernatural) and cultivated hydroponically. Tomatoes were harvested, freeze dried, and ground into a powder. Lycopene was extracted twice from 0.1 g tomato powder using hexane/acetone/ethanol. Distilled water was added and the non-polar layer containing lycopene was collected. The absorbance at 503 nm was measured spectrophotometrically. Results showed that Black Krim grafted onto Arnold exhibited significantly higher ($p<0.001$) lycopene compared to WT and Supernatural rootstocks. Green Zebra showed a similar tendency with higher lycopene content when grafted on Arnold. However, the difference was not statistically significant. The lycopene content was not changed for any of the Big Beef cultivars. Taken together, these results indicate that the type of grafting rootstock influences the total lycopene content of certain heirloom tomato varieties. These results may be valuable to producers of hydroponic heirloom tomatoes to ensure maintenance of marketable antioxidant content.

Investigation of Electronic Parameters in Oxidopyrylium Based [5+2] Cycloadditions

Adam J. Youman, Samantha N. Rokey, John R. Goodell, and T. Andrew Mitchell
Illinois State University

The generally accepted thermal activation mechanism of silyloxy pyrones proceeds via a zwitterionic oxidopyrilium intermediate en route to the corresponding [5+2] cycloadducts. Recently, our group has explored a series of [5+2] cycloaddition precursors with a focus on olefin electronics and silyl transfer group steric hindrance. In order to further these endeavors, a series of styrenyl precursors was subjected to uniform reaction conditions and evaluated using Hammett plot analysis. Under thermal activation, Hammett plot analysis revealed a non-linear relationship where increasing electron withdrawing potential resulted in a positive slope, and increasing electron donating potential resulted in a negative slope. Conversely, under TBSOTf activation which proceeds via a bis-silylated cationic intermediate, Hammett plot analysis revealed a negatively sloped linear correlation across the entire series. It is proposed that a positive slope is analogues to normal demand Diels-Alder reactions whereas a negative slope is comparative to an inverse electron demand Diels-Alder. Taken together, the current data suggests that a more complex mechanistic picture exists with a dependence on both electronics and sterics.

Emerging Contaminants in the Kinnickinnic River - Metals

Patricia Zamora, Erika Olvera, Ana Olvera, and Alex Blom
Alverno College

The project consisted of finding a suitable method to monitor the levels of metals such as iron, sodium, copper, magnesium, calcium, and lead in the water from the Kinnickinnic River using atomic absorption spectroscopy. For seven weeks water samples from Jackson, Wilson and Zablocki parks were collected and analyzed using atomic absorption spectroscopy with an air/acetylene flame, emission and absorbance were used to analyze the water samples. In addition, since lead is present at lower amounts, the standard addition method was used to avoid matrix interferences. Results for iron, sodium, and magnesium produced inconsistent plots hence no further investigations were done. Initial results for copper showed no significant amounts of this metal in any of the water samples, therefore, no further analysis was performed. However, an accurate linear plot was obtained for calcium by adding lanthanum chloride to the water samples and shifting the instrument's flame 30 degrees. The results for lead were higher than expected being in Jackson park 1.346 ppm, Wilson 1.448 ppm, and Zablocki 1.186 ppm. Also, the water from the three parks showed roughly 100 ppm calcium.

A High-throughput MALDI-ToF MS-based Screening Method for Medium-chain Fatty Acid Detection

Linzixuan (Rhoda) Zhang, Pu (Mason) Xue, and Huimin Zhao
University of Illinois at Urbana-Champaign

Free fatty acids (FFAs) are significant products that exist in crucial nutrients, soaps, and fuels. This attracts extensive investigation on the production and selection of FFAs in fungi. Specifically, controlling chain length compositions of the FFAs is desired to achieve efficient formation of valuable biofuels and chemicals. However, current method for selection of shorter-chain length FFAs, which involves esterification and derivatization in gas chromatography mass spectrometry (GC-MS), is time-consuming and labor-intensive. Here, we report an MS-based high-throughput screening method for detecting medium-chain fatty acids (MCFAs) in *Saccharomyces cerevisiae* by using lipids as a proxy. Four key residues in the fatty acid synthase (FAS) were genetically modified with site-saturation mutagenesis. Achieving 95% library coverage, 288 colonies were screened by matrix-assisted laser desorption/ionization time-of-flight (MALDI-ToF) MS in the downstream phenotypic analysis. The results showed significant improvements in shorter acyl-chain phosphatidylcholine (PC) production in all the mutants compared to the wild-type (WT). We further correlated the lipids with MCFAs by GC-MS characterization. Among all the mutants, the M1251S mutant presented almost 400-fold improvement in octanoic acid production than the WT. This generalizable detection technology could be widely applicable for controlling FFA compositions in a high-throughput manner for various yeast species.

Rational Design and Synthesis of a Red-Fluorescent Probe for Aldehyde Dehydrogenase 1A1

Guadalupe Aguirre-Figueroa, Thomas E. Bearrood, and Jefferson Chan
University of Illinois at Urbana-Champaign

Cancer stem cells (CSCs) make up only a small percentage of all cancer cells, but they are believed to be the root cause of the problems associated with cancer including recurrence and metastasis. With functional roles in endogenous and xenobiotic aldehyde detoxification and cellular signaling, Aldehyde Dehydrogenase (ALDH) 1A1 is an important marker upregulated by these CSCs. The Chan Lab recently reported AlDeSense, a highly selective, activity-based probe for ALDH1A1 that allowed for in vivo imaging. A red-shifted version based on the TokyoMagenta (TM) dye platform was proposed to reduce the limitations of AlDeSense including an overlapping absorbance and emission profile with FITC and GFP and a lack of permeability. With a 100 nm bathochromic shift, the new probe required rational design of the d-PeT quenching benzaldehyde to achieve a good fluorescence turn on while maintaining selectivity. Furthermore, the higher pKa of the TM platform makes the final probe cell permeable, negating the previous need for an enzyme-responsive capping group. With this new probe for ALDH1A1 paired with previously developed green-fluorescent chemical biology tools, we are actively pursuing simultaneous multianalyte imaging of ALDH1A1 and other biological species of interest in CSCs.

Chemoselective Differentiation of Bis(monoacylglycero)phosphate (BMP), Phosphatidylglycerol (PG)

Fatima Akili, Justin T. Mohr, Stephanie Cologna, and Melissa Pergande
University of Illinois at Chicago

Bis(monoacylglycero)phosphate (BMP) and phosphatidylglycerol (PG) are isomeric lipids found in endosomal membranes. The objective of this project is to distinguish the two isomers as they are not readily differentiated by mass spectroscopy. We propose to discern isomeric 1,2-diols via chemoselective reactions by using a pair of phosphoryl diglycerides differing in acylated hydroxyl groups as primary model for this investigation. The diols selectively cyclize into carbonates which are observed in mass spectroscopy on the isomer lacking adjacent hydroxyl groups. Further investigations with larger ring carbonates will be explored to predict hydroxylation patterns and ultimately differentiate BMP and PG. With this knowledge, we hope to be able to tag various biological lipids in membranes using selective chemical reactions to further understand membrane composition and functionality of these lipids.

How to Create a GTA Manual - Investigation of Best Practices in GTA Training and Departmental Needs.

Ahmad H. Alfoudari, Charles R. Enlow, and Franziska K. Lang
Purdue University

Graduate Teaching Assistants (GTAs) are a vital means for teaching undergraduate students at universities and colleges, particularly in large-enrollment introductory courses. Although GTA training manuals are a useful and effective means of communicating relevant skills and resources, one size does not fit all. We present a model for the development of a GTA training manual that is informed by the existing literature and meets the specific needs of our department. Firstly, we performed a thematic analysis of 102 articles on GTA training to determine which topics related to GTA training are discussed in the literature. Secondly, we consulted 8 experts involved in GTA training within our department to gauge topics they identified as necessary for GTAs to learn. Preliminary findings show both alignment and differences between the topics that are reported in the literature and the topics that the department's experts identified as important. This suggests that a GTA manual could benefit from incorporating voices in the department to increase its relevance and utility. Future work will involve collecting data to investigate the goals and perceptions for other stakeholders, such as graduate students and research advisors. Through the process discussed above, we propose a model for the development of departmental resources such as GTA manuals and hope to empower other departments to utilize the same process for creating their own contextualized and relevant GTA training guides.

Chiral Auxiliaries for Diastereoselective γ-Functionalizations of Carbonyl Substrates

Anh M. Bui, Sara Y. Siddiqui, and Justin T. Mohr
University of Illinois at Chicago

Stereodefined γ-functionalized carbonyls are prominent functionalities amongst several valuable bioactive molecules. However, synthetic pathways for preparing these carbonyls remain a relatively underdeveloped topic in organic synthesis. Consequently such transformations are scarce, let alone stereoselective. Amidst a shortage of these transformations, recent literature published by the Mohr Group provides effective methodologies for various regioselective heteroatomic γ-functionalizations. Control over the diastereotopic faces of the reactive intermediates has proven to be a challenge, and therefore we have proposed employment of chiral auxiliaries to enhance this selectivity. Auxiliaries of the oxazolidinone class have remained a classic choice in asymmetric synthesis, however their efficacy is only proven for substrates bearing α- and β- relationships. We have begun synthesis of novel oxazolidinone chiral auxiliaries, with which we intend to quantify and refine the diastereomeric ratios of our γ-functionalized products.

Iterative Stereospecific Csp3-Csp3 Coupling Using Bifunctional Carbenoid-Boronate Building Blocks

Sriyankari Chitti, David Kostrya, V. Mubayi, Daniel J. Blair, and Martin D. Burke
University of Illinois at Urbana-Champaign

The building block based approach - or the iterative assembly of interchangeable parts is increasingly being recognized as a highly flexible and efficient method for the construction of small molecules. For biopolymers such as polypeptides, oligosaccharides and oligonucleotides the common linkages between building blocks is easy to recognize. This has led to the development of automated platforms which have broadly enabled both experts and non-experts to explore biopolymer chemical space. If a similar strategy could be applied to small organic molecules the societal impact would be tremendous as it would address a key bottleneck in the development and discovery of new drugs, fragrances, fertilizers and materials. A building block based analysis of small organic molecules is substantially more challenging as the repeating units are not obvious. However, if C-C bond forming reactions could be rendered sufficiently general, then essentially any C-C bond could be regarded as a common linkage. Toward this objective, we are developing bifunctional building blocks which contain a protected boronate and a masked chiral carbenoid. Treatment of these carbenoids with a simple Grignard reagent promotes a stereospecific coupling reaction with an unprotected boronate such that a C-C bond is formed with near-perfect stereocontrol. After having developed conditions for iterating this method, we are exploring how this method can be applied within the context of total synthesis.

Environmental Ruggedness of a Portable MS System Coupled With Paper Spray Ionization During Field Operation

Phoebe C. Clowser, Jessica M. Holtz, Ashley R. Stelmack, Shahnaz Muktah, William L. Fatigante, and Christopher C. Mulligan
Illinois State University

Combining mass spectrometric (MS) instrumentation with ambient ionization sources increases screening time which in turn allows brisk analysis of samples. Applying this to a portable MS system can be beneficial in both forensic and environmental applications. Groups such as law enforcement and environmental scientists can take advantage of this idea in on-scene analysis of substances which appear in minute quantities. Environmental effects can influence portable instrumentation performance which can influence the acceptability of the data collected. In this work, the performance of a portable MS system featuring a homebuilt paper spray ionization (PSI) sources is determined across a wide range of environmental factors such as ambient temperature, relative humidity, and wind speed/direction.

POSTER SESSION II: POSTER 43

Evaluating Biotransformation Efficiency of Oleic Acid to10-Hydrodroxystearic Acid by Two Secondary Alcohol Dehydrogenase Knockout Mutants of Nocardia cholesterolicum NRRL5767

Lilliana Dunterman, Alice Axline, Lisa Wen, and Jenq-Kuen Huang
Western Illinois University

Hydroxy fatty acids (HFAs) have potential industrial applications. Most renewable plant oils(corn and soybean oil) contain little HFAs. The unsaturated fatty acids from plant oils can be converted to value-added HFAs chemically or enzymatically. We are interested in improving Nocardia cholesterolicum NRRL5767 (NC NRRL 5767) for several reasons: it is a stable industrial microorganism, it converts oleic acid and linoleic acid to corresponding HFAs in high yield with minor keto fatty acids. We intend to improve NC NRRL 5767 by CRISPR/Cas9genome editing to knockout the secondary alcohol dehydrogenase (2 o -ADH) gene, thus blocking the conversion of hydroxy fatty acids to their keto derivatives. We have recently obtained two knockout mutants of 2 o -ADH of NC NRRL5767. We are now evaluating the biotransformation efficiency of oleic acid to10-hydrodroxystearic acid (10-HSA)by these two knockout mutants. The two mutants and wild-type NC NRRL 5767 were cultured. Individual cell pellet was used to set up biotransformation reaction containing one mL of 100mM sodium phosphate buffer (pH 6.8) and 5 ÂµL oleic acid (as substrate). Biotransformation was carried at 37 o C for 8 hrs. The yield of biotransformation products was analyzed by TLC and will be further quantified by Gas chromatography (GC). Our preliminary results from TLC analysis indicated that there is a similar yield of 10-HSA from the knockout mutants and the wild-type NC NRRL 5767.

Unknown Nepetalactone Isomer Elucidated from Nepeta citriodora Extract

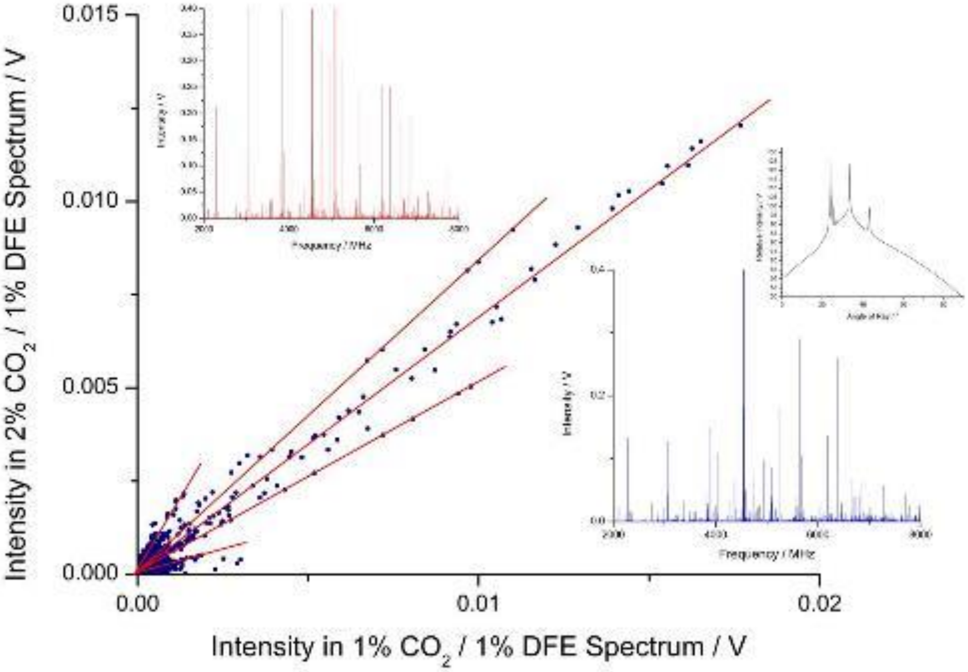
Jeffrey Dykstra, Laila Nawab, Tia L. Walker, and Ian S. Taschner
Indiana University Northwest

Many species within the Nepeta genus, commonly referred to as catnip, biosynthetically produce a mixture of diastereomeric monoterpenes, known as nepetalactones. Deep Water Culture and Flood and Drain hydroponic systems were constructed and five Nepeta speciesâ€”N. cataria, N. citriodora, N. clarkei, N. faassenii, and N. parnassicaâ€”were grown from seed. Each cultivar was subjected to sonication in hexanes for terpene extraction, and potential nepetalactones identified via gas chromatography in tandem with mass spectrometry (GCMS). The trans-cis and cis-trans nepetalactones were extracted via steam distillation and separated from N. cataria. A nepetalactone with unknown stereochemistry was extracted via steam distillation from N. citirodora and purified. The isolated nepetalactones were subjected to CHN elemental analysis to be used as analytical standards. A dynamic through-space NMR NOESY experiment was conducted to determine the stereochemistry of the unknown nepetalactone isomer. Nepetalactone was quantified via GCMS for each Nepeta species, and multiple extraction techniques were tested for maximization. Multiple N. cataria cultivars were subjected to varying pH conditions for evaluating the effect of pH on nepetalactone expression.

Implementing Extended Cross Correlation as a Tool to Identify Patterns in Microwave Spectra, and its Application to Fluoroethylene/Carbon Dioxide Clusters

Hannah L. Fino, Rebecca A. Peebles, Sean A. Peebles, Channing T. West, and Brooks H. Pate
Eastern Illinois University

Extended cross correlation (XCC), originally implemented by Professor Robert Field at MIT, is an analytical technique that extracts subgroups of related data to provide separated spectra for different species. XCC correlates the intensities of peaks between two spectra recorded with one varying experimental parameter in order to identify patterns of transitions for which this variation leads to similar changes in intensities. Efficiently analyzing the components of complex mixtures has many different applications, such as determination of impurities that may result during pharmaceutical synthesis. This project investigated automation of the XCC method by implementing programming in Mathcad, Python, and Excel. The developed XCC tools were applied to spectra of clusters containing 1,1-difluoroethylene and carbon dioxide. The separation of experimental microwave spectroscopy data for different sized clusters, when comparing spectra recorded with varying carbon dioxide concentrations, was probed.



The Search for New Solid-State Electrolytes: Investigating the Structural Properties of Substituted Li_5MO_4 or Li_6MO_4 Antifluorite Materials

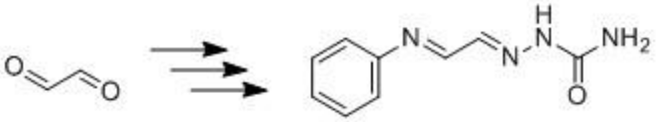
Matthew A. Frank and Paris W. Barnes
Millikin University

Lithium ion batteries have been studied since the early 1970s and have undergone limited change in regard to the advancements in other fields. Mobile battery power is a necessary aspect of modern living, but the current battery model has limitations. As part this project, different potential solid-state electrolytes – Li_5MO_4 (M = Al, Ga, In, or Sc), Li_6ZnO_4, Sc^{3+}-doped Li_5AlO_4, and Ti^{4+}/Zn^{2+}-doped Li_5AlO_4 – were synthesized and analyzed using X-ray powder diffraction (XRPD). Data collected on materials that were previously reported in the literature were compared to published XRPD data. Li_5AlO_4 and Li_6ZnO_4 were likely synthesized whereas Li_5InO_4 and Li_5GaO_4 did not appear to adopt the antifluorite structure. XRPD data for the Sc^{3+}-doped materials suggested that the Sc^{3+} was not successfully doped into the antifluorite material. However, initial XRPD data for the Ti^{4+}/Zn^{2+}-doped Li_5AlO_4 suggested that the materials were successfully incorporated into the antifluorite structure.

Preparing Imine Analogues of Cinnamaldehyde Semicarbazone to Explore Their Photochromicity

Kaylee D. Fuller-Svarz and Edward M. Treadwell
Eastern Illinois University

Compounds undergo a reversible color change when exposed to and removed from light, and are commonly used in transition lenses, energy-saving windows, and optical switches. Photochromicity in the solid state is rare, with cinnamaldehyde semicarbazide being one example. This research seeks to determine if cinnamaldehyde semicarbazone analogues where the vinylic unit is replaced by an imine are also photochromic. A direct pathway to these 2-(phenylimino)acetaldehyde semicarbazones, where p-anisidine, glyoxal, and semicarbazone HCl were all mixed together, together gave a complex mixture, while combining p-anisidine and glyoxal gave only the dimer in 17.8 % yield. Reaction of glyoxal and semicarbazone gave a solid that has been difficult to characterize. `Stepwise pathways where glyoxal dimethyl acetal was reacted with either m-anisidine or semicarbazone HCl are currently being explored.



POSTER SESSION II: POSTER 48

Polyurethane Hugoniot for Polymer-Bonded Explosives

Hoya Ihara, Belinda P. Johnson, and Dana D. Dlott
University of Illinois at Urbana-Champaign

Our group has developed a Shock Compression Microscope (SCM) to investigate explosive materials under extreme conditions. The purpose of my current work is to construct a Hugoniot for a polyurethane elastomer which is commonly used in munitions to bind explosive crystals together. The SCM utilizes a 1064 nm Nd:YAG laser to eject a 25 Âµm aluminum impactor, or flyer plate. The laser-driven flyer plate hits the polymer surface and shock compresses a sample up to tens of GPa. The entire process starting from the flyer launching to the shock impact was characterized by an 8 GHz fiberoptic photon Doppler velocimeter. The shock velocity was obtained from Al flyer and the particle velocity was obtained from the gold-coating under the sample allowing us to calculate the shock transit time through the sample. Elucidating the Hugoniot for polymers allows us to determine pressures during shock experiments which in turn allow us to characterize the behavior of explosives under shock.

2,6-Didehydropyridinium Cations Can React From An Excited Triplet State

Hanning Jiang, Xin Ma, Erlu Feng, John J. Nash, and Hilkka I. Kenttämaa
Purdue University

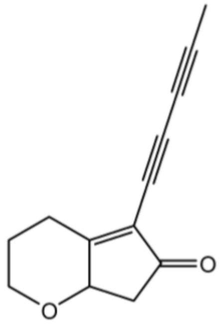
The 2,6-didehydropyridinium cation, a protonated aromatic carbon-centered σ,σ-biradical with a singlet ground state, was reported to react with many reagents via predominant proton transfer that occurs from an excited triplet state. Based on calculations, the triplet state of the neutral biradical has a lower proton affinity (PA) of 196.9 kcal/mol than that of the singlet state (209.7 kcal/mol). The biradical differs from all other meta-benzyne type biradicals studied thus far in that it has the smallest singlet-triplet splitting (-11 kcal/mol). To explore similar biradicals with small singlet-triplet splittings, several substituted (-Cl, -CN, -OH) 2,6-didehydropyridinium cations were studied in a linear quadrupole ion trap mass spectrometer. Proton transfer to allyl iodide (PA = 193.4 kcal/mol) indicated that both the 4-hydroxy- and the 3-chloro-2,6-didehydropyridinium cations reacted from their triplet states. Although the 3-cyano- and 4-cyano-2,6-didehydropyridinium cations (triplet state PAs of neutral biradicals 183.5 and 185.0 kcal/mol, respectively) showed fast H+ transfer to allyl iodide, they likely reacted from their singlet states due to the relatively low PAs of the singlet states of the neutral biradicals (PAs194.8 and 196.9 kcal/mol, respectively). On the other hand, both cations transferred a proton to ethanol with a lower PA (185.6 kcal/mol), which confirmed that proton transfer occurred from the triplet states of these protonated biradicals.

POSTER SESSION II: POSTER 50

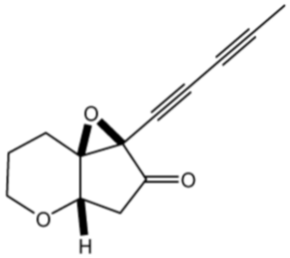
Synthesis of Chrysindin A and B via the Pauson-Khand Reaction

Rida Khan and Justin T. Mohr
University of Illinois at Chicago

Active ingredients of the Chrysanthemum indicum plant, from which the natural products chrysindin A and B were extracted, have been used in traditional Chinese medicine to treat vertigo, headaches, and various inflammatory conditions. Although not yet evaluated in pure form, the chrysindins are expected to possess similar bioactive properties. The chrysindins pose a synthetic challenge to organic chemists due to the presence of a conjugated diyne functional group and bicyclic core structure. We have proposed the synthesis of these compounds through the use of an atypical adaptation of the Pauson-Khand reaction (PKR). This requires employment of the PKR on a conjugated triyne instead of a simple alkyne. Thus, these syntheses will allow us to explore the limitations of the PKR while providing essential insight on polyyne reactivity for further syntheses of complex compounds.



Chrysindin A



Chrysindin B

Structural-Activity Relationship Campaign Leads to a Novel Chain of Fusidic Acid with an Improved Resistance Profile

Kailey Komnick, Martin Garcia Chavez, and Paul J. Hergenrother
University of Illinois at Urbana-Champaign

Multi-drug resistant bacteria are a major threat to human health worldwide. Specifically, methicillin-resistant S. aureus (MRSA) was reported as a high priority pathogen by the World Health Organization in 2017. As a result, classes of antibiotics with efficacy against these problematic Gram-positive strains are urgently needed. Fusidic acid is a gram-positive only antibiotic that has been used to treat MRSA infections. Although fusidic acid has been efficacious in the clinic since its introduction in the 1960s, it requires a high dosing regimen due to its high resistance frequency. We herein report a SAR activity campaign, resulting in the synthesis of the first equipotent derivatives of fusidic acid. Our derivatives show potent whole cell activity and an improved resistance profile. Lastly, our lead derivative displays improved efficacy *in vivo* against a fusidic acid resistant strain.

Determination of Cell Binding Properties of a Novel Pancreatic Cancer Targeting Phage

Anna Larsen, Mallika Asar, and Mette Soendergaard
Western Illinois University

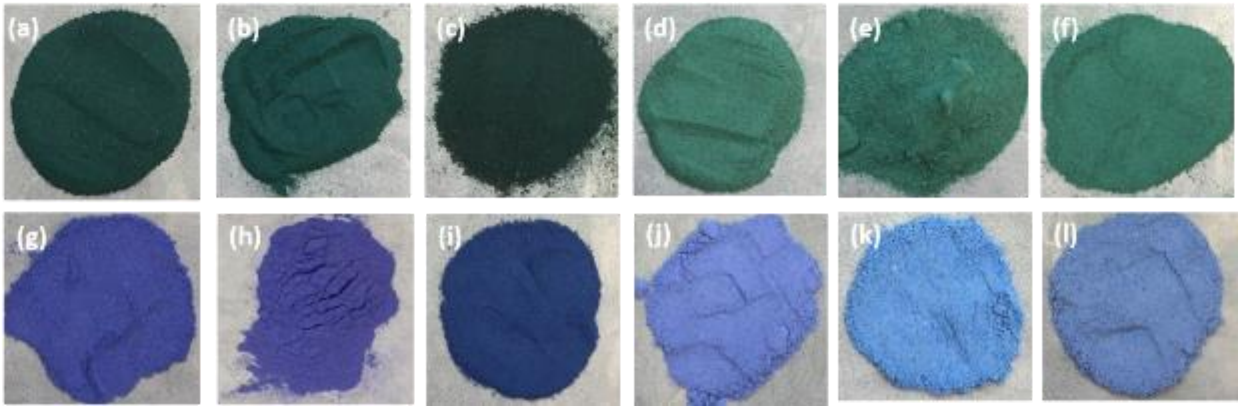
In the 21st century, pancreatic cancer continues to be one of the most lethal forms of cancer. The disease is estimated to cause 30,000 deaths per year the United States and have a five-year survival rate of less than 5% due to poor detection. Thus, new methods of detection and diagnosis is needed. Phage display technology has been used to discover peptide ligands that target cancer cells and have been used in detection of various malignancies. Such peptides may be utilized while displayed on the phage as detection and imaging agents. Previously, we carried out phage display selections against pancreatic cancer (Mia-Paca-2) cells, and identified a peptide (MCA1) that exhibit binding and specificity to this cell line. he particles of pMCA1 were amplified in E. coli K91BK and isolated using polyethylene glycol (PEG) NaCl. Mia-Paca-2 cells were grown in DMEM supplemented with 10% FBS and 5% horse serum at 37Â°C, 5% overnight, and then incubated with 1010 virions per mL (v/mL) wild type (WT) or pMCA1 phage for 1 h. Wells are washed three times with TBS and ABTS was added for a half hour at room temperature and read at 405 nm. When analyzed, it was found that there was a statistically significant different between pMCA1 and WT. Through this we find that the pMCA1 had significantly more binding than that of the WT. Proving that through further research, increased detection of Pancreatic cancer can ensue.

POSTER SESSION II: POSTER 53

Designing Novel Tunable Inorganic Pigments

Brianna Lehr and Eirin Sullivan
Illinois State University

The oxyfluoride Sr3MO4F (M = Al, Ga) is a known phosphor host lattice where the photoluminescent output can be altered dramatically by subtle structural changes in the host lattice such as creating anion defects or changing cation sizes. Substitution of Mn2+ for Sr2+ according to Sr3xMnxMO4F (M = Al, Ga) produces vivid green coloration in these materials with hue varying slightly between Al and Ga compositions, whilst reductively annealed samples are brilliant blue-purple in color. A systematic study was carried out to determine the range of shades of green and blue that could be produced by substitution of Ca2+ or Ba2+ for Sr2+ and subsequent reductive annealing of these materials. As transition metals are renowned for producing colored complexes, the incorporation of other divalent first row transition metals were investigated. Powder X-ray diffraction (PXRD) confirmed that Fe2+, Co2+, and Ni2+ could be successfully incorporated into the crystal lattice, producing khaki green, black and brown phases respectively.



Colors of Mn(II)-containing $Sr_{2.4}A_{0.5}Mn_{0.1}MO_4F$ and $Sr_{2.4}A_{0.5}Mn_{0.1}MO_{4-\alpha}F_{1-\delta}$ (A = Ca, Sr, Ba; M = Al, Ga): (a) A = Ca, M = Al, (b) A = Sr, M = Al, (c) A = Ba, M = Al, (d) A = Ca, M = Ga, (e) A = Sr, M = Ga, (f) A = Ba, M = Ga, (g)-(l) same compositions as (a)-(f) with post-synthesis reductive annealing.

Co-base catalyst in ORR

Alexis Magaña, Anne Marie Esposito, and Andrew A. Gewirth
University of Illinois at Urbana-Champaign

Fuel cells are able to provide energy that is clean, can be taken off grid, and more efficient than current combustion engines. Fuel cells require the oxygen reduction reaction (ORR) at the cathode. However, the ORR requires a catalyst to complete the reaction. Due to high temperature synthesis conditions, the active site structure of Co-based catalysts is not well understood. By controlling the Co content in the catalyst, it will be producing different onset potentials. One of the CoNC is capable of produce an onset potential of 0.82 V vs RHE, with an error of +/- 0.1V. CoNC is then able to be improved by adding a surfactant. By adding a surfactant to Co-ZIF-8 mixture, it is capable of producing an onset potential of 0.85 V vs RHE, with an error if +/- 0.1V. I used small molecule attachment to the surface of my catalyst to probe the changes is active site structure between CoNC and CoNCCTAB. The addition of a surfactant prior to pyrolysis changes the carbon active site structure of my catalyst.

Targeting the Class II HMG-CoA Reductase Enzyme for the Development of Novel Antimicrobials

Brittany Meyer, Miri Niedrauer, Mark Lipton
Purdue University

Bacterial resistance to antibiotics has become a major issue. According to the World Health Organization, it is one of the biggest threats to global health. Our lab has identified a new potential drug that inhibits II-HMGR in gram-positive bacteria such as Methicillin-resistant Staphylococcus Auereus (MRSA). II-HMGR is a reductase enzyme that is responsible for catalyzing the reduction of HMG-CoA to mevalonate. Mevalonate is an essential precursor to isopen-tenyl disphosphate (IPP), a component of un-decaprenol that acts as a lipid carrier in bacterial cell-wall synthesis. We are currently working to optimize the inhibitory activity of our lead compounds.

POSTER SESSION II: POSTER 56

Effects of Sample Storage and Handling on Jet Fuel Composition and Flash Point

Sarah Nowling, Brent Modereger, Jeff Zhang, Gozdem Kilaz, and Hilkka Kenttamaa
Purdue University

Quality jet fuel is essential to the safe operation of any aircraft, which is why its physical and chemical properties are regularly measured. If these properties are measured in a laboratory, samples should be stored and handled in a way that minimizes changes to the properties. It is possible that the most volatile fuel constituents evaporate during sample storage or handling, which would impact the fuel's chemical composition and physical properties (such as flash point). We monitored the chemical composition and flash point of (1) fuels kept in room temperature storage for up to 6 months and (2) fuels left uncapped for up to 24 hours. Three types of containers were used (Mason Jars, amber glass bottles, and F-style cans). Chemical composition was determined via GCxGC-FID and flash point was measured with a TAG 4 flash point tester. Minimal changes occurred during 6 months of storage for all container types. Samples stored in amber glass bottles exhibited the largest average increase in flash points while the samples stored in F-style cans exhibited the most deviation in flash point. Mason jars were the best containers for preventing evaporative losses in storage but, were the worst at preventing losses during sample handling. The amber glass bottles proved to be an adequate intermediate in both tests.

Emerging Contaminants in the Kinnickinnic River - Inorganic Anions and Pesticides

Ana Olvera, Erika Olvera, Patricia Zamora, and Alex Blom
Alverno College

Water samples from three locations, along the Kinnickinnic River, Jackson, Wilson and Zablocki parks were tested for water contaminants: fluoride, chloride, nitrate, phosphate, and sulfate. Ion Chromatography with the Dionex IonPac AS 18 and AG 18 (Guard) columns, sodium hydroxide as an eluent, and a suppressor were used to evaluate the samples. A combined five anion standard with a modified method for anions were used. Due to excess chloride, a separate set of standards were prepared. Throughout the research Chloride concentrations in Jackson park fluctuated the most, Zablocki did fluctuate but had the lowest amounts, and Wilson park remained mostly constant. For nitrate, Zablocki was consistent and had the lowest amounts, Wilson and Jackson fluctuated significantly, yet Wilson had the highest concentrations. The peak integrated as phosphate greatly varied in results for all three parks. Fluoride and sulfate were not detected. In addition, the water samples were evaluated for volatile organic compounds using Gas-Chromatography-Mass-Spectrometry (GC-MS) and solid-phase microextraction (SPME) immediately after each sampling. The fiber used in the analysis was composed of Divinylbenzene (DVB), Carboxen (CAR) and polydimethylsiloxane (PDMS). GC-MS results showed no evidence of volatile organic compounds in Wilson and Zablocki parks. However, the GC-MS results of the Jackson park showed the presence of 1,2 dichlorobenzene and methoxy phenyl oxime and other volatile compounds.

Biosynthetic Models of Unique Structural Features in Cytochrome Oxidases Found in Pathogens

Stephanie Ouchida, Sudharsan Dwaraknath, and Yi Lu
University of Illinois at Urbana-Champaign

Breaking the O2 double bond to form water through a four electron mechanism is the fundamental reaction of cellular respiration - a necessary process to produce fuel for cellular processes and survival. Cytochrome c oxidase, a type of heme-copper oxidase, is the terminal enzymatic complex in cellular respiration. These proteins are large and complex making it extremely difficult to study structural and functional features. A smaller scale biosynthetic model of heme-copper oxidases (HCOs) has been made in myoglobin to better study specific structure-function relationships necessary for optimal enzymatic activity. Cbb3 oxidase is a particularly interesting HCO as it occurs in many deadly pathogens that have the ability to survive under low oxygen conditions. This oxidase has a proximal hydrogen bonding His-Glu-Trp triad that is unique amongst HCOs. In order to study the role of the proximal hydrogen bond triad, we have modeled in wild type myoglobin. This structural modification showed an increased proportion of water production over reactive oxygen species. We have determined the redox potential and O2 affinity of our model and used Resonance Raman spectroscopy as well as electron paramagnetic resonance to determine structural changes.

Engineering an O2 transport protein into a CO2 reduction biocatalyst

Owen Ouyang, Sudharsan Dwaraknath, and Yi Lu
Washington University in St. Louis

Climate change has already become one of the biggest environmental concerns since the end of 20th century. As one of the main byproducts during combustion, CO2 was considered as a substance that was difficult to be re-utilized due to its stable chemical properties. Besides that, poor selectivity of catalysis also challenges the idea of reducing CO2. In this study, we aimed to recycle atmospheric CO2 into useful chemicals by introducing enzymes, a kind of biocatalyst which is known to be highly selective and eco-friendly. Myoglobin, an O2 transport protein found in muscle tissue, was used due to its well-characterized property and easily engineerable scaffold. We engineered myoglobin into a light-driven CO2-to-CO reduction biocatalyst by engineering the native metal center, an additional non-native metal center, and active-site amino acid residues. The experiment was then conducted under anaerobic environment to detect the product and measure the rate of the reaction. The data collected indicates that by introducing novel mutations among the scaffold, the resulting enzyme is among the fastest artificial CO2-reduction biocatalysts and exhibits high selectivity for CO over H2. In conclusion, the resulting system demonstrates its strong catalytic ability in producing CO. In the long term, this result also indicates the possibility of further reducing CO2 to generate other valuable chemicals such as formate and methanol.

Fast Mechanochromism of Regioisomeric Oxazines in Polymer Network

Nathan S. Purwanto, Hai Qian, Doug Ivanoff, Nancy R. Sottos, and Jeffrey S. Moore
University of Illinois at Urbana-Champaign

The activation of photochromic molecules by mechanical force through bulk material has been increasingly investigated in the field of polymer mechanochemistry. So far, there are only three reported mechanochromic molecular scaffolds, all with slow mechanical response. Here, we introduce a new class of color-changing mechanophore of the benzo[1,3]oxazine moiety. Computational DFT simulations were performed to demonstrate that the mechanochemical activation of the oxazine mechanophores is highly dependent on regioisomeric effect. To further validate such hypothesis, three oxazine regioisomers and one control compound were synthesized and examined in polydimethylsiloxane (PDMS) matrix. One intriguing property of this new system is the instantaneousl mechanochemical response without any sign of fatigue.

Synthesis of Iridium and Rhodium Pincer Complexes to Catalyze Parahydrogen Induced Polarization (PHIP)

Steven Ramirez, Safiyah Muhammad, and Alison Fout
University of Illinois at Urbana-Champaign

Magnetic resonance imaging (MRI) is a powerful diagnostic tool that allows physicians and radiologists to carefully examine tissues in the body with great detail. However, due to MRI's low sensitivity, gadolinium, a toxic heavy metal, is utilized to enhance images, owing to its strong paramagnetic characteristics. Gadolinium metal poses a significant risk to individuals with limited kidney function, as reduced excretion of metal in urine leads to a buildup in tissues and could ultimately result in toxicity. An alternative approach to resolving MRI's sensitivity issue is using parahydrogen to hyperpolarize signals of biologically relevant substrates. This method, known as Parahydrogen Induced Polarization (PHIP), has been shown to amplify signals by over 5 orders of magnitude in NMR. Our approach makes use of a CCC pincer ligand to increase electron density on metal centers in the catalyst complexes. Our rhodium complexes, (MesCCC)Rh(L) where L = ligand, will be applied towards the signal amplification of substrates via the parahydrogenation of olefins, transferring magnetic info from parahydrogen to the hydrogenated substrate. Our iridium complexes, (MesCCC)Ir(L), will be applied towards signal enhancement of nitrogen-based substrates and olefins via SABRE, Signal Enhancement by Reversible Exchange, a method that enhances signals without substrate hydrogenation. Finally, the efficiency of our synthesized complexes and other existing complexes used for PHIP will be compared.

Investigation of Polarization Effects on Intramolecular Oxidopyrylium-Alkene [5+2] Cycloadditions

Samantha Rokey, John Goodell, and T. Andrew Mitchell
Illinois State University

The Diels-Alder reaction is a reliable way to synthesize six-membered rings with good control over stereochemistry. Less known are the mechanistic aspects of seven-membered ring construction. In contrast to Diels-Alder [4+2] cycloadditions, [5+2] cycloaddition mechanisms are less established and also thus have greater limitations such as dimerization and variable regioselectivity and diastereoselectivity. Nevertheless, [5+2] cycloadditions are important reactions to synthesize polycyclic ring structures that are part of many biologically active natural products. Some examples include (-)-englerin A, toxicodenane A, and santalin Y which all possess polycyclic caged ethers. For this study, both kojic acid and maltol based derivatives were synthesized and evaluated in relative reaction rate studies utilizing an internal standard for a reliable comparative analysis. From this collected data, a Hammett plot was established giving preliminary insight into potential mechanism pathways dependent upon substituent electronics.

The Structure-Activity Relationships of Enterococcal Cytolysin

Alondra Sanchez, Imran Rahman, Weixin Tang, and Wilfred A. van der Donk
University of Illinois at Urbana-Champaign

Enterococcal cytolysin is a two-component hemolytic virulence factor produced by pathogenic strains of Enterococcus sp. that has been found to be responsible for an increased likelihood of fatal infections. In addition to targeting eukaryotic cells, cytolysin also exhibits antimicrobial activity against Gram-positive bacteria. Due to this unique dual specificity of cytolysin, we investigated the structural basis of these activities. To determine which amino acid residues of cytolysin are necessary, we prepared alanine scanning mutagenesis of every residue on each peptide, purified, and tested for both antimicrobial and hemolytic activity. We observed that some mutations completely abolish activity on both cell types, whereas other mutations specifically reduce activity on only one cell type. Understanding the mechanism by which cytolysin targets bacterial and eukaryotic cells allows will allow for better understanding of how this virulence factor works and potentially inform on anti-virulence therapies for antibiotic resistant infections.

Ion Exchange Reaction and its Influence on Network Ionic Polymer

Naisong Shan, Chengtian Shen, and Christopher M. Evans
University of Illinois at Urbana-Champaign

Ionic polymer networks have attracted increasing research attention due to its unique way (using covalent crosslinker) of decoupling mechanical strength and ionic conductivity. By crosslinking low Tg ionic polymer, one can achieve liquid-like ionic conductivity and solid-like mechanical property to make robust film, membrane, and so on. Thus, ionic polymer network has being widely used in electrochemical applications such as: solid electrolyte to suppress dendrite formation in Li-metal batteries; solid electrolytes for ionic polymer soft actuators; all solid-state supercapacitor; ion exchange membranes for fuel cell battery and so on. The synthesis of anionic or cationic polymers involve an important ion exchange step where the counter-ion was exchanged to a target ion for their specific application. For example, a Li+ conducting electrolyte needs to have Li+ as the mobile ion whereas a fuel cell membrane needs OH- as the counter ion. To the best of our knowledge, there is a lack of systematic study of how ion concentration and network structure influence the kinetics as well as the extent of ion exchange. Furthermore, how exactly does the residual ion impact the materials' properties we aim to design. A class of back bond ammonium ionic polymer networks is synthesized with different carbon spacer between ionic group and the Br counter ion was exchanged to TFSI with different concentration of salts (1.5 to 10 eqiuv.).

High Pressure Freezing/Freeze Substitution Combined with Correlated Imaging Techniques for Investigating the Intracellular Lipid & Protein Distributions

Daphne Shen, Brittney Gorman, and Mary L. Kraft
University of Illinois at Urbana-Champaign

Direct imaging of stable isotope-labeled lipids in cell membranes with high-resolution secondary ion mass spectrometry (NanoSIMS) can afford insight into plasma membrane organization. The depth profiling mode enables visualization of intracellular lipid distributions by rastering across the surface multiple times at various depths to probe composition of organelle membranes. To preserve cellular integrity under the ultra-high vacuum employed by NanoSIMS, samples are generally fixed with conventional chemical fixatives. High-pressure freezing/freeze substitution (HPF/FS) offers better cellular preservation by executing ultra-rapid freezing with subsequent organic solvent substitution and fixation that allow instantaneous molecule fixation and crossing-linking to reduce cell autolysis and fixation artifacts. The samples can be processed into ultra-thin resin embedded sections for analysis of intracellular structures with fluorescence microscopy and transmission electron microscopy. Alternatively, the samples can be critical-point dried or air-dried with hexamethyldisilazane and analyzed with scanning electron microscopy (SEM) for evaluation of membrane structural integrity. SEM images show improved plasma membrane integrity with the addition of glutaraldehyde to fixatives routinely used in FS. Combining HPF/FS with correlated imaging techniques provides improved preservation of the internal cell membranes, thus yielding enhanced preservation of membranes for NanoSIMS analysis.

Chemistry Laboratory Experiment: Molecular Interactions in Liquid Crystals

Kylie H. Smith, Carissa K. Gettelfinger, and Gudrun Schmidt
Purdue University

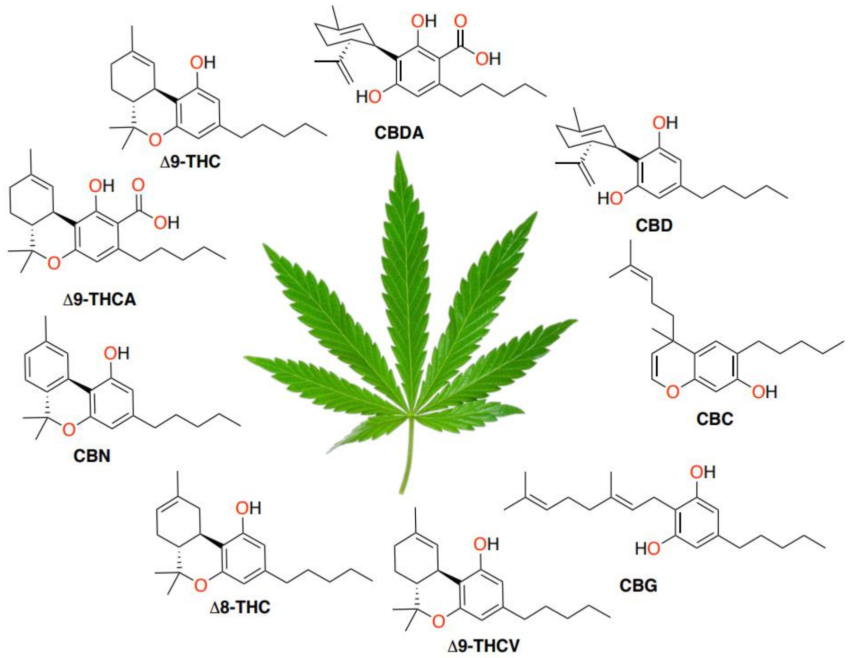
We are presenting a general chemistry laboratory experiment that relates optical properties of liquid crystals to molecular interactions. For example, the wavelength of reflected light can be changed by liquid crystal molecules in a film when the molecules interact and arrange in a specific way. As a result, a change in color can be observed as a function of mechanical stimulation, electricity or temperature. Applications for liquid crystals are plentiful including liquid crystal displays for computers, sensors for electronics or simple fever thermometers. This chemistry laboratory experiment has three objectives. i) Develop hands-on skills on how to prepare and formulate liquid crystal mixtures that will change colors. ii) Observe and record color changes of liquid crystal mixtures as a function of temperature. iii) Analyze and evaluate results in terms of molecular interactions and generate evidence supported conclusions. Students learn about the anisotropic structures of rigid liquid crystal molecules. The polar and nonpolar parts of these molecules may lead to hydrogen bonds, ionic interactions, dipole-dipole and dipole-induced dipole interactions. The molecular arrangements in liquid crystals are important in controlling optical properties for specific applications.

POSTER SESSION II: POSTER 67

Quantification of Phytocannabinoids in CBD Products

Alex Solivais and Ian S. Taschner
Indiana University Northwest

Cannabidiol, or CBD, is a phytocannabinoid that has surged in popularity due to the 2018 legalization of hemp cultivation and CBD product distribution. However, CBD extraction and isolation is still an emerging field. There is little consistent federal regulation of these products, and few large-scale operations exist. Previous studies have shown 69% of products have CBD concentrations different than advertised. More alarming, Δ9-tetrahydrocannabinol (Δ9-THC), the compound responsible for the psychoactive effect of cannabis, has been found in excess of 1%. A method was developed for the separation of various phytocannabinoids, including Δ9-THC, Δ8-THC, CBD, CBDV, CBC, CBG, CBDA, and THCA through high pressure liquid chromatography in tandem with a triple quadrupole mass spectrometer (HPLC-MS/MS). Various CBD infused products were purchased from local vendors, analyzed for cannabinoid concentration, and evaluated for accuracy in labelling.



POSTER SESSION II: POSTER 68

Magnetic properties of Co-doped Nickel Aluminides, DyNi3-x-yCoxAly

Justin Shing Him Wong, George Agbeworvi, and Corey M. Thompson
Purdue University

Recently, rare earth-transition metal (R-T) intermetallic compounds have been investigated because of their fascinating magnetic properties, such as high magnetoresistance, magnetic pole reversal, Kondo effect, large magnetostriction, superconductivity, and giant magnetocaloric effects. The RNiAl2 (R = Gd, Tb, Ho, and Er) system has attracted interests due its potential for magnetic refrigeration technology. These compounds crystallize in the orthorhombic structure, Cmcm, with magnetic entropy values of 16.0 J/kgÂ·K, 14.0 J/kgÂ·K, and 21.2 J/kgÂ·K for GdNiAl2, HoNiAl2, and ErNiAl2, respectively. However, the magnetic entropy of the Dy-analog is not known. Here, we have synthesized DyNiAl2 to investigate its structural and magnetic properties. We report on the structural and magnetic behavior of DyNiAl2 and the influence of substituting Co for Ni and Al on the observed properties.

POSTER SESSION II: POSTER 69

Phage Display Selection of a Hemagglutinin Targeting Peptide

Che Woodson, Taylor Gunby, Jessica Newton-Northup, and Mette Soendergaard
Western Illinois University

Affinity chromatography is among a common protein isolation method that often employs antibodies. However, these are expensive to produce. Bacteriophage (phage) display has been widely used to develop peptide ligands, which is significantly more cost and time efficient. Thus, phage display technology may be used to develop peptides that target recombinant protein tags such as the hemagglutinin (HA) epitope. Phage display using a fUSE5 15-mer peptide library was conducted to identify a HA targeting peptide. Four positive selection rounds (0.04-4 Î¼g/mL HA peptide) was carried out, and peptides were identified by next generation sequencing. Results identified a peptide (TG1) that occurred more than 4*106 times and was thus selected for further analysis. TG1 was sequenced with an N-terminal biotin and GSG spacer. To validate binding, 25 ug/mL HA peptide was immobilized onto the surface of an amine reactive plate and blocked using 3% bovine serum albumin (BSA). TG1 or a non-relevant peptide J18 (15.6-250 ng/mL) was then added for 1 h. The plate was washed with PBS, and streptavidin-HRP was added for 30 min. After washing, 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulphonic acid) (ABTS) was added and allowed to develop for 30 min. The absorbance at 405 was determined spectrophotometrically. Results showed that at 250 ng/mL TG1 bound significantly higher ($p<0.05$) to the HA epitope compared to J18, indicating that the former demonstrates binding affinity for the peptide tag.

Metal Substrates Modulation of Outer-Sphere Electron Transfer Kinetic on Single Layer Graphene

Chang Xia, Jingshu Hui, and Joaquín Rodríguez-López
University of Illinois at Urbana-Champaign

Single layer graphene (SLG), as a new generation carbon material, has attracted a great deal of attention in recent years. Due to its electrochemically active basal plane and extreme thinness, SLG can be used as an ideal platform to explore new concepts in electrochemical reaction kinetics. Previous studies have shown a ~ 5-fold increase of outer-sphere electron transfer kinetics of graphene when modified with a Au metal substrate.1 Scanning electrochemical microscopy (SECM) was used to characterize the graphene's electrochemical activity locally with high accuracy and spatial resolution. Graphene was transferred into the patterned metal substrate via wet transfer. Multiple metals are being tested including Palladium, Nickle, Silver, and Chromium. SECM was used to detect local reactivity changes of each metal substrate-patterned graphene electrode. Kinetic contour map is being crafted afterwards to monitor the outer-sphere electron transfer kinetics change of patterned graphene system using ferricyanide/ferrocyanide redox couple. Overall the result shows that kinetic transfer is significant enhanced by metal substrate underneath single layer graphene due to electronic donation, which also had positive relationship with metal-graphene interaction strengths.

Synthesis of Polypeptides with Complex Architectures Through SIMPLE Strategy

Xuetao Zheng, Ziyuan Song, and Jianjun Cheng
University of Illinois at Urbana-Champaign

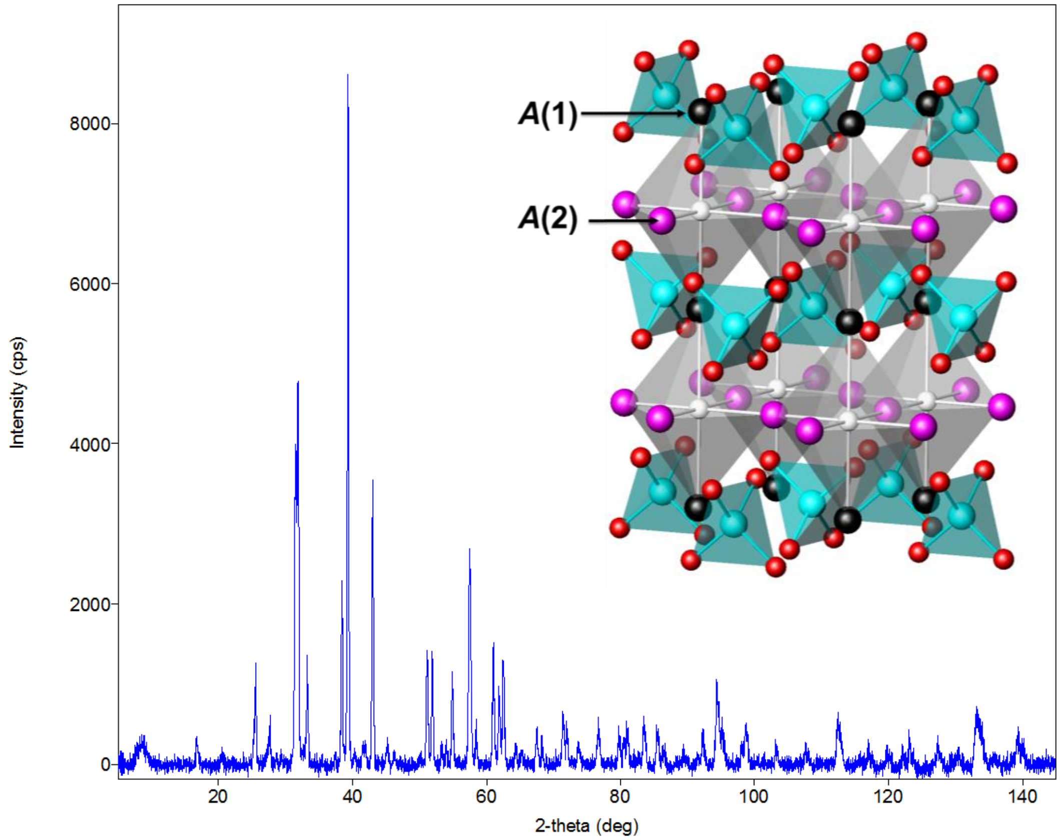
Synthetic polypeptides with complex architectures, including brush-like polypeptides and star-shaped polypeptides, have drawn increasing attentions due to their unique self-assembly behaviors and promising biomedical performance compared with their linear analogues. The synthesis of these polypeptides from ring-opening polymerization (ROP) of N-carboxyanhydrides (NCAs), however, was limited to complicated macroinitiator designs and stringent requirements on monomer purity. Herein we report the fast and controlled synthesis of polypeptides with complex architectures through the segregation-induced monomer-purification and initiator-localization promoted rate-enhancement (SIMPLE) strategy. By directly dissolving various multi-amine based macro-initiators in the aqueous phase, well-defined star-shaped or brush-like polypeptides with predictable molecular weights and narrow dispersity were obtained. The obtained polypeptides can form uni-molecular micelles when the side chains are properly modified, offering a series of promising polypeptide materials for assembly and biomedical applications.

POSTER SESSION II: POSTER 72

Exploring the Structure-Property Relationship in Oxyfluoride Pigments

George Zurowski, Brianna Lehr, and Eirin Sullivan
Illinois State University

The $\mathrm{Sr}M\mathrm{O_4F}$ oxyfluoride (M=Al, Ga) is a known phosphor host lattice and it has been demonstrated that structural changes in lattice significantly alter photoluminescent behavior. This material has three distinct cation lattice sites and due to the presence of mixed anion charges and high tolerance for defects in the anti-perovskite type structure is amenable to a variety of iso- and aliovalent cation substitutions. Substitution of dopant quantities of transition metal cations such as $\mathrm{Mn^{2+}}$ has been shown to produce a variety of vivid green and blue colors in this material. Experiments were performed to test the subtle variation in shades of green that can be accomplished by altering the size of group 2 cations and group 13 metals and monitoring corresponding changes induced in the crystal lattice according to $\mathrm{Sr}_{3-x}A_x\mathrm{Mn}_xM_{0.25}\mathrm{Al}_{0.75}\mathrm{O_4F}$ (A=Ca, Sr, Ba) (M=B, In). Powder X-ray diffraction (PXRD) was used to determine that the $\mathrm{Mn^{2+}}$ could be successfully incorporated into the lattice within these conditions. The variation in these structures produced a wide assortment of shades of green with the source of variation linked to the metals involved in the structure. Boron tended to produce lighter shades of green while indium in the structure resulted in darker coloration. Color differences can also be observed in the varying cations with larger ionic radii producing darker colored product.



Optimization of Photoacoustic Probes for Nitric Oxide Detection

Ruiwen Xu, Christopher J. Reinhardt, and Jefferson Chan
University of Illinois at Urbana-Champaign

Nitric oxide (NO) is an essential signaling molecule involved in many physiological and pathological processes. Due to its free-radical nature, NO is innately unstable and requires sensitive detection methods for studying its functions within living systems. Photoacoustic (PA) imaging is a noninvasive technology that utilizes near-infrared light excitation and ultrasonic detection for deep-tissue imaging. In 2018, the first activatable contrast agent for NO, APNO-5, was reported for imaging lipopolysaccharide-derived inflammation in mice. To enable the detection of lower concentrations of NO (e.g., in cancer), we proposed to optimize the compound by red-shifting the absorbance maxima into the detectable range of commercial PA tomographers (680-950 nm). We hypothesized that planarization would occur following the relaxation of the steric clash on the boron-azadipyrromethene dye platform, thereby resulting in a redshift and a corresponding increase in the sensitivity. Through systematic replacement of the thienyl rings we evaluated the effect of the location and number of thiophenes on the photophysical properties, both before and after N-nitrosation by NO. The lead compound, thioAPNO, enabled more rapid detection of inflammatory NO and the increased sensitivity allowed for the first detection of cancer-derived NO in a mouse breast cancer model.

Lipidomic Profiling in Amyloid Beta-Treated BV2 Microglia

Elizabeth A. Thayer, Priya Prakash, Jonathan A. Fine, Christina R. Ferreira, and Gaurav Chopra
Purdue University

Microglia – the brain's resident immune cells, are responsible for maintaining tissue homeostasis by engulfing cellular debris and protein aggregates through the process of phagocytosis. Microglia in Alzheimer's disease (AD) show functional impairment and altered phenotypes and contribute to the accumulation of amyloid beta (Aβ) peptide resulting in neuronal death. In addition to genes and proteins, lipids play crucial roles in regulating microglial function, however, the specific lipids involved in Aβ response are not well understood. In this study, we determined the lipidomic signature of BV2 microglia upon time-dependent exposure to aggregated Aβ. Total lipids were extracted from the Aβ-treated microglia using the Bligh and Dyer method and Multiple Reaction Monitoring profiling was used to evaluate the cellular lipid content. Interestingly, our data revealed various lipid classes (phosphatidylserines, free fatty acids, ceramides, etc.) that were downregulated in Aβ-treated microglia compared to the control microglia. These results highlight various lipids that are implicated in microglial immune response to Aβ over time. Ongoing studies involve determining the functional roles of the identified lipids. In conclusion, we propose that lipidomic profiling reveals novel metabolic pathways in microglia that may be useful in developing therapeutic strategies to combat AD.

Computational Analysis of Potential Small Molecule Therapeutics for Myotonic Dystrophy Type 1

Philip A. Kocheril, Sarah E. Bonson, Lauren D. Hagler, and Steven C. Zimmerman
University of Illinois at Urbana-Champaign

Myotonic dystrophy type 1 (DM1) is an autosomal dominant genetic disease characterized by muscle wasting, myotonia, cardiac defects, and more. DM1 symptoms are caused by expanded RNA, r(CUG)^{exp}, that exist as imperfect hairpin structures that sequester RNA-binding proteins, such as muscleblind-like protein 1 (MBNL1), that are involved in the regulation of alternative splicing. Our therapeutic approach is to rationally design small molecules that target r(CUG)^{exp} and release MBNL1. One of the most accessible methods to assess probable ligand-RNA interactions is computational modeling. Molecular dynamics simulations allow for visualization of the possible binding modes of ligands and computations to assess their relative stabilities; coupled with experimental data, these simulations can provide useful insights to explain the relative binding strengths of different ligands. We have synthesized a novel ligand, assessed its binding via isothermal titration calorimetry (ITC), and performed modeling studies on both the novel ligand and previously reported ligands. Although a strong binding interaction was not observed for the first generation novel ligand, modeling studies revealed structural shortcomings which reasonably explained the observed lack of binding. A modified ligand was designed that appears promising from preliminary modeling and ITC studies. This method will be used to develop a systematic approach for broad application to small molecule therapeutics.

Uncovering Lipophilicity Rules for Small-Molecule Mediated Transmembrane Metal Transport

Peng-Jui Chen, Andrew D. Blake, Daniel J. Blair, and Martin. D. Burke
University of Illinois at Urbana-Champaign

In the traditional paradigm of pharmacology, diseases arising from excess protein function are treated through potent and selective inhibitors. In contrast, diseases originating from lack of protein function are refractory to this approach and present a tremendous unmet medical need. In the Burke lab, we propose that small molecules can directly replace missing proteins, acting as a prosthesis on the molecular scale. We have identified hinokitiol, a tropolone natural product capable of the replacement of missing iron transporters. In order to understand hinokitiol's activity and enable the development of a clinically relevant therapeutic, we seek to understand the atomistic underpinnings (SAR) that govern its transport activity. We synthesized an array of tropolones with differing alkyl substituents and branching patterns at various positions in order to systematically analyze the impact of both lipophilicity and substituent constitution. We have also shown that other scaffolds capable of iron binding can be engineered for transport and follow the same rules we uncovered for tropolones. Using our synthetic route, we have synthesized uniformly 13C-labelled tropolones, which will serve as valuable mechanistic probes in solid-state NMR paramagnetic relaxation enhancement (PRE) experiments. The understanding gained from our SAR studies will allow for rational design of an optimized hinokitiol-inspired derivative with optimal transport capability.

PAST AWARD RECIPIENTS

ECI Outstanding Oral Presentation Awards

2018	Clare Gallagher
2018	Alayna Johnson
2017	Alayna Johnson
2017	Travis Lantz

ECI Outstanding Poster Awards

2018	Sriyankari Chitti
2018	Mara Fattah
2018	Jake Grabowski
2018	Daniel Olson
2017	Dominic Aiello
2017	Michael Niederbrach
2017	Matthew Clawson
2017	Terry Kim
2017	Eliot Rapoport
2016	Thomas Dieter
2016	Brenton Hull
2016	William Lau
2016	Kang Yong Loh
2016	Nathan Reed
2016	Steven Szymanski

NOBCChE Outstanding Poster Awards

New for 2019

SACNAS Outstanding Poster Awards

2018	Heriberto Flores Jr.
2018	Jose Ignacio Vergara Panzone
2017	Amanda Cowfer
2017	Luis Curet
2016	Amanda Cowfer
2016	Christian Ocampo
2016	Andrea Salazar

WCC Outstanding Poster Awards

2018	Jonathan Hicks and Cheyanne Woolwine
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2018	Gina Partipilo
2018	Andrea Perry
2018	Elizabeth Thayer
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2017	Sarah Ackenhusen
2017	Jonathon Adams
2017	Hannah Frerker
2017	Gina Partipilo
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Wolfram Awards

2018	Heriberto Flores Jr.

SUPPORTING GROUP DETAILS

American Chemical Society – The mission of ACS is to advance the broader chemistry enterprise and its practitioners for the benefit of Earth and its people. This includes advancing science, advocating for chemistry, enabling career development, educating the public, supporting future chemists, and promoting diversity. For more than 140 years ACS has been improving people's lives through the transforming power of chemistry.

East Central Illinois – Local Sections help chemists stay active and involved in their communities by providing a forum for networking and collaboration and by supporting chemists' efforts to educate their community about chemistry. The East Central Illinois (ECI) Local Section of the American Chemical Society has over 500 members from Effingham to Champaign. The list of institutions that our chapter serves includes the University of Illinois at Urbana-Champaign, Eastern Illinois University, and Parkland College. We encourage fellow chemists, other scientists, students, and the interested public to meet us at our public lectures and special events.

NOBCChE at Illinois – The National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE) is a non-profit professional organization dedicated to assisting black and other minority students and professionals in fully realizing their potential in academic, professional, and entrepreneurial pursuits in chemistry, chemical engineering, and allied fields.

UIUC ACS Student Chapter - The ACS Student Chapter (ACS-SC) at the University of Illinois offers many networking, educational, and professional opportunities. The goal of ACS-SC is to promote personal, professional, and scientific development through organized events and individualized mentoring. The chapter primarily serves as a support group for chemistry and chemical engineering majors. Whether it is for a career in industry, pursuit of higher education, or an interest in science, there is a spot for any individual in the organization.

UIUC SACNAS Chapter - Society for the Advancement of Chicano/Hispanic and Native Americans in the Sciences (SACNAS) is an inclusive society of scientists dedicated to fostering the success of scientists of diverse backgrounds including those of Hispanic/Chicano and Native American descent. Our mission is to increase the diversity of the scientific community by mentoring and sharing science at all levels of education. We are dedicated to helping underrepresented groups obtain advanced degrees, careers, and positions of leadership in science in order to increase resources, eliminate barriers, and achieve greater equality.

UIUC Women Chemists Committee - The UIUC Women Chemists Committee was founded in the fall of 2005 to promote the advancement of women in the chemical sciences. With the support of our local section and the University of Illinois Department of Chemistry, we have planned professional and social events that benefit graduate students, faculty, staff, and undergraduates.

Younger Chemists Committee - YCC advocates for and provides resources to students, early-career chemists, and professionals in the chemical sciences and related fields. YCC also addresses specific issues facing younger chemists within ACS and serves as their voice in ACS. Past events have included industry tours, webinars, networking events, and professional development.

2019 COMMITTEE

This conference would not be possible without the planning and hard work of all the committee members. Thank you!


Sarah Bonson (co-chair)


Rebecca Ulrich (co-chair)


Thomas Bearrood


Edzna Garcia


Gabriela Ibarra


Safiyah Muhammad


Elizabeth Murphy

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East Central Illinois Local Section
Undergraduate Research Conference

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