

**CONTROL ID:** 2209123

**TITLE:** [Structural study of Mongolian tourmaline in the electric power saving system with infrared spectroscopy](#)

**CONTACT (NAME ONLY):** [Ki-Seog Chang](#)

**ABSTRACT STATUS:** decisioned\_accepted

**INSTITUTIONS (ALL):** 1. Bio. & Chemical Engineering, Hongik University, Sejong, Jochiwon-eup, Korea (the Republic of).

**AUTHORS (LAST NAME, FIRST NAME):** [Chang, Ki-Seog](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** This Fourier Transformation Infrared (FTIR) experiment investigates the relevance of H<sub>2</sub>O and other components' structural environments. Four element materials, tourmaline, ferrite, NaCl, and H<sub>2</sub>O, comprised the electronic power saving system. FTIR spectroscopy in the range of 3,000 to 4,000 cm<sup>-1</sup> was used to examine the hydroxyl ions of H<sub>2</sub>O and Mongolian tourmaline. The tourmaline crystal was polar and therefore pyroelectric, electrical charges developing at the ends of the polar axis and temperature changing from the IR activation with H<sub>2</sub>O in the system. As a result, the tourmaline was shown to be related to the activation of H<sub>2</sub>O as a pyroelectric substance.

**CONTACT (COUNTRY ONLY):** Korea (the Republic of)

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**SESSION HOST:** Organizer (Sherine Obare)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Hongik University

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**CONTROL ID:** 2210996

**TITLE:** [Calculation of the anharmonic effect of elementary reactions of high-temperature combustion reaction](#)

**CONTACT (NAME ONLY):** [Li Yao](#)

**ABSTRACT STATUS:** decisioned\_accepted

**INSTITUTIONS (ALL):** 1. Department of Physics , Dalian Maritime University, Dalian, Liaoning, China.

**AUTHORS (LAST NAME, FIRST NAME):** [Yao, Li](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Abstract

Combustion plays an important role in engineering and our life. Today, about 90 percent of the energy is generated by the combustion in our world [1]. Focusing on the chemistry of combustion of fuels, it is of great significance to design the combustion chamber, control pollutants and research on alternative fuels [3-4]. The chemical kinetic mechanism of combustion of fuels is composed of a series of elementary reactions. Therefore, to better grasp the mechanism of combustion reaction, it is necessary to investigate the elementary reaction process. Being the key parameters of the chemical kinetic mechanism of the combustion reactions, the rate constant are calculated using RRKM theory, transition state theory and our own method. Most results are similar with those of accurate quantum dynamics (QD). At the same time, the RRKM theory, the intramolecular vibration theory, and the vibrational transition state theory for large molecule reaction systems, or the gas-phase reaction kinetics that are difficult to investigate by using accurate quantum dynamics and quasi classical trajectory method provide the feasibility of estimating. We investigate the anharmonic effect of the canonical and the microcanonical systems, and calculate the total number of states, the density of the states, the partition function and the rate constant. From the various calculation results, we get the following conclusions. First, the anharmonic effect is significant for the weak binding force of microscopic reaction systems. Second, the error of harmonic approximation is larger in high temperature, which is announced for the kinetic mechanism of the combustion reactions. Third, when the molecular

reaction is 2000 K, the anharmonic rate constant is smaller than the harmonic rate constant ranging from 2 times to thousands times. The anharmonic effect increase with the increasing temperatures. Forth, the anharmonic effect is not only related to the intramolecular bond length and binding energy, but also with the symmetry of the molecular structure. We will focus on the developing the anharmonic model of high-temperature combustion reactions in the following days, high-temperature non-resonant correction calculation methods and apply the method and parameters to building and optimizing the kinetic mechanism of the high-temperature combustion of hydrocarbons.

**CONTACT (COUNTRY ONLY):** China

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Dalian Maritime University

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**CONTROL ID:** 2211208

**TITLE:** [Development and implementation of a summer camp for high school students based on the applications of analytical instrumentation in forensic chemistry](#)

**CONTACT (NAME ONLY):** [Jennifer Batten](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Physical Sciences, Grand Rapids Community College, Jenison, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Batten, Jennifer H.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Chemistry in the real world is now permanently merged with technology and it is the goal of the Forensic Chemistry Summer Camps at Grand Rapids Community College to show area high school students how instrumentation is a key component in modern chemical analysis. The premise of the camps is that an arson crime (simulated) has been committed at an area college chemistry lab and it is the students' responsibility to analyze the crime scene evidence and identify a likely suspect. The students use procedures, which have elements of inquiry based discovery, to analyze ink, soil, accelerants, and DNA using UV-vis and atomic absorption spectroscopy, gas chromatography- mass spectrometry, and gel electrophoreses, respectively. This presentation will address the preparation, operation, and outcomes of the camps including the recruitment of student attendees, the laboratory investigations, and student feedback.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** High School, Community College, and Undergradate Education - Oral

**SESSION HOST:** Organizer (Thomas Higgins)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Grand Rapids Community College

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**CONTROL ID:** 2231671

**TITLE:** [Integrating gas chromatography-mass spectrometry into organic chemistry to improve student interest in and skill with this technique and beyond](#)

**CONTACT (NAME ONLY):** [Jennifer Batten](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Physical Sciences, Grand Rapids Community College, Jenison, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Batten, Jennifer H.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The recent acquisition of a gas chromatograph-mass spectrometer (GC-MS) through the National Science Foundation Grant DUE 1140509 has allowed the faculty at Grand Rapids Community College to incorporate this instrument across the two-year curriculum. This technique was used in the organic chemistry lab sequence to highlight the mass spectrometry data of functional groups and to introduce basic quantitative methods. With the goal of improving interest in and comprehension of a variety of chemistry related topics including cation stability and resonance, seven experiments were adapted or developed to include GC-MS. The methods and outcomes of this work will be presented including curriculum development, student feedback, and assessment of student achievement.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** High School, Community College, and Undergraduate Education - Oral

**SESSION HOST:** Organizer (Thomas Higgins)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Grand Rapids Community College

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**CONTROL ID:** 2211445

**TITLE:** [X-ray crystallographic structure of BshC: A unique enzyme involved in bacillithiol biosynthesis](#)

**CONTACT (NAME ONLY):** [Paul Cook](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry, Grand Valley State University, Allendale, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Cook, Paul D.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Bacillithiol is a low molecular weight thiol produced by many Gram-positive bacteria such as *Bacillus anthracis* and *Staphylococcus aureus*. The compound is involved in the maintenance of redox homeostasis and resistance to the FDA-approved antibiotic fosfomycin. It is produced via a pathway utilizing the enzymes BshA, BshB, and BshC. The structures and functions of enzymes similar to BshA (glycosyltransferase) and BshB (deacetylase) have been reported, but very little is known about BshC, the putative cysteine ligase in bacillithiol production. Here we report the first ever structure of BshC from *B. subtilis* to a resolution of 1.77 Å. The structure reveals that BshC contains a core Rossmann fold with extended connecting peptide motifs (CP1 and CP2) and an  $\alpha$ -helical coiled-coil domain that facilitates dimerization. The structure contains citrate and glycerol in the canonical active site and ADP in a second ligand binding site. The overall structure and bound ligands give insight into the function of this unique enzyme.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Mechanisms of Antibiotic Resistance - Oral

**SESSION HOST:** Organizer (Rachel Powers)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Grand Valley State University

**CONTROL ID:** 2212323

**TITLE:** [Synthesis and applications of oxoquinonacyclophane macrocycles](#)

**CONTACT (NAME ONLY):** [Jay Wackerly](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry, Central College, Pella, IA, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Wackerly, Jay W.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** This presentation will feature research in our lab on the synthesis of a new class of redox active [1<sub>4</sub>]oxacyclophanes that contain *p*-benzoquinones. These macrocycles can be accessed in one-pot base catalyzed reactions of 2,3-dichloronaphthoquinone and various diphenols. Modifications to the electrophile and reactions conditions were also explored to access similar structures. Subsequently, each macrocycle was investigated for its ability to act as a supramolecular host for host-guest binding.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Jay Wackerly)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Central College

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**CONTROL ID:** 2213282

**TITLE:** [Vibrational spectroscopy of asparagine in acidic, neutral, and basic solutions](#)

**CONTACT (NAME ONLY):** [Joong-Won Shin](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Division of Science, Governors State University, University Park, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Dandurand, Daniel](#)<sup>1</sup>; [Shin, Joong-Won](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Fourier transform infrared spectroscopy (FTIR) utilizing attenuated total reflectance (ATR) was carried out to analyze changes in vibrational bands of asparagine (L-Asn) at 0.20 M concentration in acidic, neutral, and basic solutions in the pH range of 1 to 14. The spectra show evolution of peaks near 1730, 1680, 1260, and 1228 cm<sup>-1</sup> at pH values below 2, suggesting protonation of the carboxylic acid on the backbone of the molecule. The appearance of peaks near 1530, 1400, and 1360 cm<sup>-1</sup> at pH values in the 2 - 8 range implies that the amino acid adopts a zwitterionic structure.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Governors State University

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**CONTROL ID:** 2214001

**TITLE:** [Coulometric titration of thiosulfate ion in shampoo](#)

**CONTACT (NAME ONLY):** [Thomas Kuntzleman](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Spring Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Francis, Jessica](#)<sup>1</sup>; Kuntzleman, Thomas S.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Thiosulfate ion in Ultra Swim shampoo was determined coulometrically. In a single cell reaction, triiodide ion was generated at a carbon anode, while hydrogen gas was formed by the reduction of acid protons at a platinum cathode. Excess triiodide ion generated after equivalence reacted with starch indicator, causing the color of the solution in the reaction cell to darken. End point detection was accomplished by measuring light absorbance through the reaction cell. This detection process was also done visually. This method was also used to titrate ascorbic acid in other experiments.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Spring Arbor University

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**CONTROL ID:** 2227648

**TITLE:** [A simple mechanism for fog formation in the dry-ice-in-water experiment](#)

**CONTACT (NAME ONLY):** [Thomas Kuntzleman](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Spring Arbor, MI, United States.

2. Jackson College, Jackson, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Kuntzleman, Thomas S.](#)<sup>1</sup>; Ott, Mark E.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** When solid carbon dioxide (dry ice) is placed in water, a cloudy white fog results. It is often assumed that this fog results from atmospheric water vapor condensing on cold carbon dioxide gas that escapes the bulk water. However, simple experiments indicate that this fog originates from the bulk water into which the dry ice is placed. By observing the characteristics of the fogs formed when dry ice is placed in various liquids, insight is gained into the molecular events that lead to fog formation when dry ice is placed in water. Fog formation seems to be related to physical properties of the bulk liquid, such as vapor pressure and surface tension. Additional clues about fog formation in this experiment are gained by viewing high-speed, slow motion video of the fog-filled bubbles that form at the dry ice / water interface.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Spring Arbor University

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**CONTROL ID:** 2214639

**TITLE:** [Modified Sonogashira- and Glaser-type couplings: Reaction methodology for undergraduate research](#)

**CONTACT (NAME ONLY):** [Matthew Mio](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry and Biochemistry, University of Detroit Mercy, Berkley, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Mio, Matthew J.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Due to their structural rigidity, conjugation and unique bond torsion, sequence-specific arylethynylene and arylbutadiyne oligomers are excellent scaffolds for the study of shape-persistent supramolecular and nanoscale systems. With the ultimate goal of improving the generation of these important architectures, new synthetic methodologies have been developed utilizing an in situ ethynylsilane deprotection reaction. While synthetic strategies for the alkylation of aryl moieties (Sonogashira) or the homocoupling of alkynes (Glaser) traditionally involve iterative pathways, the use of an in situ ethynylsilane deprotection reaction has been shown to allow for the rapid construction, often in one pot, of complex arylethynylene and arylbutadiyne oligomers. Key to the protocol is the inclusion of a mixture of amidine base, such as 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU), CuI and substoichiometric amounts of water. The use of trimethylsilylacetylene versus bis-trimethylsilylacetylene, base toggling, inclusion of dioxygen for homocoupling, sterics of silylacetylene protection and CO insertion projects will be discussed.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Jay Wackerly)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Detroit Mercy

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**CONTROL ID:** 2220589

**TITLE:** [Design and synthesis of nitrogen rich porous organic polymers](#)

**CONTACT (NAME ONLY):** [Mohammad Rabbani](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.  
2. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.  
3. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.  
4. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.  
5. Chemistry, University of Wisconsin-Platteville, Platteville, WI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Rabbani, Mohammad](#)<sup>1</sup>; Heitsman, Jessica<sup>2</sup>; Roe, Brittany<sup>3</sup>; Moore, Ashley<sup>4</sup>; Boushley, Michael<sup>5</sup>

**ABSTRACT BODY:**

**Abstract:** Recently porous organic polymers have been widely studied because of their multifunctionality. They have potential uses in areas such as storage, separation, and catalysis. It has been found that nitrogen rich porous organic polymers play significant roles in gas storage capacity and selectivity. We report here the synthesis of benzimidazole-linked polymers. Synthesized polymers are chemically and thermally stable due to the stability of benzimidazole moiety. Suitable building unit have been selected and synthesized to enrich the overall nitrogen heterogeneity in the frames. The polymers have moderate surface areas of around 500 m<sup>2</sup>g<sup>-1</sup>. Details synthesis and porous studies will be reported in poster presentation.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** University of Wisconsin-Platteville

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**CONTROL ID:** 2235959

**TITLE:** [An international perspective on green chemistry and sustainability education](#)

**CONTACT (NAME ONLY):** [George Bodner](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Dept of Chemistry, Purdue University, W Lafayette, IN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Bodner, George M.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The literature on Green Chemistry and Sustainability (or Sustainable Development) suggests that these terms are often used as if they were synonymous. The results of a Symposium on Science Education Research and Education for Sustainable Development held at the University of Bremen, last summer, clearly showed that they are not. This paper will use the results of this symposium to look at efforts to bring Green Chemistry and/or Sustainability Education into the chemistry curriculum under the context of “relevance” in diverse cultures around the world. If time permits, the author will also reflect on a recent study done by the ACS Green Chemistry Institute of the state of Green Chemistry education in the U.S.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**SESSION HOST:** Organizer (Sherine Obare)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Purdue University

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**CONTROL ID:** 2221483

**TITLE:** [Synthesis and characterization of trimetallic Cu\(I\), Au\(I\) and Ag\(I\) complexes](#)

**CONTACT (NAME ONLY):** [Ahmad Samin](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Math and Science, American University of Afghanistan , Saint George, UT, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Samin, Ahmad](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The design and preparation of multinuclear metal complexes or coordination polymers containing direct metal-metal interactions, such as Pt-Ag, Pt-Tl, Pt-Pt, Pt-Pd, Au-Au, Ag-Ag, and Cu-Cu has received considerable attention. Among them, emissive copper(I) complexes are expected to be key materials for preparation of organic light emitting diodes likely because copper(I) is more cost-effective than the other precious metal complexes. In these systems metallophilicity plays an important role in assembling close M...M interactions.

Earlier our group reported the application of the 2-picoyl substituted NHC ligand toward stabilizing Ag(I)-Ag(I) interactions. The simple reaction of the NHC ligand precursor 1,3-bis(2-pyridinylmethyl)-1H-imidazolium tetrafluoroborate, [H(pyCH<sub>2</sub>)<sub>2</sub>im]BF<sub>4</sub> with silver oxide in acetonitrile produces the unusual



triangulo-Ag<sub>3</sub> cluster, [Ag<sub>3</sub>((pyCH<sub>2</sub>)<sub>2</sub>im)<sub>3</sub>](BF<sub>4</sub>)<sub>3</sub>, with unusually short Ag-Ag separations (2.72 to 2.78 Å). We have now extended this chemistry to explore the electronic alteration of the ligand on the metal-metal separation. Additionally, we were able to produce mixed metal systems, and copper triangulo-Cu<sub>3</sub> clusters.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** American University of Afghanistan

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**CONTROL ID:** 2223811

**TITLE:** [Nucleoside ribohydrolases as targets for \*Trichomonas vaginalis\* therapeutic agents](#)

**CONTACT (NAME ONLY):** [Brian Stockman](#)

**ABSTRACT STATUS:** decisioned\_accepted

**INSTITUTIONS (ALL):** 1. Department of Chemistry, Adelphi University, Garden City, NY, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Stockman, Brian J.](#)<sup>1</sup>; Beck, Sierra<sup>1</sup>; Bekker, Simona I.<sup>1</sup>; Benzie, Annie Laurie<sup>1</sup>; Humes, Colleen S.<sup>1</sup>; Muellers, Samantha N.<sup>1</sup>; Rosario, Irving<sup>1</sup>; Shea, Tara A.<sup>1</sup>; Violo, Victoria L.<sup>1</sup>; Parkin, David W.<sup>1</sup>; Vanalstine-Parris, Melissa A.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Trichomoniasis is the most prevalent non-viral sexually transmitted disease. Resistance to the 5-nitroimidazole class of therapeutic agents in use for the past 50 years has increased markedly, indicating the need for new therapies with novel mechanisms of action. *Trichomonas vaginalis* is an obligate parasite that relies on purine and pyrimidine salvage pathway enzymes to obtain its nucleobases. Nucleoside salvage pathway enzymes used by *T. vaginalis* are distinct from the pathway involved in activation of the 5-nitroimidazole drugs, and do not have mammalian counterparts, thus representing excellent targets for developing new antitrichomonal agents. The first step in this pathway is the hydrolysis of nucleosides to release the nucleobases. Uridine nucleoside ribohydrolase (UNH) and adenosine/guanosine preferring nucleoside ribohydrolase (AGNH) have been characterized and found to have distinct substrate specificities and thus recognize distinct pharmacophores. The druggability of the two enzymes was tested by developing an <sup>19</sup>F NMR-based activity assay to monitor the hydrolysis of 5-fluorouridine, and a <sup>1</sup>H NMR-based activity assay to monitor the hydrolysis of adenosine, and then screening the NIH Clinical Collection for inhibitors. Different classes of inhibitors were identified for the two enzymes confirming that they represent distinct, druggable targets. The best inhibitors were obtained commercially, structurally validated using 2D <sup>1</sup>H-<sup>13</sup>C NMR methods, and rank-ordered using IC<sub>50</sub> values determined by NMR. Suspected aggregators were also examined by assaying in the presence of detergent. Benzimidazole-containing proton-pump inhibitors were identified as μM inhibitors of UNH. Dipine-containing calcium channel blockers were also identified as UNH inhibitors, but these compounds were determined to be active in their phenylpyridine forms rather than the parent compounds. Flavonoid-based compounds were identified as μM inhibitors of AGNH. Active compounds are being further explored using a combination of activity assays, binding assays, fragmentation, and medicinal chemistry to define structure-activity relationships, as well as biological assays to correlate enzyme inhibition with antitrichomonal activity.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Upjohn, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Jed Fisher)|Organizer (Mike Barbachyn)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Adelphi University



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**CONTROL ID:** 2227284

**TITLE:** [Election of acs directors-at-large by a minority of voters in five of the last six years: A possible solution to the problem, multiple instant run-off voting](#)

**CONTACT (NAME ONLY):** [Wendell Dilling](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, Central Michigan University, Mt. Pleasant, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Dilling, Wendell L.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** In five of the last six years ACS elections for Directors-at-Large (*Chem. Eng. News*, Nov. 23, 2009, p 7; Nov. 28, 2011, p 9; Nov. 26, 2012, p 7; Nov. 25, 2013, p 5; Nov. 24, 2014, p 3) one of the elected candidates received votes from <50% of the voters (Councilors). In each election two Directors-at-Large were elected from a slate of four or five candidates. A method is proposed to carry out elections in which two or more candidates are elected with each being elected by a majority of the voters. The method (multiple instant run-off) involves voters prioritizing their votes. The first Director-at-Large is elected by a majority in exactly the same way a single candidate would be elected from three or more candidates by the instant run-off procedure. In the instant run-off procedure the candidate with the fewest first-choice votes is eliminated, and the second choice votes on those ballots where the eliminated candidate was the first choice are added to the first choice votes for the other candidates. This procedure is repeated until one candidate has a majority of the votes. Then, in the multiple instant run-off procedure, all the votes for the first candidate elected are removed from the voting priority list of each voter. The second successful candidate is then determined in exactly the same manner as the first using the new prioritized list of each voter. Thus both candidates are elected by a majority in a single election. If more candidates are to be elected, the preceding procedures are repeated.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Central Michigan University

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**CONTROL ID:** 2230854

**TITLE:** [Enantiodifferentiating \[4+4\] photocyclodimerization of 2-Anthracene-carboxylate catalyzed by 6<sup>A</sup>,6<sup>X</sup>-Diamino-6<sup>A</sup>,6<sup>X</sup>-dideoxy- \$\gamma\$ -cyclodextrins: Misinterpretation of the sign of differential entropy of activation](#)

**CONTACT (NAME ONLY):** [Wendell Dilling](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, Central Michigan University, Mt. Pleasant, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Dilling, Wendell L.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Inoue and coworkers reported the title reactions in which the four dimers **1-4** are formed (*J. Photochem. Photobiol. A: Chem.* **2005**, *173*, 375-383). The relative yields of dimers **1-4** and the enantiomeric excesses of dimers **2** and **3** (as high as 37%) could be controlled within limits by varying the catalyst, temperature, and solvent composition. Linear plots of the relative rate constants for the formation of the

enantiomers of **3** against the reciprocal temperature in various concentrations of aqueous methanol gave data from which the differential enthalpy of activation and the differential entropy of activation could be calculated. These authors report the signs (+ or -) of these differential activation parameters. The absolute values of these signs are completely arbitrary. Only the relative values have significance.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Central Michigan University

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**CONTROL ID:** 2227328

**TITLE:** [How to report the results of an instant run-off election](#)

**CONTACT (NAME ONLY):** [Wendell Dilling](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, Central Michigan University, Mt. Pleasant, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Dilling, Wendell L.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** A clarification of the results of the 2013 ACS President-Elect election was reported in C&EN, March 10, 2014, p 2. The results of that election are shown in the table. The original report in C&EN, November 25, 2013, p 5, reported only total votes for the three candidates, first-choice votes plus second-choice votes for two of the candidates and only first-choice votes for the third candidate. Even though the correct order of finish was reported initially, the total vote counts gave a distorted view of the results. The original report implied that Balazs was supported by 3126 (9638 – 6512) more voters than Kolb was, whereas the difference was only 192 (6704 – 6512) votes. The 42%, 35%, and 23% reported are not pertinent because two of the total vote counts included both first-choice and second-choice votes and the third included only first-choice votes. The last (second in this case) stage of an instant run-off election is between only two candidates (Schmidt and Balazs) and always results in one candidate receiving a majority (>50%) of the votes unless there is a tie. Schmidt received 55% [ $11623 \times 100 / (11623 + 9638)$ ] of the vote in the run-off portion of this election. Kolb was not involved in this second stage. Also the total number of voters, 21659 (8443 + 6704 + 6512), could not be determined from the initial set of numbers reported, which implied 27773 (11623 + 9638 + 6512) voters if one does not recognize that some voters were counted twice.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Central Michigan University

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**CONTROL ID:** 2227569

**TITLE:** [A valine catabolic enzyme could be a potential target for altering the lipid or protein content in an oilseed](#)

**CONTACT (NAME ONLY):** [Kerry Rouhier](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry Department, Kenyon College, Gambier, OH, United States.  
2. University of Minnesota, Minneapolis, MN, United States.  
3. The JM Smucker Company, Orville, OH, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Rouhier, Kerry A.<sup>1</sup>; Gipson, Andrew B.<sup>1,2</sup>; Pena, Mithzy<sup>1,3</sup>; Rhee, Rachel<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Seeds use storage reserves, such as lipids and protein, to fuel the early stages of germination, prior to the commencement of photosynthesis. These necessary reserves accumulate through various metabolic reactions during embryo development and seed maturation. One such reaction catalyzed by methylmalonate semialdehyde dehydrogenase (MMSDH) looks to play an important role in both lipid production and protein content in *Arabidopsis thaliana* seeds. MMSDH catalyzes an energy intensive step in valine catabolism by converting methylmalonate to propionyl-CoA (as well as malonate to acetyl-CoA). Recent results reveal decreased lipid and protein content in seeds lacking MMSDH. Other phenotypes such as seed viability, physical characteristics, and metabolic profiles also support its role in seed development. Based on these results, potential applications of an overexpression seed line could lead to seeds with increased lipid and protein content – something of interest to those seeking alternative biofuel mechanisms or food sources with altered protein content.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Kenyon College

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**CONTROL ID:** 2249836

**TITLE:** [Results from an external review of the Kenyon College Summer Scholars Program: an ongoing discussion between faculty and administration](#)

**CONTACT (NAME ONLY):** [Kerry Rouhier](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry Department, Kenyon College, Gambier, OH, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Rouhier, Kerry A.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Undergraduate research in the sciences has been an integral part of applied learning at Kenyon College for more than 30 years. Students participate as "... partners in inquiry..." (Kenyon's mission statement) during the academic year and throughout the summer. This academic year, the Department of Chemistry has more than thirty students working in our labs on various projects as volunteers or for course credit. During the summers, students apply to participate in our Kenyon Summer Science Scholars program (KSSS). What started as a small research program funded through external grants (NSF, NIH, and HHMI), the KSSS program is now entirely supported by the college. More than thirty students and their faculty mentors are provided stipends to conduct research for 8-10 weeks each summer. Student-faculty teams hail from all departments in the Natural Science Division (Chemistry, Physics, Biology, Mathematics and Statistics, and Psychology) and the Department of Anthropology. In 2014, members of the KSSS program conducted a thorough self-study and underwent an external review. We sought feedback in these broad areas- 1) meeting the needs of the students, 2) meeting the needs of the faculty, and 3) best practices for a sustainable and high-quality program. I will be sharing the results of our Review, including feedback from our subsequent discussions with the administration.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Research at Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Bradley Wile)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Kenyon College

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**CONTROL ID:** 2227722

**TITLE:** [A search for novel rifamycins and small molecule leads against \*M. tuberculosis\* RNA polymerase](#)

**CONTACT (NAME ONLY):** [Hollis Showalter](#)

**ABSTRACT STATUS:** decisioned\_accepted

**INSTITUTIONS (ALL):** 1. Medicinal Chemistry, University of Michigan, Ann Arbor, Ann Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Showalter, Hollis D.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Rifampin, a semisynthetic rifamycin, is the cornerstone of current tuberculosis treatment. Among many derivatives the benzoxazinorifamycins (bxRIFs), characterized by the clinical agent rifalazil, have great potential for tuberculosis (TB) treatment due to their superior affinity for wild-type and rifampin-resistant (Rif<sup>R</sup>) *Mycobacterium tuberculosis* RNA polymerases and their reduced hepatic Cyp450 induction activity. This presentation will detail x-ray crystal structures of *Escherichia coli* RNA polymerase complexed with two newer generation benzoxazinorifamycins. Consistent with our structure-base design approach, these structures show the C3'-tail of the benzoxazinorifamycin located in a gap between the  $\beta$  subunit fork loop 2 and  $\sigma$  finger of the polymerase. We will also discuss more recent work involving the development of an *in vitro* RNAP transcription assay that uses a fluorescent probe to detect transcription of RNA aptamers to the probe. This assay is being utilized in HTS against a clinically relevant Rif<sup>R</sup> RNAP mutant to search for novel inhibitory scaffolds. Preliminary results from the HTS will be discussed.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Parke-Davis, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Michigan, Ann Arbor

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**CONTROL ID:** 2227756

**TITLE:** [Quantification of chromium in biological matrices](#)

**CONTACT (NAME ONLY):** [Jacqueline Arroyo](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Loyola Univ, Chicago, IL, United States.

2. Chemistry and Biochemistry, Loyola University of Chicago, Chicago, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Arroyo, Jacqueline](#)<sup>2</sup>; Schmeling, Martina<sup>1</sup>; Batycki, Jacob<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** Chromium exposure happens in several ways, it is in the food and water we ingest, consumer products, and it is released by industrial activities. Measuring the exposure a person has had to a toxic element requires the sampling of tissues and fluids, such as those found in the ocular system. The human lens

is of particular interest because it grows over an entire lifetime beginning from embryo and continuing through adulthood, therefore reflecting a lifetime of exposure. Chromium has two main oxidation states: trivalent and hexavalent, the trivalent form is necessary for glucose metabolism while the hexavalent form is toxic. The goal of this work is to develop a sample preparation protocol and method of analysis that can accurately quantify both states of chromium in biological matrices. Biological samples have a complex matrix that can include proteins, organic acids, and metals, all of which can effect the analysis. The current method uses cation exchange prior to the quantification of trivalent chromium by graphite furnace atomic absorption spectroscopy. Several studies designed to simulate the analysis of biological samples have been completed in order to evaluate the method's capabilities in four main criteria: interference of the sample matrix, limit of detection, specificity, and reproducibility.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Loyola University of Chicago

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**CONTROL ID:** 2228362

**TITLE:** [Self-cleaning surface by growing hierarchical ZnO nanowire coatings on micro-scale PMMA](#)

**CONTACT (NAME ONLY):** [Jun Li](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemical Engineering, University of Michigan, Ann Arbor, MI, United States.  
2. Chemical Engineering, Harbin Institute of Technology, Harbin, Heilongjiang, China.

**AUTHORS (LAST NAME, FIRST NAME):** [Li, Jun](#)<sup>2, 1</sup>; Wang, Lijun<sup>2</sup>; Hu, Zhen<sup>2</sup>; Huang, Yudong<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** In recent years, self-cleaning materials with lotus-effect, namely superhydrophobicity, and photocatalysis are attractive because of their eco-friendly characters. In this study, a hierarchical superhydrophobic and photocatalytic surface was constructed by growing various lengths of zinc oxide (ZnO) nanowires on micro-scale polymethyl methacrylate (PMMA) surface that produced by electrostatic adherence and chemical etching. Firstly, the ZnO nanowires are applied as a coating onto PMMA substrates, and then silanization was used to offer enhanced water-repellence and hydrophobicity. At last, a hierarchical surface similar to lotus was obtained. The nano-size effect on wettability of nano/micro complex structures has been investigated by adjusting the ZnO nanowire length. As the nanowire length on the PMMA surface increases, a transition from the Wenzel state to the Cassie state occurs. A water contact angle as high as 155.7° was formed by growing ZnO nanowires of a suitable length on the micro-scale PMMA surface. Moreover, this material shows a high light transmission. Compression and impact experiments further demonstrate the robust superhydrophobicity of PMMA/ZnO nanowire hierarchical structures. The presented transparent materials offer an attractive alternative for surface treatments of glass, avoiding the use of environmental unfriendly chemicals.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**SESSION HOST:** Organizer (Sherine Obare)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Harbin Institute of Technology

**CONTROL ID:** 2228425

**TITLE:** [In situ generated metal nanoparticles as two-dimensional assemblies, core-shell structure and biosensor](#)

**CONTACT (NAME ONLY):** [Krisanu Bandyopadhyay](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Natural Sciences , University of Michigan-Dearborn, Dearborn, MI, United States.

2. Department of Natural Sciences , University of Michigan-Dearborn , Dearborn , MI, United States.

3. Department of Natural Sciences , University of Michigan-Dearborn , Dearborn , MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Bandyopadhyay, Krisanu](#)<sup>1</sup>; Renard, David<sup>2</sup>; Teh, Ruishen <sup>1</sup>; Alexander, Celeste<sup>3</sup>

**ABSTRACT BODY:**

**Abstract:** Metallic and bi-metallic nanoparticles like gold, platinum, palladium, Au-Pt and Au-Pd of specific size immobilized on solid support has seen remarkable growth due to their different potential applications. Thus, there is a considerable interest for investigating a general preparative route to engineer aggregation-resistant metallic nanoparticles for various applications. The present study deals with *in situ* formation of two-dimensional assemblies of metallic and bi-metallic nanoparticles on functionalized surfaces. Electrochemical investigations of these nanoparticles revealed a highly efficient catalytic activity for many long-chain and poly alcohols including methanol, ethanol, 1-propanol, 2-propanol, ethylene glycol, and glycerol. In another application of this *in situ* metal nanoparticle synthesis, gold and palladium nanoshells have been synthesized successfully by reducing surface bound palladium and gold ions onto ~200 nm diameter silica core. The method for generating such nanoshells is based on seed-mediated growth technique. This present method reports the first time synthesis of palladium nanoshell from surface bound palladium nanoparticles seeds compare to earlier reports that use gold nanoparticles as seed to generate final palladium shell. In addition, the current study also involves synthesis of gold nanoshells on silica cores that are less than 100 nm diameter. Previous work has shown the successful synthesis of gold nanoshell on a ~200 nm silica core using the present seed mediated synthesis procedure. Gold nanoshells with a smaller core may find increased application in photo-thermal therapeutic studies. Finally, palladium nanoparticle assemblies generated on indium tin oxide (ITO) coated glass surfaces are applied towards detection of Dopamine (DA), an important neurotransmitter in the mammalian central nervous system. The sensing performance of the present biosensor is measured electrochemically using differential pulse voltammetry (DPV) and impedance spectroscopy, at different concentrations of dopamine in solution. The biosensor has shown a remarkably low detection limit for DA and a linear response over a wide concentration range. In addition, specificity of this biosensor for DA detection is also explored in presence of ascorbic acid (AA).

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Research at Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Bradley Wile)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Michigan-Dearborn

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**CONTROL ID:** 2229237

**TITLE:** [Silver nanoshells synthesis by \*in situ\* generation of silver seeds on silica nanoparticle cores](#)

**CONTACT (NAME ONLY):** [Krisanu Bandyopadhyay](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Natural Sciences , University of Michigan-Dearborn, Dearborn, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Siblini , Tamara](#)<sup>1</sup>; Teh, Ruishen<sup>1</sup>; Bandyopadhyay, Krisanu<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Recently, several differing core-shell combinations of nanoshells have been fashioned by the bottom-up approach and are finding prospective applications in cancer treatment as well as solar energy absorbers. The synthesis procedure to generate this silica nanoparticle is well documented in literature. Most metal nanoshells such as gold and palladium have been published. Silver nanoshells are still a work in progress. Silver nanoparticles are known for its anti-bacterial properties, that are beneficial for the health of human being. Currently, silver seeds are formed externally and then adsorbed onto a surfactant functionalized silica core surface which then proceed to its final growth stage. The present research deals with a more efficient method of synthesizing these silver nanoshells by eliminating the need of pre-synthesized silver seed in solution. The reason for a different method is to help shorten the overall synthesis process. This efficient route to generating silver nanoshells will improve their candidacy for various potential applications in the medical field and solar energy harvesting.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** University of Michigan-Dearborn

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**CONTROL ID:** 2229235

**TITLE:** [Catalytic assessment and characterization of \*in-situ\* generated gold-palladium bimetallic nanoparticles on functionalized surfaces](#)

**CONTACT (NAME ONLY):** [Krisanu Bandyopadhyay](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Natural Sciences , University of Michigan - Dearborn , Canton , MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Hales, Joshua](#)<sup>1</sup>; Renard, David<sup>1</sup>; Peer, Aileen<sup>1</sup>; Bandyopadhyay, Krisanu<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The use of nanoparticle-based heterogeneous catalysts has grown immensely in recent years due to their high surface area and unique chemical and physical properties. While many noble metal nanoparticles (such as gold, platinum, palladium, and silver) have proven to be promising catalytic systems, a combination of these materials may prove to be an even better option, combining the advantages of each metal individually. The present work involves the *in-situ* generation of 2D gold-palladium (Au-Pd) bimetallic nanoparticle assemblies on functionalized silicon and indium-tin oxide (ITO) coated glass substrates. Varying ratios of gold and palladium are used to produce a set of catalysts, ranging from only gold to only palladium. Atomic Force Microscopy (AFM) is used to characterize the physical structure of the nanoparticles while zeta potential measurements are used to track the change in surface charge throughout the generation process. UV-Visible (UV-Vis) spectroscopy is used to observe the optical properties of the bimetallic nanoparticles, giving insight to their morphology. The catalytic properties of the nanoparticle arrays are assessed electrochemically through the oxidation of ethanol and ethylene glycol using cyclic voltammetry. Additionally, the catalytic abilities of these bimetallic nanoparticles assemblies are assessed through the catalytic reduction of 4-nitrophenol to 4-aminophenol in the presence of excess borohydride. This reaction is monitored through UV-Visible response, allowing for the calculation of the apparent rate constants of the reaction. Through the use of these various characterization techniques, we hope to understand the morphology of these nanostructures



and tune their catalytic abilities.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** University of Michigan - Dearborn

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**CONTROL ID:** 2229131

**TITLE:** [Non-enzymatic glucose biosensing using gold nanoparticles](#)

**CONTACT (NAME ONLY):** [Krisanu Bandyopadhyay](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. University of Michigan-Dearborn, Dearborn, MI, United States.

2. Department of Natural Sciences , University of Michigan - Dearborn , Dearborn, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Yang, Pheng](#)<sup>1</sup>; Alexander, Celeste<sup>2</sup>; Bandyopadhyay, Krisanu<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Diabetes is a common long term disorder characterized by high blood glucose concentration. Commonly known ways of detecting glucose levels involve the enzymatic approach of undergoing rapid redox reactions with Glucose Oxidase (GOx) and a small mediator molecule such as ferrocyanide or other ferrocene derivatives. Furthermore, there are other known ways of detecting glucose but all methods require the GOx enzyme. The issues involving stability of this enzyme leads to a short shelf life in the products used to detect blood glucose concentrations. The present research identify a non-enzymatic way of glucose sensing that excludes the need of any mediator and GOx, subsequently reducing costs and eliminating conditions required to keep GOx stable during sensing process. We have used our own method to generate in situ gold nanoparticles assemblies on indium tin oxide (ITO) coated glass surfaces. These newly synthesized gold nanoparticles is used as sensing platform in conjunction with electrochemical impedance spectroscopy and cyclic voltammetry to measure electrochemical response with varying concentration of glucose to probe for a linear range between concentration and electrochemical parameters. Fitting Impedance response to an appropriate equivalent circuit shows an increase in inverse of charge transfer resistance with increasing glucose concentrations which reveal a systemic non-enzymatic method of detecting glucose with two dimensional assemblies of gold nanoparticles. Additionally, cyclic voltammograms show a consistent trend of increasing current with increase in glucose concentration that supports the general applicability of this method of glucose sensing.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** University of Michigan-Dearborn

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**CONTROL ID:** 2228578

**TITLE:** [Progress toward the syntheses of novel monocyclic  \$\beta\$ -lactam antibiotics](#)

**CONTACT (NAME ONLY):** [Serena Carosso](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Rempex Pharmaceuticals -The Medicines Company, San Diego, CA, United States.

2. Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Carosso, Serena](#)<sup>2</sup>; Miller, Marvin J.<sup>2</sup>; Hecker, Scott<sup>1</sup>; Glinka, Tomasz<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The clinical introduction of penicillin in the 1940s is a milestone in the history of mankind since it led to a drastic decrease of the mortality rate caused by bacterial infections and also to an unprecedented improvement in the quality of life. The two decades between 1940 and 1960 have been defined as the “golden era of antibiotics” in which several new classes of antibiotics were developed and introduced on the market. However, infectious diseases have not been eradicated since bacteria progressively developed a wide variety of mechanisms to survive antibiotics, giving rise to the growing phenomenon of bacterial resistance. As a consequence the commonly used antibiotics are becoming less and less effective and the need for new antibiotics, with novel structures and/or mechanism of action, become every year more pressing.

My work in the Miller group deal with the development of new methodologies to be applied to the synthesis of monocyclic  $\beta$ -lactam antibiotics. In particular, we are interested in the synthesis of  $\beta$ -lactams which display a sulfur-containing side chain at the C4 position and an ATMO side chain at the C3 position. Several analogs have been generated through a synthetic route in which a bromine-induced cyclization is used for the construction of the  $\beta$ -lactam ring. The biological activity of the final compounds has been also evaluated. Efforts have also been directed to the synthesis of monocyclic  $\beta$ -lactams containing an ATMO side chain at the C3 position and a 1,2,3-triazole moiety at the C4 position, which is introduced through the use of click chemistry. The biological activity of the final compounds will also be evaluated using in house agar diffusion essays.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** University of Notre Dame

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**CONTROL ID:** 2228725

**TITLE:** [Red Dyes in North and South American Archaeological Textiles by DART-MS](#)

**CONTACT (NAME ONLY):** [Ruth Ann Armitage](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry, Eastern Michigan University, Ypsilanti, MI, United States.

2. The Ohio State University, Columbus, OH, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Armitage, Ruth Ann](#)<sup>1</sup>; Jakes, Kathryn A.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** We report here on the application of direct analysis in real time – time-of-flight mass spectrometry (DART-MS) to both comparative materials and archaeological fibers to investigate the sources of red dye colorants in ancient textile objects. DART-MS has significant advantages compared to existing ones used in the analysis of dye colorants in that the analyses are rapid and require little or no sample preparation. Chemical standards, botanical materials and comparative reference samples characteristic of dyes from regions of both North and South America, including both plant and insect dyes, were investigated. We have applied DART-MS to three fragments shed from red and yellow colored textiles recovered from Seip Mound in southern Ohio (100 BC- 400 AD), and to red fibers obtained from several different textiles within two different funerary bundles recovered from the Paracas Necropolis in Peru (400 BC – 400 AD). The presence

of a specific set of anthraquinones to the exclusion of others supports previous studies suggesting the prehistoric use of *Galium* and *Relbunium* species as dye plants in Eastern North America and South America.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Eastern Michigan University

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**CONTROL ID:** 2260980

**TITLE:** [DART-MS: A Confirmatory Test for Heme in Bloodstains on Fabric](#)

**CONTACT (NAME ONLY):** [Ruth Ann Armitage](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry, Eastern Michigan University, Ypsilanti, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Torres, Sylvia](#)<sup>1</sup>; Armitage, Ruth Ann<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Presumptive blood tests on crime scenes are used to identify wet or dry stains that potentially may be blood. Each presumptive test must be followed by a confirmatory test. Confirmatory tests are implemented to confirm the presence of blood and can help determine its origin. In this study, three common presumptive tests – Kastle-Meyer, tetramethylbenzidine (TMB), and luminol – were compared to determine their sensitivity to heme (the catalyst in the reactions) in dry bloodstains. Of the three tests performed, TMB was found to be the most sensitive. Direct analysis in real time mass spectrometry (DART-MS) was applied to the bloodstains to evaluate its use as a confirmatory test. Heme was readily detected using the DART-MS method even at low concentration in dried bloodstains on fabric, potentially leading to a new confirmatory test in forensic science.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Eastern Michigan University

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**CONTROL ID:** 2229075

**TITLE:** [Single atom alloys as a strategy for selective heterogeneous hydrogenations](#)

**CONTACT (NAME ONLY):** [E Charles Sykes](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Tufts University, Medford, MA, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Sykes, E Charles H.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Hydrogenation reactions are central to the petrochemical, fine chemical, pharmaceutical, and food industries and are of increasing interest in energy production and storage technologies. Typical heterogeneous

## JGLCRM March 23, 2015 Submitted Abstracts

catalysts often involve noble metals and alloys based on platinum, palladium, rhodium and ruthenium. While these metals are active at modest temperature and pressure, they are not always completely selective and are expensive. We have demonstrated that single palladium atoms can convert the otherwise catalytically inert surface of an inexpensive metal into an ultrasensitive catalyst. We used high resolution imaging to characterize the active sites and temperature programmed reaction spectroscopy to probe the chemistry. The mechanism involves facile dissociation of molecular hydrogen at individual palladium atoms followed by spillover onto the copper surface, where ultrasensitive catalysis occurs by virtue of weak binding. The reaction selectivity is in fact much higher than that measured on palladium alone, illustrating the unique synergy of the system.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Catalysis and Surface Science to Advance Energy Efficiency - Oral

**SESSION HOST:** Organizer (Daniel Killelea)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Tufts University

---

**CONTROL ID:** 2230847

**TITLE:** [Natural colors for food and beverages](#)

**CONTACT (NAME ONLY):** [Deepti Dabas](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Colors, Kalsec, Kalamazoo, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Dabas, Deepti](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Color is the most important component influencing the purchase of food. Colors are added to food for consistency and to meet customer expectations among other reasons. Natural Colors are coming to the forefront replacing synthetics. Natural colors, with the use of appropriate technology and know-how of applications, can perform at par with synthetics. Different pigments can provide with different hues required for color match. Carrot and turmeric provide yellow color to foods with the coloring pigments being beta-carotene and curcuminoids respectively. Annatto can be used as yellow or orange colorant depending on concentration and application, with the active component being bixin. Paprika can provide a red or orange hue to foods, owing to compounds- capsorubin and capsanthin. Anthocyanins are a bigger class of compounds with pigments providing different hues in red-purple family depending on their structure. Betalains and lycopene can also provide red colors isolated respectively from beet and tomatoes. Chlorophyll is the green colored pigment but is not allowed for use in the USA. Depending on desired hue, the physical properties of pigments can be changed or suitable stabilizers can be added which impart better performance. Depending on the nature of pigments, two or more pigments can be mixed to provide the desired color. Knowing about application matrix is very important for the pigment to perform successfully in that application. Today natural colors are growing fast as more and more consumers are seeking them over synthetic colorants.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Color Your Food: Meeting the Challenges of Natural Food Colors - Oral

**SESSION HOST:** Organizer (Shane McDonald)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Kalsec

**CONTROL ID:** 2230995

**TITLE:** [Rhodium-catalyzed C-C single bond activation: Using mechanistic understanding to guide reaction development](#)

**CONTACT (NAME ONLY):** [Jeffrey Johnson](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Hope College Chemistry Dept, Holland, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Johnson, Jeffrey B.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Methodology achieving the activation and functionalization of carbon-carbon single bonds holds the promise to unveil previously unforeseen retrosynthetic disconnects. This presentation will summarize ongoing mechanistic investigations of rhodium-catalyzed carbon-carbon bond activation methodologies and outline successful efforts to utilize the resulting quantitative insight to develop new transformations.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Jay Wackerly)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Hope College Chemistry Dept

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**CONTROL ID:** 2231227

**TITLE:** [Combined QM/MM study of the isomerization of 1-Deoxy-D-Xylulose 5-Phosphate \(DXP\) catalyzed by DXP reductoisomerase \(DXR\)](#)

**CONTACT (NAME ONLY):** [Yirong Mo](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Western Michigan University - Mailstop 5413, Kalamazoo, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Mo, Yirong](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The conversion of 1-deoxy-D-xylulose 5-phosphate (DXP) to 2-C-methyl-D-erythritol 4-phosphate (MEP) catalyzed by DXP reductoisomerase (DXR) is the committing step in the biosynthesis of terpenoids. This MEP pathway is essential for most pathogenic bacteria but absent in human, thus is an attractive target for the development of novel antibiotics. To this end, it is critical to elucidate the conversion mechanism and identify the transition state, as many drugs are transition state analogues. Here we performed extensive combined quantum mechanical (density functional theory B3LYP/6-31G\*) and molecular mechanical molecular dynamics simulations to elucidate the catalytic mechanism. Computations confirmed the transient existence of two metastable fragments of DXP by the heterolytic C3-C4 bond cleavage, namely 1-propene-1,2-diol and glycoaldehyde phosphate, in accord with the most recent kinetic isotope effect (KIE) experiments. Significantly, the heterolytic C3-C4 bond cleavage and C2-C4 bond formation are accompanied by proton shuttles, which significantly lower their reaction barriers to only 8.2-6.0 kcal/mol, compared with the normal single carbon-carbon bond energy 83 kcal/mol. This mechanism thus opens a novel way for the design of catalysts in the cleavage or formation of aliphatic carbon-carbon bonds.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Western Michigan University - Mailstop 5413

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**CONTROL ID:** 2231232

**TITLE:** [The directionality of non-covalent bonds](#)

**CONTACT (NAME ONLY):** [Yirong Mo](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Western Michigan University - Mailstop 5413, Kalamazoo, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Mo, Yirong](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The recently proposed s-hole concept by Clark, Politzer and their coworkers not only reinforces the contribution of electrostatic attraction to non-covalent bonds, but implies the angular dependency of the electrostatic force. To probe the magnitude of covalency, i.e., the electron transfer interaction, and its contribution to the directionality in non-covalent bonding, we investigated a small group of exemplary molecules which include hydrogen bonding, halogen bonding, chalcogen bonding and pnictogen bonding systems. The computational study is based on the block-localized wavefunction (BLW) method which decomposes the binding energy into the steric energy, which is a combination of electrostatic, Pauli repulsion, polarization and electron correlation effects, and the electron transfer (hyperconjugation) energy. The uniqueness of the BLW method is that it can provide optimal geometries with only steric effect included but electron transfer interaction excluded. On one hand, computations show that when only steric effect rules with the electron transfer interaction quenched, the bonding distances are about 0.5~0.8 Å shorter than the sum of van der Waals atomic radii due to the electrostatic attraction, and the overall steric effect exhibits the angular dependency notably in halogen bonding, chalcogen bonding and pnictogen bonding systems. On the other hand, the electron transfer interaction significantly shortens non-covalent bonding distances. This bond shortening enhances the Pauli repulsion which subsequently offsets the electrostatic attraction, and in the end the contribution of the steric effect to bonding is diminished. For instance, in the halogen bonding system H<sub>3</sub>N···ClF, the steric effect is even destabilizing and the binding is completely contributed by the electron transfer interaction. In several other systems particularly hydrogen bonding systems, the steric effect nevertheless still plays the major role while the electron transfer interaction is minor. However, in all cases, the electron transfer exhibits strong directionality, suggesting that the linearity or near linearity of non-covalent bonds is largely governed by the electron transfer interaction whose magnitude determines the covalency in non-covalent bonds.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Western Michigan University - Mailstop 5413

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**CONTROL ID:** 2236925

**TITLE:** [Finding motivation and inspiration in assessment work](#)

**CONTACT (NAME ONLY):** [Christine Rener](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Pew FTLC, Grand Valley State University, Allendale, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Rener, Christine](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:**

Over my 18 years of involvement in educational assessment efforts, I have challenged myself and my colleagues to view assessment as significant, enjoyable, and motivating. While my zeal is often met with initial skepticism, I have developed a rationale and framework that most faculty can connect with and benefit from. The framework outlines a set of constituencies impacted by our deep engagement with assessment and details the potential sources of motivation and inspiration for those engaged in this work. For example, authentic engagement in assessment can contribute to:

- (a) faculty-student engagement, with increased transparency of teaching and learning processes
- (b) an inclusive classroom environment that honors a diverse student body
- (c) stimulating departmental conversations about what matters: student learning
- (d) sustainable faculty engagement in their profession
- (e) robust connections of teaching practices to student learning
- (f) relevant and consistent curricula
- (g) learning from and with the wider chemical education enterprise
- (h) greater community understanding (on and off campus) of what we do, why and how it works

While certainly focused on student learning outcomes, this session will make the case for viewing assessment efforts in this larger context.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Assessment in Chemical Education - Oral

**SESSION HOST:** Organizer (Francis Burns)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Grand Valley State University

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**CONTROL ID:** 2253986

**TITLE:** [Syntheses and Characterization of Ferrocenophanes](#)

**CONTACT (NAME ONLY):** [Marwan Joudah](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Marshall Univ, Huntington, WV, United States.

2. Chemistry, Marshall University, Huntington, WV, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Joudah, Marwan T.](#)<sup>2</sup>; [Calvary, Caleb A.](#)<sup>1</sup>; [Wilson, Benjamin M.](#)<sup>1</sup>; [Castellani, Michael P.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Previous metallocenophanes were prepared by harsh methods and only work to form ferrocenophanes. Sodium cyclopentadienide reacts with  $[\text{Br}-(\text{CH}_2)_n-\text{Br}]$ , (where  $n = 4, 5$ ), to make  $[(\text{C}_5\text{H}_5)(\text{CH}_2)_n(\text{C}_5\text{H}_5)]$ . After deprotonation with  $n\text{-BuLi}$ , this compound reacts with  $\text{FeCl}_2(\text{THF})_{1.5}$  to yield  $[(\text{C}_5\text{H}_4)(\text{CH}_2)_n(\text{C}_5\text{H}_4)]\text{Fe}$ . In addition, two equivalents of  $(\text{H}_3\text{C}-\text{CH}=\text{CCH}_3\text{Li})$  react with dimethyl adipate and dimethyl pimelate to form  $[(\text{C}_5\text{R}_4\text{H})(\text{CH}_2)_n(\text{C}_5\text{R}_4\text{H})]$  (where  $\text{R} = \text{CH}_3$ ,  $n = 4, 5$ ). After deprotonation with  $n\text{-BuLi}$ , this compound reacts with  $\text{FeCl}_2(\text{THF})_{1.5}$  to form  $[(\text{C}_5\text{R}_5)(\text{CH}_2)_n(\text{C}_5\text{R}_5)]\text{Fe}$ .

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Call for Papers Inorganic Chemistry - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Brian Eklov)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Marshall University



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**CONTROL ID:** 2232300

**TITLE:** [Fifty year retrospective on the synthesis of corannulene](#)

**CONTACT (NAME ONLY):** [Paul Rasmussen](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Vinazene Inc, Ann Arbor, MI, United States.

2. Chemistry, University of Michigan, Ann Arbor, MI, United States.

3. Chemistry, University of Michigan, Ann Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Rasmussen, Paul G.<sup>1,2</sup>; [Lawton, Richard](#)<sup>3,1</sup>

**ABSTRACT BODY:**

**Abstract:** In 1965, the first synthesis of the highly strained, bowl shaped hydrocarbon corannulene, was completed at the University of Michigan by Prof. Richard G. Lawton and graduate student Wayne E. Barth. Corannulene, C<sub>20</sub>H<sub>10</sub>, is one-third of C-60 buckminsterfullerene and was the prototype for the synthesis of Eulerian shaped hydrocarbons. The original synthesis required some 17 steps, starting from acenaphthene. In the ensuing fifty years, many derivatives, both organic and organometallic, have been synthesized, and the synthesis improved by methods that use flash vapor pyrolysis and cleverly redesigned starting materials. As a result of these efforts, corannulene is now poised to become an important molecular building block for energy storage, and as an intermediate for the synthesis of more complex materials. The story and narrative of the early synthetic path, stumbling blocks, history of the beginning chemistry and the recounting of developments to the present day will be presented by Professor Lawton.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** History of Chemistry - Oral

**SESSION HOST:** Organizer (Seth Rasmussen)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Vinazene Inc

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**CONTROL ID:** 2236963

**TITLE:** [Water adsorption on Pt\(111\) and stepped Pt surfaces](#)

**CONTACT (NAME ONLY):** [Rachael Farber](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Loyola University Chicago, Chicago, IL, United States.

2. LIC / CASC, University Leiden, Leiden, Zuid Holland, Netherlands.

3. Leiden Institute of Chemistry, Leiden, Netherlands.

**AUTHORS (LAST NAME, FIRST NAME):** [Farber, Rachael G.](#)<sup>1</sup>; Killelea, Daniel R.<sup>1</sup>; Juurlink, Ludo B.<sup>3</sup>; Kolb, Manuel J.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** The interaction of water with metal surfaces has attracted much attention in the field of surface science. Water is ubiquitous on earth and is therefore of high significance to a wide range of fields, from studies of material aging and corrosion to atmospheric science. Studies of the adsorption, wetting, and desorption of water on metal surfaces continues to reveal new, and sometimes surprising, information about this deceptively simple system. Most relevant to this work are more recent advances in understanding the structures formed by submonolayer coverages of water on metal surfaces. Progress in this avenue has been facilitated by a combination of atomically resolved imaging experiments with density functional theory (DFT) calculations to elucidate how the balance of the water-water and water-surface interactions yield the

bonding patterns and behavior of water on regular metal surfaces [1]. As the application of these methods continues to develop, the understanding of 2-D water cluster formation and bonding behavior has given greater insight into the unique chemistry displayed by water on metal surfaces. Thus far, most studies have focused on the interaction of water with flat, regular metal surfaces; the still emerging studies of water on terrace step edges has further added to this already rich field [2]. In this project, we will study the arrangements of small clusters of water molecules on highly stepped Pt surfaces and compare the submonolayer coverage clusters on the stepped surfaces to those found on planar surfaces. We begin our study by first imaging water clusters on a Pt(111) crystal surface using an ultra-high vacuum scanning tunneling microscope (UHV-STM). We will then move on to studying the stepped surfaces. We will compare our observations to the predictions from DFT calculations of the same system [3]. The information gathered in this project will not only give further insight into water's unique behavior on metal surfaces, but also provide information on water's behavior on more reactive surface sites. An understanding of how steps and defects perturb the delicate balance of water-water and water-substrate interactions will result from this study.

References:

- [1] A. Hodgson; S. Haq; *Surf. Sci. Rep.* **64** 381 (2009).  
[2] M. van der Niet; A. den Dunnen; L.B.F. Juurlink; M.T.M. Koper; *PCCP* **13** 1629 (2011)  
[3] M.J. Kolb; F. Calle-Vallejo; L.B.F. Juurlink, M.T.M. Koper; *JCP* **140** 134708 (2014)

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Loyola University Chicago

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**CONTROL ID:** 2239410

**TITLE:** [Synthesis of glycine phthalimide using a heat gun](#)

**CONTACT (NAME ONLY):** [Elizabeth Brueggeman](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Jackson, MI, United States.

2. Spring Arbor University, Spring Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Brueggeman, Elizabeth A.](#)<sup>1</sup>; Baldwin, Bruce W.<sup>1</sup>; Schaerer, Charles L.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** Reactions between phthalic anhydride and various amides to create imide acids were studied. A heat gun was used to supply energy to drive the reaction. Phthalic anhydride and glycine reacted to produce glycine phthalimide. Because it has been observed that energy from microwave ovens increases the rates of these reactions (1), a study of the effect of the energy supplied by the heat gun on the control of the reaction will be conducted. In addition to glycine, other amides may be used as reactants in this study. References: 1. Bari, S., Bose, A., Chaudhary, A., Manhas, M., Raju, V., & Robb, E. Reactions Accelerated by Microwave Radiation in the Undergraduate Organic Laboratory. *J. of Chem. Ed.*, 1992, 69, 938-939.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Spring Arbor University

**CONTROL ID:** 2242075

**TITLE:** [Drugging the undruggable: Therapeutic potential of targeting the protein tyrosine phosphatases](#)

**CONTACT (NAME ONLY):** [Zhong-Yin Zhang](#)

**ABSTRACT STATUS:** decisioned\_accepted

**INSTITUTIONS (ALL):** 1. Biochemistry and Molecular Biology, Indiana University School of Medicine, Carmel, IN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Zhang, Zhong-Yin](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Aberrant tyrosine phosphorylation has been linked to the etiology of many human diseases including cancer, diabetes/obesity, neurodegenerative and autoimmune disorders. Notable success has been achieved in targeting signaling pathways regulated by protein tyrosine phosphorylation, with more than a dozen of small molecule kinase inhibitors already in the clinic. However, despite the fact that protein tyrosine phosphatases (PTPs) have been garnering attention as potential therapeutic targets, they remain largely an untapped resource. In fact, PTP-based drug discovery programs have historically been shrouded with difficulty in inhibitor selectivity and bioavailability, both of which are related to the intrinsic PTP active site properties.

We apply a novel approach for the design of potent and specific PTP inhibitors by tethering appropriately functionalized moieties to a nonhydrolyzable pTyr mimetic in order to engage both the active site and nearby unique peripheral binding pockets. By targeting less conserved interactions outside of the pTyr-binding cleft, increased affinity and selectivity can be obtained. Several novel nonhydrolyzable pTyr mimetics have been developed over the last few years offering potential solutions to overcome the bioavailability issue that has long plagued the PTP drug discovery field. Our recent work demonstrate that phosphonodifluoromethyl phenylalanine (F<sub>2</sub>Pmp), a well-established nonhydrolyzable pTyr surrogate, and bicyclic salicylic acid pharmacophores are sufficiently polar to bind the PTP active site, yet remain capable of efficiently crossing cell membranes, offering PTP inhibitors with both high affinity and selectivity and excellent *in vivo* efficacy in animal models of oncology, diabetes/obesity, autoimmunity, and tuberculosis. Current work is focused on advancing our lead generation paradigms and create a 'PTP-based drug discovery platform' that will ultimately impact broadly the portfolio of tomorrow.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Academic Drug Discovery: Challenges, Successes, Private Partnerships - Oral

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Indiana University School of Medicine

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**CONTROL ID:** 2259396

**TITLE:** [ACS CHAS: Where chemistry and safety meet](#)

**CONTACT (NAME ONLY):** [Kenneth Fivizzani](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Division of Chemical Health and Safety, Naperville, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Fivizzani, Kenneth P.](#)<sup>1</sup>

**ABSTRACT BODY:**

JGLCRM March 23, 2015 Submitted Abstracts

**Abstract:** The American Chemical Society Division of Chemical Health and Safety (CHAS) provides expertise in laboratory safety, chemical management, and safe chemical work practices to the Society and the general public. The division organizes technical symposia at ACS National and Regional Meetings and offers workshops in specific areas of chemical safety. Two CHAS awards recognize outstanding contributions to the field of chemical health and safety; a third award recognizes comprehensive lab safety programs in higher education. The CHAS website and Listserv offer on-line information and discussion of relevant topics. The division publishes the *Journal of Chemical Health and Safety* six times per year.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Current Issues in Chemical Lab Safety - Oral

**SESSION HOST:** Organizer (Kenneth Fivizzani)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Division of Chemical Health and Safety

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**CONTROL ID:** 2259400

**TITLE:** [Safety attitudes, awareness, and ethics](#)

**CONTACT (NAME ONLY):** [Kenneth Fivizzani](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Division of Chemical Health and Safety, Naperville, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Fivizzani, Kenneth P.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Solid safety awareness and attitudes are as important to chemistry as are following experimental procedures and keeping good records of conducted experiments. Building safety awareness is a long-term project - safety must be highlighted repeatedly. Faculty and staff members as well as industrial employers have an ethical obligation to teach students (chemistry majors and non-chemistry majors) and new employees about the need for a positive, proactive attitude about safety while conducting chemistry experiments. To set a good example, everyone who teaches, trains, or manages others in chemistry must know and follow all appropriate safety practices in the laboratory.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Current Issues in Chemical Lab Safety - Oral

**SESSION HOST:** Organizer (Kenneth Fivizzani)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Division of Chemical Health and Safety

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**CONTROL ID:** 2242205

**TITLE:** [Synthesis of pyrido lentzium](#)

**CONTACT (NAME ONLY):** [Haley Coggins](#)

**ABSTRACT STATUS:** re

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Spring Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Coggins, Haley N.](#)<sup>1</sup>; Schaerer, Charles<sup>1</sup>; Baldwin, Bruce W.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The focus of this experiment is to change a dianhydride into a diimide product. This will be done

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using 4-aminomethyl piperidine and imidazole as a catalyst. The energy supply for the procedure will come from heated air. The goal of this experiment is to verify the synthesis of the target molecule, and to attempt to increase the yield and purity of the compound through recrystallization.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Preferred

**CONTACT (INSTITUTION ONLY):** Spring Arbor University

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**CONTROL ID:** 2242347

**TITLE:** [Hydrogenation of tetraphenylcyclopentadione](#)

**CONTACT (NAME ONLY):** [SydneyChanel Price](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Detroit, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Price, SydneyChanel](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** This experiment is a hydrogenation reaction using Tetraphenylcyclopentadione. The Tetraphenylcyclopentadione will be reacting with H<sub>2(g)</sub> and 5% Pd/C in CH<sub>2</sub>CL<sub>2</sub>. The starting material is purple solid and the reaction creates a different white solid. Analysis of the reactions will be done by testing in IR and TLC analysis. The hydrogen adds anti but because of the metal center it should add syn. The experiment also should yield a trans-product but it makes a cis-product. I will change the source of hydrogen using gas and ammonium formate to find out if that makes a difference.

Ref. Mohrig, J. R.; Hammond, C. N.; Schatz, P.F.; Davidson, T. A. J. *Chem. Ed.* **2009**, 86, 243-239

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Spring Arbor University

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**CONTROL ID:** 2259110

**TITLE:** [Bouncing Batteries: Exploring the Chemistry of Alkaline Cells](#)

**CONTACT (NAME ONLY):** [Johnathon Hall](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Spring Arbor, MI, United States.

2. Natural Sciences, Spring Arbor University, Rockford, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Hall, Johnathon](#)<sup>2</sup>; Kuntzleman, Thomas S.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Alkaline batteries have been observed to bounce higher as the amount of charge delivered increases. Also, water is shown to be consumed in the overall chemical reaction for alkaline cells<sup>1,2,3</sup>. The

purpose of this study is to quantify and investigate the potential correlations between bounce height, charge delivered, and water consumed in alkaline batteries. AA alkaline batteries were obtained, labeled, and drained using a prototype MicroLab Resistive Load module supplied by our collaborators at MicroLab. Bounce heights were determined by recording and reviewing slow-motion videos of fresh and spent alkaline batteries as they were dropped from 60 cm. The batteries were then cut open with a hack saw. Percent mass lost after heating the inner battery contents at 90 degrees Celsius overnight was calculated. Additionally, Fourier Transform Infrared (FTIR) spectra were analyzed for the inner contents of the batteries. The bounce heights for alkaline batteries increased greatly as charge was delivered. In some cases, the dead batteries bounced up to 25 cm (opposed to the average 1 cm bounce height of the fresh batteries). Inner contents of fresh batteries lost a significantly higher amount of mass than spent batteries after heating overnight. This loss of mass was presumed to be from water evaporation. FTIR spectra consistently indicated a decreased water peak at  $3350\text{ cm}^{-1}$  in dead batteries as well. All collected data support that water is consumed as the chemical reaction progresses in alkaline batteries, which can aid in a student's understanding of the chemistry behind alkaline cells.

#### References

Energizer Battery Manufacturing Inc. *Alkaline Manganese Dioxide Handbook*. **2012**.  
Vincent, C. A.; Smith, M. J. *J. Chem. Ed.* **2002**, (79), 851-853.  
Kozawa, A.; Powers, R. A. *J. Chem. Ed.* **1972**, (49), 587-591.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Spring Arbor University

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**CONTROL ID:** 2244148

**TITLE:** [The effect of polyphenols on abeta aggregation](#)

**CONTACT (NAME ONLY):** [Colin Agatisa-Boyle](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Case Western Reserve University, Shaker Heights, OH, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Agatisa-Boyle, Colin](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Alzheimer's Disease, which is caused partially by the aggregation of the abeta peptide, is a major and growing public health concern. The abeta peptide initially exists in a monomeric random coil configuration, but transitions into a beta sheet conformation and oligomerizes as it aggregates. This presentation will examine if natural products could play a role in treating Alzheimer's Disease. Polyphenols from spices such as resveratrol, curcumin and capsaicin can potentially inhibit the aggregation of the abeta peptide. Circular dichroism was used to track the secondary structure conformation change of the peptide. NMR techniques were used to examine the interactions of the natural products with specific amino acids of abeta. Finally, atomic force microscopy was used to observe oligomer and fibril formation of abeta controls versus abeta treated with the various natural products.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Health Benefits of Natural Products in Spices: The Past, Present and Future - Oral

**SESSION HOST:** Organizer (Raul Juarez)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Case Western Reserve University

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**CONTROL ID:** 2245843

**TITLE:** [Esterification of Vanillin with Succinic Anhydride](#)

**CONTACT (NAME ONLY):** [Rachel Hayes](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Wyoming, MI, United States.  
2. Spring Arbor University, Spring Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Hayes, Rachel](#)<sup>1</sup>; Baldwin, Bruce W.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** The esterification of vanillin can be made more efficient and environmentally friendly by using a cyclic anhydride instead of acetic anhydride. Succinic anhydride, a solid, has far less danger of inhalation than acetic anhydride, which is most commonly used in this kind of reaction. This research will esterify vanillin by using succinic anhydride, an imidazole catalyst, and a heat gun. The procedure produces a vanillyl hydrogen succinate ester of vanillin, an environmentally safe spice. A successful reaction can be confirmed by IR analysis, as it will show three different carbonyl peaks in IR--acid, ester, and an aldehyde

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Spring Arbor University

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**CONTROL ID:** 2246175

**TITLE:** [Molecular crystals: A different take on surface science](#)

**CONTACT (NAME ONLY):** [Jacob Ciszek](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, Loyola University, Chicago, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Ciszek, Jacob W.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Science naturally gravitates towards well-defined systems of societal relevance. As such, the field of surface science arose from classical elemental surfaces and industrially relevant systems (e.g. silicon and catalytic surfaces). But as technologies change, new materials beckon to inquisitive scientists. As such, we have been recently studying organic semiconductors, with a surface chemistry as robust as their predecessors, and applications across all modes of electronic devices. We find that both single crystal and polycrystalline organic substrates are amenable to surface functionalization, and that many of the classical surface science tools (XPS, PM-IRRAS, etc.) can elucidate the structural features (density, chemical bonding, etc.) of these reacted surfaces. Interestingly, the unique composition of the surface (anisotropic building blocks held together by intermolecular forces) results in many features not displayed by traditional systems, including extreme differences in reactivity of the various facets.

**CONTACT (COUNTRY ONLY):** United States



**ABSTRACT SYMPOSIUM NAME:** Catalysis and Surface Science to Advance Energy Efficiency - Oral

**SESSION HOST:** Organizer (Daniel Killelea)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Loyola University

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**CONTROL ID:** 2247067

**TITLE:** [Adsorption of atomic oxygen on Ag\(111\)](#)

**CONTACT (NAME ONLY):** [Jonathan Derouin](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Loyola University Chicago, Chicago, IL, United States.

2. Chemistry, Loyola University Chicago, Palatine, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Derouin, Jonathan](#)<sup>2</sup>; Farber, Rachael G.<sup>1</sup>; Killelea, Daniel R.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Understanding the interaction of oxygen with transition metal surfaces is important in many areas including corrosion and catalysis. The oxygen/silver system in particular has been studied extensively both experimentally and theoretically. Interest is driven largely by the role of silver in two widely used industrial reactions: the epoxidation of ethylene to produce ethylene oxide and the partial oxidation of methanol to produce formaldehyde. The oxygen/silver system can also serve as a model for the dissociative chemisorption of diatomic molecules on close packed metal surfaces. Despite extensive research, the oxygen/silver system is still not well understood. To better understand this system, we use UHV-STM, AES and TPD to study the adsorption of atomic O on an Ag(111) crystal. Atomic O is generated by thermally cracking O<sub>2</sub>. By varying the power of the thermal cracker we are able to change the flux and energy of atomic O reaching the Ag surface. Using lower power, in addition to large p(4x4), p(4x5√3), c(3x5√3), and c(4x8) domains, a previously unseen adsorbate structure was identified. When higher power was used to thermally crack O<sub>2</sub>, another oxide structure with a significantly higher temperature desorption peak was formed. All of the adsorbate structures were characterized using AES, TPD and STM.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Catalysis and Surface Science to Advance Energy Efficiency - Oral

**SESSION HOST:** Organizer (Daniel Killelea)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Loyola University Chicago

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**CONTROL ID:** 2247939

**TITLE:** [Soluble Phthalocyanine: Catalyst for Selective Oxidation of Organic Sulfides and Building Block for "Molecular Panel" MOFs](#)

**CONTACT (NAME ONLY):** [Sarut Jianrattanasawat](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Western Michigan University, Kalamazoo, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Jianrattanasawat, Sarut](#)<sup>1</sup>; Mezei, Gellert<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The conversion of organic sulfides to sulfoxides and sulfones reduces the emission of sulfur from petroleum products. In addition, organic sulfides are important intermediates for pharmaceuticals. Metal salts of phthalocyanine (Pc), a thermally and chemically stable planar molecule, are known to catalyze the

oxidation of organic sulfides. Due to Pc's low solubility, many studies use Pcs as heterogeneous catalysts. Here, we describe the use of soluble phthalocyanine-2,3,9,10,16,17,23,24-octacarboxylic acid and its metal salts ( $\text{Fe}^{2+}$ ,  $\text{Cu}^{2+}$ ,  $\text{Zn}^{2+}$ ), as catalysts for sulfide oxidation reactions using aqueous hydrogen peroxide and methanol as solvent, at ambient conditions. The reactions are monitored in real-time by  $^1\text{H-NMR}$ . The results are compared using the rate constants of the non-catalyzed reactions versus the catalyzed reactions. Through the  $^1\text{H-NMR}$  studies, we have learned that steric hindrance has little effect on the rate of oxidation. However, electron-ing substituents lower the rate of oxidation. Furthermore, we have observed that our soluble Pc catalysts are selective for the oxidation of sulfides to sulfoxides, as no sulfones were detected. The increased solubility of Pc in organic solvents enables the efficient preparation of symmetrically functionalize Pcs, used as building blocks for metal-organic frameworks (MOFs). Our approach is to use robust, appropriately functionalized Pcs as "molecular panels", in place of traditional "struts", to build 3D MOFs. Pc-MOFs offer high capacity and large cavities, which can be exploited for catalysis applications. We have prepared several different Pc-MOFs and tested their catalytic activity in the oxidation of organic sulfides.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Call for Papers Inorganic Chemistry - Oral

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Brian Eklov)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Western Michigan University

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**CONTROL ID:** 2248057

**TITLE:** [Theoretical interpretation of atomic and ionic size](#)

**CONTACT (NAME ONLY):** [Roger Dekock](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Calvin College, Grand Rapids, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Weidman, Jared D.](#)<sup>1</sup>; [Dekock, Roger L.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Central to an understanding of electronic behavior upon ionization of atoms is the concept of atomic and ionic size. This concept is qualitative, resulting in many different ways of calculating the "radius" of an atom. Our lab has utilized the quantum chemistry software GAMESS to model the electron densities of atoms and their ions in order to calculate theoretical radii. We are interested in two groups of these radii, those that align more closely with covalent radii, and those that align with van der Waals radii, both of which are derived from experiment. Our results show that a single theoretical calculation method does not correlate with both experimentally-derived atomic and ionic radii.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Calvin College

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**CONTROL ID:** 2248542

**TITLE:** [Investigating the foundational layer formation of metal-organic coordinated thin films](#)

**CONTACT (NAME ONLY):** [Brandon Bowser](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Hope College, Midland, MI, United States.  
2. Chemistry, Hope College, Holland, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Bowser, Brandon<sup>1</sup>; Ohnsorg, Monica L.<sup>1</sup>; Anderson, Mary E.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** This research explores layer-by-layer (LBL) assembly for two types of metal-organic coordinated thin films, multilayers (ML) and frameworks (MOF). Controlled step-wise assembly defines the resulting film structure, presenting an opportunity to design these materials for specific applications, such as sensing and gas storage. Towards this realization, both films are fabricated by alternating, sequential solution phase deposition. Both systems were synthesized beginning with a 16-mecaptohexadecanoic acid (MHDA) self-assembled monolayer on gold. ML were composed of  $\alpha,\omega$ -mercaptoalkanoic acids and Cu (II) ions forming a conformal film. MOF were composed of 1,3,5-benzenetricarboxylic acid and Cu (II) ions (HKUST-1) yielding a porous crystalline framework. Both films were characterized using ellipsometry to measure film thickness and scanning probe microscopy (SPM) to map topographical morphology of film growth LBL. Using image analysis software, quantitative data regarding the growth of these thin films based on the images was procured (e.g. Particle Analysis and Percent Area Coverage). Ellipsometry suggests both ML and MOF form continuous, conformal layers that are each about 2 nm thick, respectively. However, SPM images elucidate two distinct systems, one that forms a semi-continuous film with distinct "islanding" (ML) and one that forms a rough surface of nucleating crystallites (MOF). The effects of deposition conditions, such as temperature and solution concentration, have been investigated in order to tailor film morphology for specific applications. Preliminary findings will be presented for utilizing infrared spectroscopy to study gas absorption within the MOF. Future work includes observing continued MOF growth to monitor at what point it becomes continuous and to investigate how the film forms beyond the threshold of complete surface coverage. Further studies will investigate other metal-organic coordinated thin film systems to understand the chemical and physical processes by which different film morphologies arise.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Hope College

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**CONTROL ID:** 2248760

**TITLE:** [A new class of mTOT-modulating thiazolidinedione insulin sensitizers](#)

**CONTACT (NAME ONLY):** [Steven Tanis](#)

**ABSTRACT STATUS:** decisioned\_accepted

**INSTITUTIONS (ALL):** 1. SPTanis PharmaChem Consulting LLC, Carlsbad, CA, United States.

2. Metabolic Solutions Development Company, Kalamazoo, MI, United States.

3. Kalexsyn, Portage, MI, United States.

4. Department of Medicinal Chemistry, College of Pharmacy, University of Michigan, Ann Arbor, MI, United States.

5. Jim Zeller Consulting LLC, Scottsdale, AZ, United States.

6. Kalexsyn, Portage, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Tanis, Steven P.<sup>1</sup>; Colca, Jerry R.<sup>2</sup>; Parker, Timothy T.<sup>3</sup>; Scott, Larsen D.<sup>4</sup>; Adams, Wade J.<sup>2</sup>; McDonald, William<sup>2</sup>; Kletzien, Rolf F.<sup>2</sup>; Zeller, James B.<sup>5</sup>; Gadwood, Robert C.<sup>6</sup>

**ABSTRACT BODY:**

**Abstract:** Early thiazolidine (TZD)-containing antidiabetic agents such as ciglitazone, pioglitazone (Actos®), rosiglitazone (Avandia®), and troglitazone (Rezulin®) were all discovered empirically, as a result of whole

animal testing. Consistent with the Medicinal Chemistry drumbeat for a defined mechanism, the mid-1990's saw a strong case being made that these compounds exerted their activity by a direct activation of the nuclear transcription factor peroxisome proliferator-activated receptor  $\gamma$  (PPAR $\gamma$ ). This testing paradigm led to numerous, potent PPAR $\gamma$  activators (and dual PPAR $\alpha/\gamma$  activators) entering development without success. Over the past 10 years or so evidence for a mitochondrial target for TZD's has emerged, called mTOT (*mitochondrial target of thiazolidinediones*), with PPAR activation associated with the undesired effects (weight gain, increase in intravascular volume, peripheral oedema, and congestive heart failure), this new mitochondrial target provided a potential new approach diseases associated with insulin resistance. A medicinal chemistry program targeting antidiabetic activity with a greatly reduced PPAR $\gamma$  liability while maintaining the insulin sensitizing pharmacology led to the selection of **MSDC-0160** and **MSDC-0602** for development. These compounds have active metabolites with further reduced capability to activate PPAR $\gamma$ . To date, these compounds have been through Phase 2b clinical development and they exhibit insulin sensitizing pharmacology similar to pioglitazone (Actos®) without the adverse effects associated with PPAR $\gamma$  agonists thus providing a new approach for treating metabolic diseases.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Upjohn, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Jed Fisher)|Organizer (Mike Barbachyn)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** SPTanis PharmaChem Consulting LLC

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**CONTROL ID:** 2249862

**TITLE:** [Stereoselective synthesis of cyclopentanoid monoterpene natural products and the elucidation of their roles as insect semiochemicals](#)

**CONTACT (NAME ONLY):** [John Hofferberth](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry Department, Kenyon College, Gambier, OH, United States.

2. Institute for Zoology, Chemical Ecology Group, University of Regensburg, Regensburg, Germany.

**AUTHORS (LAST NAME, FIRST NAME):** [Hofferberth, John E.](#)<sup>1</sup>; Adler, Snow<sup>1</sup>; Fischman, Clara<sup>1</sup>; Weiss, Ingmar<sup>2</sup>; Ruther, Joachim<sup>2</sup>; Stökl, Johannes<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** This presentation will highlight the divergent diastereoselective synthesis of iridomyrmecin, isoiridomyrmecin, and actinidine from the common starting material citronellol. These natural products have recently been identified in the semiochemical repertoire of the parasitic wasp *Leptopilina heterotoma* and several related wasp species. Using a similar synthetic approach, isomerically pure samples of two structurally related phytochemicals from *Teucrium marum* (Cat Thyme), teucriumlactone and dolicholactone, have also been prepared. These synthetic projects and the results of subsequent biological studies will be described.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Jay Wackerly)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Kenyon College

**CONTROL ID:** 2249929

**TITLE:** [Acyclic acid functionalized porphyrins for dye-sensitized solar cells](#)

**CONTACT (NAME ONLY):** [Hongshan He](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Eastern Illinois University, Charleston, IL, United States.  
2. School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou, Guangdong, China.

**AUTHORS (LAST NAME, FIRST NAME):** Wang, Xiangli<sup>1,2</sup>; klfout, Hafsa<sup>1</sup>; Salinas, Michael<sup>1</sup>; [He, Hongshan](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Dye-sensitized solar cell (DSC) is an electrochemical device that has a great potential to convert solar energy into electricity cost-effectively. Dyes are of importance to DSCs. Among numerous dyes investigated, porphyrins have emerged as one type of most efficient dyes for DSCs. Presently, a donor- $\pi$ -acceptor structure has been identified as a premium model for porphyrin-sensitized solar cells. In this model, a donor is usually a diphenylamine derivative, and an acceptor is an ethynylbenzoic acid in two opposite meso positions of a porphyrin ring. Though the energy efficiency up to 13% has been reported, it is still challenging to broaden the absorption capability to a longer wavelength. In this study, we designed and synthesized several porphyrin dyes with an acrylic acid as an acceptor. This design shortened the distance between porphyrin dye and titanium dioxide nanoparticle surface; therefore could facilitate the electron injection to increase the energy conversion efficiency. The detailed synthesis, characterization, photophysical and photovoltaic measurements will be presented.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Call for Papers Inorganic Chemistry - Oral

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Brian Eklov)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Eastern Illinois University

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**CONTROL ID:** 2250048

**TITLE:** [Only culinary?: Early modern medicinal uses of spice](#)

**CONTACT (NAME ONLY):** [Erika Olbricht](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. English, Case Western Reserve University, Cleveland, OH, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Olbricht, Erika](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Current alternative medicinal practice includes many plant-based remedies, but many of these plants and the knowledge about their medicinal properties are ancient. This paper explores what early English herbalists knew about spices and the plants that produce them, and in doing so, will also refer to classical writers, especially Galen and Dioscorides, who were important to early English herbalists. While today, we are likely to make distinctions between culinary and medicinal uses of various plants, there are several instances in early periods that show they did not make such distinctions. For example, at medieval feasts, often courses were served in order of the food's Galenic properties: hot and moist foods were generally followed by cold and dry foods. There is also evidence that such meals included plates of spices alongside the final course that were eaten to aid digestion. While this paper draws on scholarly work about the role of spices in culture and trade, it focuses primarily on the use of black pepper as a culinary spice and object of trade, but primarily as an herbal remedy—as a hot, dry choleric spice, it played a particular role in the

physiological balance of the humors and was an expensive, prized spice often kept under lock and key.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Health Benefits of Natural Products in Spices: The Past, Present and Future - Oral

**SESSION HOST:** Organizer (Raul Juarez)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Case Western Reserve University

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**CONTROL ID:** 2250408

**TITLE:** [Continuous flow chemistry for the synthesis of amides from nitriles and amines](#)

**CONTACT (NAME ONLY):** [Alan Medina-Gonzalez](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Augsburg College, Roseville, MN, United States.

2. Chemistry, Augsburg College, Minneapolis, MN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Medina-Gonzalez, Alan M.](#)<sup>2</sup>; Wentzel, Michael T.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:**

Amide bonds are a significant functional group of biological relevance in peptides and proteins, which are significant to pharmaceutical drugs. Amides are formed conventionally in condensation reactions using an amine and carboxylic acid in the presence of strong acid, forcing conditions, and from the acid chloride. However, usages of these chemicals can be highly expensive, waste generating, and less efficient. We have developed an alternative method to produce amides using a continuous flow reactor that is composed of a HPLC column packed with a titanium dioxide catalyst. Numerous variables such as flow rate, temperature, and pressure can be investigated rapidly with this method. By using phenylacetylnitrile, a benzylic nitrile, and various amines numerous amides have been synthesized.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Augsburg College

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**CONTROL ID:** 2250481

**TITLE:** [Modification and Green Synthesis of Sustainable Tri-block Copolymers](#)

**CONTACT (NAME ONLY):** [Zachary Swingen](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Augsburg College, Roseville, MN, United States.

2. Chemistry, Augsburg College, Minneapolis, MN, United States.

3. Chemistry, University of Minnesota, Plymouth, MN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Swingen, Zachary](#)<sup>2</sup>; Wentzel, Michael T.<sup>1</sup>; Wissinger, Jane E.<sup>3</sup>

**ABSTRACT BODY:**

**Abstract:** The importance of green polymer synthesis and sustainable polymers is the focus in a new experiment developed as a guided-inquiry polymer lab for undergraduate organic chemistry courses at all types of institutions. The lab highlights the fact that the various incorporation of monomers derived from renewable feedstocks, such as *L*-lactide,  $\delta$ -dodecalactone, and dodecalactone, are related to the physical and mechanical properties the polymer displays. This experiment not only introduces students to the fundamentals of polymer chemistry, but also instills quantitative data analysis techniques through analysis of  $^1\text{H}$ -NMR spectra of the synthesized polymer to calculate the composition and molecular weight of the product.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Augsburg College

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**CONTROL ID:** 2250784

**TITLE:** [Research from high school to grad school](#)

**CONTACT (NAME ONLY):** [Desmond Murray](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry & Biochemistry, Andrews University, Berrien Sprgs, MI, United States.

2. BEST Early, Berrien Springs, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Murray, Desmond H.](#)<sup>1, 2</sup>

**ABSTRACT BODY:**

**Abstract:** Not many teachers have the opportunity to concurrently engage high school through graduate school students in research. This presentation will describe approaches used and experiences had along the continuum of guided inquiry to independent research.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** High School, Community College, and Undergraduate Education - Oral

**SESSION HOST:** Organizer (Thomas Higgins)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Andrews University

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**CONTROL ID:** 2251346

**TITLE:** [Calcium oxide as a base in organic synthesis](#)

**CONTACT (NAME ONLY):** [Desmond Murray](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry & Biochemistry, Andrews University, Berrien Sprgs, MI, United States.

2. BEST Early, Berrien Springs, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Murray, Desmond H.](#)<sup>1, 2</sup>



**ABSTRACT BODY:**

**Abstract:** Calcium oxide is a cheap, abundant, stable, safe, nontoxic, and environmentally friendly heterogenous base that has been used in organic chemistry. We are currently exploring its applications across a spectrum of base-promoted organic reactions to determine the suitability, effectiveness and versatility of calcium oxide. We will present the results of our work to date.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**SESSION HOST:** Organizer (Sherine Obare)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Andrews University

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**CONTROL ID:** 2250904

**TITLE:** [The race to discover Element 61](#)

**CONTACT (NAME ONLY):** [Vera Mainz](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. School of Chemical Sciences, University of Illinois at Urbana-Champaign, Urbana, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Mainz, Vera V.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** B Smith Hopkins joined the University of Illinois faculty in 1912. At Illinois, Hopkins conducted research on beryllium, yttrium, columbium (now called niobium), tantalum, and the rare earths. He specialized more and more in the chemistry of the rare earths, which was the field in which he made his greatest contributions to chemistry.

At that time, separating rare earths from each other was a long and tedious process, depending on repeated recrystallizations. In some cases, thousands of recrystallizations were necessary. In 1926, Hopkins with Leonard Yntema and J. Allen Harris announced the discovery of the long sought element 61, which they named "illinium." Hopkins and his co-workers were in a race for this discovery with two other groups: 1) Charles James of the New Hampshire College of Agriculture and Mechanical Arts in Durham, N.H. (in 1923 the University of New Hampshire), who was "scooped" by Hopkins, and 2) Luigi Rolla and Lorenzo Fernandes of the University of Florence, who in 1922, undertook an immense investigation in a search directed at the isolation of element 61, which they dubbed florentium. Rolla contested the precedence of Hopkins' discovery but neither group could duplicate the isolation of element 61. Eventually it was determined that element 61 (now known as promethium) was highly radioactive and did not exist in nature. Hopkins had considered the discovery of illinium the climax of his career, and was bitterly disappointed that his work was not accepted.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** History of Chemistry - Oral

**SESSION HOST:** Organizer (Seth Rasmussen)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Illinois at Urbana-Champaign

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**CONTROL ID:** 2251042

**TITLE:** [Drug discovery at the University of Notre Dame: The Warren Family Research Center and the Indiana Drug Discovery Alliance](#)

**CONTACT (NAME ONLY):** [Richard Taylor](#)

**ABSTRACT STATUS:** decisioned\_accepted

**INSTITUTIONS (ALL):** 1. Warren Center for Drug Discovery and the Department of Chemistry Biochemistry, University of Notre Dame, Notre Dame, IN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Taylor, Richard E.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Built upon an historical research strength within the Department of Chemistry & Biochemistry, the University of Notre Dame recently established the Warren Family Research Center for Drug Discovery and Development. The Warren Center is focused towards the discovery and development of new therapeutic leads for the treatment of unmet clinical needs in cancer, infectious disease, stroke, and rare diseases. This collaborative program brings together chemical and biological expertise and technologies to through partnerships with researchers within the biomedically-focused centers at the University of Notre Dame including the Harper Cancer Institute, the Eck Institute for Global Health, the Center for Rare and Neglected Disease and external partners such as the Indiana CTSI. Over the past few years, many of the top research universities have created academic drug discovery programs in an attempt to replicate corporate capability in an academic setting. An alternative approach, like the one being implemented in Indiana, has university-based programs working collaboratively with the pharmaceutical industry to take full advantage of their complementary cultures, expertise, and resources to promote early stage discovery and to shepherd potential chemotherapeutic leads through the long and difficult path to the clinic. An overview of the Warren Center at Notre Dame and it's role in the Indiana Drug Discovery Alliance will be presented.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Academic Drug Discovery: Challenges, Successes, Private Partnerships - Oral

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Notre Dame

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**CONTROL ID:** 2251983

**TITLE:** [Thermal and flammability properties of bis-phosphorus derivatives of isosorbide](#)

**CONTACT (NAME ONLY):** [Yoseph Daniel](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Science of Advanced Materials, Central Michigan University, Mount Pleasant, MI, United States.

2. Center for Applications in Polymer Science, Department of Chemistry, Central Michigan University, Mount Pleasant, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Daniel, Yoseph](#)<sup>1,2</sup>; Howell, Bob A.<sup>1,2</sup>

**ABSTRACT BODY:**

**Abstract:** For applications in printed circuit boards, most traditional flame retardant additives contain bromine and are derived from petroleum. Bromine compounds are coming under increasingly severe regulatory pressure and alternatives are being sought. To generate non-toxic replacements, additives derived from renewable biosources are being developed. In this case, bis-phosphorus derivatives of isosorbide have been prepared, fully characterized, and examined as flame-retarding additives in DGEBA epoxy resin. These additives display good polymer compatibility, good thermal stability and enhancement of char formation. The flammability of blends of the additives with epoxy resin have been studied using limiting oxygen index (LOI), pyrolysis combustion flow calorimetry (PCFC) and vertical burn (UL94) test methods. Blends of

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additives (up to 2% phosphorus) with epoxy displayed strongly reduced flammability compared to that for epoxy containing no additives.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Green Chemistry and Sustainability - Oral

**SESSION HOST:** Organizer (Sherine Obare)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Central Michigan University

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**CONTROL ID:** 2253181

**TITLE:** [Selective encapsulation and extraction of kosmotropic anions from water by self-assembled nanojars](#)

**CONTACT (NAME ONLY):** [Gellert Mezei](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Western Michigan University, Kalamazoo, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Mezei, Gellert](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Selective encapsulation and extraction of anions by artificial receptors is one of the most far-reaching areas of supramolecular chemistry, with implications in chemical, biological and environmental sciences. The extraction of kosmotropic anions from aqueous media is challenging, due to their large hydration energies (affinity for water). We have recently shown that a class of toroidal copper(II)-hydroxide/pyrazolate complexes (nanojars), with the formula  $[\text{Cu}(\mu\text{-OH})(\mu\text{-pz})]_n$  ( $n = 27\text{-}36$ ), totally encapsulate kosmotropic anions with an unprecedented strength. Lined by H-bond donors on the inside and hydrophobic on the outside, these ~2 nm sized assemblies selectively extract kosmotropic anions from mixtures with chaotropic anions (low hydration energies). Up to twelve hydrogen bonds from the neutral host assembly wrap around and sequester anions from aqueous solutions, similarly as in their analogs in living organisms, such as the sulfate- and phosphate-binding proteins. Tetrabutylammonium “lids” seal the nanojars and render the encapsulated anion completely buried and inaccessible, so that, for example, sulfate is not precipitated by  $\text{Ba}^{2+}$  ions. Crystallographic, mass spectrometric, nuclear magnetic resonance, as well as reactivity and selectivity studies of seventeen different anions will be discussed.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Nanophotonics for Energy and Catalysis - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Seth Rasmussen)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Western Michigan University

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**CONTROL ID:** 2253267

**TITLE:** [Mechanism-driven catalyst modification for lactide ring-expansion polymerization](#)

**CONTACT (NAME ONLY):** [Yutan Getzler](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Kenyon College, Gambier, OH, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Getzler, Yutan D.](#)<sup>1</sup>; Wright, Shannon E.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The aluminum complex (<sup>t</sup>Bu-SalAmEE)Al (<sup>t</sup>Bu-SalAmEEH<sub>3</sub> = *N,N*-bis(3,5-di-*tert*-butyl-2-hydroxybenzyl)-2-(2-aminoethoxy)ethanol) catalyzes the synthesis of cyclic poly(lactide) (cPLA) by the ring-expansion polymerization (REP) of lactide. The solid-state structure of (<sup>t</sup>Bu-SalAmEE)Al has been confirmed by X-ray crystallography, revealing a five-coordinate complex with a geometry between trigonal bipyramidal and square pyramidal ( $\tau=0.4$ ). Variable temperature <sup>1</sup>H NMR studies with added Lewis bases and solution kinetics are consistent with intramolecular loss of a datively bound ligand oxygen as the rate determining step in lactide REP. Consequently, we have undertaken modification of the ligand at this site in an effort to increase polymerization rate.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Jay Wackerly)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Kenyon College

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**CONTROL ID:** 2255516

**TITLE:** [Mechanistic Studies on the BBr<sub>3</sub>-Catalyzed Cyclization of \*o\*-Alkynylanisoles to Form Benzofurans](#)

**CONTACT (NAME ONLY):** [Richard Lord](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry, Grand Valley State University, Allendale, MI, United States.

2. Dept of Chemistry 312 Padnos Hall, Grand Valley State University, Allendale, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Barylski, Matthew E.](#)<sup>1</sup>; [Korich, Andrew L.](#)<sup>2</sup>; [Lord, Richard L.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** In a previous study in the Korich group, *o*-alkynylanisole was shown to cyclize to form benzofuran, an important pharmaceutical precursor, in the presence of BBr<sub>3</sub>. We explored mechanistic possibilities to explain this unexpected observation using computational chemistry. In particular, geometry optimizations of reactants, intermediates, products, and transition states connecting these species were optimized at the B3LYP/6-31G(d) level of theory. Based on these findings we propose a new mechanism that plausibly explains the experimental results.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Grand Valley State University

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**CONTROL ID:** 2255526

**TITLE:** [Restoring Immune Balance Through Modulation of Immune Metabolism and Cytokine Networks](#)

**CONTACT (NAME ONLY):** [Peter Toogood](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Lycera Corp, Ann Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Toogood, Peter L.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Autoimmune diseases and cancer occur in part as a result of dysregulation of the natural immune response. Autoimmune disease is characterized by chronic activation of lymphocytes that recognize and attack naturally occurring, endogenous targets. These chronically activated lymphocytes exhibit a distinct bioenergetic profile in comparison to acutely activated immune cells, which provides a target for therapeutic intervention. Lycera is developing modulators of the mitochondrial ATPase to treat autoimmune conditions such as inflammatory bowel disease (IBD). The talk will include a description of the identification and characterization of Lycera's current lead candidate for treating IBD. In contrast, it is increasingly recognized that cancer cells exploit mechanisms to suppress anti-tumor immunity. Retinoid-related Orphan Receptor gamma (ROR $\gamma$ ) is a nuclear hormone receptor that functions as the master transcription regulator for type 17 T cells. The identification of endogenous ROR $\gamma$  agonists will be described and data will be presented demonstrating that synthetic ROR $\gamma$  agonists increase the ability of type 17 T cells to inhibit tumor growth.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Parke-Davis, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Lycera Corp

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**CONTROL ID:** 2255528

**TITLE:** [Green protection of pyrazole, thermal isomerization of tetrahydropyranypyrazoles, and high-yield, one-pot synthesis of 3\(5\)-alkyl- and 3,5-dialkylpyrazoles](#)

**CONTACT (NAME ONLY):** [Basil Ahmed](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry , Westren Michigan University , Kalamazoo, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Ahmed, Basil M.<sup>1</sup>; Mezei, Gellert<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Pyrazole is a remarkably versatile moiety, and its derivatives have a wide range of applications (e.g. pharmaceuticals and dyes). Therefore, it is essential to find green approaches for the large-scale and inexpensive derivatization of pyrazole. Herein we present a new synthetic approach one-pot, highly yield derivatization of the pyrazole, which it could be applied for the large-scale applications. We illustrate the approach by the highly efficient synthesis and characterization of a series of 3(5)-alkylpyrazoles and 3,5-dialkylpyrazoles. Green protection of the pyrazole was carried out by using the relatively cheap reagent 3,4-dihydro-2H-pyran, followed by lithiation with n-BuLi, alkylation by iodo or bromoalkanes, and deprotection with aqueous HCl. Alkylpyrazoles were thus obtained in 90–100% yield. Heating the intermediate 5-alkyl-1-(tetrahydropyran-2-yl)-1H-pyrazoles leads to isomerization to 3-alkyl-1-(tetrahydropyran-2-yl)-1H-pyrazoles, which can be further derivatized to 3,5-disubstituted pyrazoles. The 5-alkyl isomers are unreactive as a result of what's known as "adjacent lone pair effect". Computational studies have shown that the deprotonation of N-protected 3-methylpyrazole occurs at an endocyclic CH group (5-position), leading to an endocyclic carbanion. In contrast, the deprotonation of methyl-substituted, six-membered aromatic molecules occurs at the benzylic methyl group, producing exocyclic benzylic carbanion.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Call for papers Organic Chemistry - Poster

**SESSION HOST:** Organizer (Brian Eklov)|Organizer (James Kiddle)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Westren Michigan University

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**CONTROL ID:** 2255541

**TITLE:** [Isocyanate anion radicals and their cyclotrimerization to isocyanurate anion radicals](#)

**CONTACT (NAME ONLY):** [Steven Peters](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Illinois State University, Normal, IL, United States.

2. Chemistry, Illinois State University, Hoffman Estates, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Peters, Steven J.](#)<sup>1</sup>; Servos, Mark<sup>1</sup>; Scholtens, Cody<sup>1</sup>; Klen, Joseph<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** The remarkable utility of isocyanates as building blocks for the production of more complex molecular systems has been realized for well over 150 years. More recently, anion radicals of isocyanates have been used to generate polyisocyanates, which exhibit unique optical properties, and have also been exploited for use as helical linkers with molecular switches attached. Our group is interested in studying isocyanate anion radicals in part because so little is known about their structure. We believe a better understanding of these anion radicals will lead to a more complete picture of how these species can be used in synthesis. Unfortunately, the high reactivity of isocyanate anion radicals makes exploring their structure extremely challenging. In our studies involving of the alkali metal reduction of alkyl- and aryl isocyanates, we found that ion association to the alkali metal counter ion plays an important role in the stability and the reactivity of these anion radicals. Under conditions where ion association is absent, the anion radical of phenyl isocyanate can be generated and observed spectroscopically. Our findings indicate that the geometry of the NCO group depends upon the amount of electron spin density residing in this moiety. Alternatively, when these reductions are carried out under conditions where strong ion association to the cation is expected, no anion radical of any isocyanate is observed. Instead, we find that a rapid cyclotrimerization occurs upon reduction leading to the formation of isocyanurate anion radicals. The enhanced reactivity of isocyanate anion radicals is due to the increased electron density in the NCO group caused by tight ion pairing to the metal cation. The focus of this presentation will be on the formation of these isocyanate anion radicals and the structure of the isocyanurate anion radicals produced upon their cyclotrimerization.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Harnessing Radicals in Organic Synthesis - Oral

**SESSION HOST:** Organizer (David Nagib)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Illinois State University

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**CONTROL ID:** 2255644

**TITLE:** [Evaluating the effects of treatment combinations on erbB2+ cancer cells.](#)

**CONTACT (NAME ONLY):** [Christopher Taylor](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Mercyhurst University, Erie, PA, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Taylor, Christopher E.](#)<sup>1</sup>; Jones, Dyan<sup>1</sup>; Walter, Autumn E.<sup>1</sup>; Kuhnheim, Catherine J.<sup>1</sup>; Steiger, Sarah N.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The growth factor receptor erbB2 is overexpressed in a variety of cancers, where it drives the development of a phenotype marked by increased metastasis and resistance to treatment. Although numerous approaches to treat erbB2+ cancer have been developed, including kinase inhibitors and monoclonal antibodies, lack of efficacy continues to be an issue. An emerging paradigm in anti-cancer research is to evaluate broad-spectrum treatments or combinations of treatments with the intent of finding combinations that have a synergistic effect and are more selective for the targeted cell population.

This presentation will cover our recent work evaluating the potential of canertinib, an irreversible inhibitor of erbB2, to produce synergistic effects in combination with drugs that target related biochemical pathways and with more broadly effective agents such as radiation. Results will be presented using current mathematical models for evaluating synergistic effects relative to the effects of individual agents. In addition to a presentation of the research itself, the logistics of carrying out cell culture work with undergraduates at a primarily undergraduate institution will be discussed.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Research at Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Bradley Wile)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** Mercyhurst University

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**CONTROL ID:** 2255841

**TITLE:** [Synthesis of Substituted Pyrazolines as Inhibitors of \*Staphylococcus aureus\*](#)

**CONTACT (NAME ONLY):** [Teage Drinnon](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Ball State Univ, Muncie, IN, United States.

2. Chemistry, Ball State University, Muncie, IN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Drinnon, Teage K.](#)<sup>2</sup>; Fullenkamp, Christopher<sup>1</sup>; Pelly, Rachel R.<sup>1</sup>; McDowell, Susan<sup>1</sup>; Sammelson, Robert E.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** One of the greatest global health concerns since the development of antibiotics has been bacteria's ability to become resistant to the drugs that are prescribed. *Staphylococcus aureus*, is one of the most common bacteria involved in infection in the United States and some strains of *S. aureus* have found ways to become resistant to many drugs. Methicillin-Resistant *S. aureus*, also known as MRSA, is resistant against beta-lactam antibiotics which include, penicillins, such as methicillin and nafcillin, and also drugs classified as cephalosporins. New treatments for MRSA infections are needed. One such compound that has shown promise as a treatment has been deemed ML 141. ML 141 is a pyrazoline derivative that was discovered to have antimicrobial activity. Research focusing on synthesizing novel pyrazoline derivatives that are as effective, if not more effective, at inhibiting *S. aureus* as the compound ML 141 has become increasingly important.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Call for Papers Medicinal Chemistry - Poster

**SESSION HOST:** Organizer (Brian Eklov)|Organizer (James Kiddle)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Ball State University



**CONTROL ID:** 2256158

**TITLE:** [Collaborative Engagement in Novel Therapeutic Research & Enterprise in Chicago: UICentre \(drug discovery @ UIC\)](#)

**CONTACT (NAME ONLY):** [Gregory Thatcher](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Univ Of Illinois At Chicago, Chicago, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Thatcher, Gregory R.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** UICentre is a campus-wide drug discovery initiative at the Chicago campus of the University of Illinois supported by the Colleges of Pharmacy, Medicine, Liberal Arts & Sciences and other university administrative units and is associated with the Center for Clinical & Translational Science CTSA. UIC is home to 7 health sciences colleges and to the largest college of medicine in the nation, providing a potentially fertile ground for translational, small molecule therapeutic discovery. UICentre was established with no infrastructure costs and modest annual support, conceived to utilize existing resources, and to leverage the expertise of teams of scientists and clinicians across campus in collaborative engagement in translational research. The Centre's disease-agnostic strategy has evolved over the first 2 years of operations from reactive to a more proactive approach in sculpting and steering drug discovery initiatives on campus. Successful projects include a funded collaboration with University of Chicago and IIT Research Institute, which engages a team of 10 faculty at UIC with complementary expertise. The vision of UICentre is to create a collaborative, entrepreneurial environment conducive both to the cutting-edge science that drives drug discovery and to the translation of this science towards clinical application benefiting society at large. A similar vision is shared by a growing legion of academic drug discovery centers; however, academic research is not traditionally complementary or comfortable with the approaches taken in industry, yet alliances with industrial partners are essential to succeed. To attain ultimate success in placing new medicines in patients' hands, transformative changes are needed in academia and in industry.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Academic Drug Discovery: Challenges, Successes, Private Partnerships - Oral

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Univ Of Illinois At Chicago

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**CONTROL ID:** 2256715

**TITLE:** [Development of a natural product as a leukemia differentiation therapy](#)

**CONTACT (NAME ONLY):** [david wald](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. case western reserve university, Cleveland, OH, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [wald, david](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** As the defining feature of Acute Myeloid Leukemia (AML) is a maturation arrest, a highly desirable therapeutic strategy is to induce leukemia maturation. This strategy has the potential of avoiding the significant side effects that occur with traditional AML therapeutics and providing superior efficacy. Though AML is a common forms of leukemia in adults; the 5 year survival is less than 20-50% in adults and significantly lower in the elderly. The remarkable success in treating one uncommon subset of AML, acute promyelocytic leukemia (APL), with the differentiation agent, ATRA, illustrates the great promise for

differentiation therapy. Utilizing ATRA, the presumed cure of 75-85% of patients is possible but only for this rare AML subset. We have found that a plant-derived alkaloid, securinine, holds promise as an AML therapeutic for non-APL leukemia due to its ability to induce differentiation. Securinine has previously been used clinically as a therapeutic for primarily neurological related diseases. Through extensive preclinical development efforts, we have identified a class of optimized securinine analogues that exhibit high clinical potential. We have also characterized the pathways through which securinine induces differentiation as well as its other anti-cancer activities and identified putative direct targets. As differentiation therapies are able to treat leukemia without the necessity for overt cytotoxicity, this work has the potential to lead to much needed more efficacious, less toxic, and better tolerated therapy for patients with AML.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Health Benefits of Natural Products in Spices: The Past, Present and Future - Oral

**SESSION HOST:** Organizer (Raul Juarez)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** case western reserve university

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**CONTROL ID:** 2256876

**TITLE:** [Crystallographic Analysis of BshB from \*Bacillus subtilis\*, the Deacetylase Involved in Bacillithiol Biosynthesis](#)

**CONTACT (NAME ONLY):** [Chelsea Meloche](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Biomedical Sciences, Grand Valley State University, Allendale, MI, United States.

2. Department of Chemistry, Grand Valley State University, Allendale, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Meloche, Chelsea E.](#)<sup>1</sup>; Cook, Paul D.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** Gram-positive bacteria such as *Bacillus subtilis*, *Staphylococcus aureus*, and *Bacillus anthracis* utilize a recently discovered low molecular weight thiol called bacillithiol to maintain the appropriate cellular redox balance. Resistance to the antimicrobial drug fosfomycin depends on a thiol-dependent enzyme FosB, which utilizes bacillithiol as a crucial substrate. The biosynthesis of bacillithiol involves a three step pathway. Briefly, BshA, the first enzyme, is a glycosyltransferase that attaches *N*-acetylglucosamine to l-malate while expelling UDP. BshB, the deacetylase, hydrolyses the *N*-acetyl moiety from *N*-acetylglucosamine-malate. Lastly, to produce bacillithiol, BshC adds cysteine. Although the structure of BshA and BshC have been determined, the structure of BshB has not yet been reported. Here we present the 1.9 Å resolution X-ray crystallographic structure of BshB, a metal-dependent deacetylase from *B. subtilis*. This structure reveals an  $\alpha/\beta$  fold, consisting of seven helices surrounding a central parallel  $\beta$ -sheet. Enclosed in a deep cavity reside three amino acid residues, His 12, Asp 15 and His 113, which constitute a metal-binding site associated with  $Zn^{2+}$ . This citrate bound structure indicates how the carboxylates of the product are accommodated. The structure of BshB gives insight into key target residues for inhibiting the production of bacillithiol, which may provide therapeutic benefits.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Grand Valley State University

**CONTROL ID:** 2257060

**TITLE:** [A remote-controlled adaptive medchem lab: an innovative model of scientific collaboration to enable Drug Discovery in the 21st Century](#)

**CONTACT (NAME ONLY):** [Thierry Masquelin](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. DCRT, Eli Lilly, Indianapolis, IN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Masquelin, Thierry](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Integrated automation technologies continue to evolve and offer an ever-expanding scope of chemical synthesis possibilities. However, these endeavors have often come with increasing complexity and sophistication without necessarily increasing the flexibility necessary for overcoming challenges presented by an ever-changing landscape in chemical synthesis. While the goal of any fully integrated automated synthesis solution is to minimize the burden of repetitive, routine, rules-based operations that surround any given synthesis objective, there is a need to influence the future of the Drug discovery/pharmaceutical industry by breaking with the traditional research paradigm of medicinal chemistry practice and allow chemists to remotely guide chemical syntheses as a virtual extension of their own lab.

During assembly of the automated Synthesis and purification Laboratory (ASPL) at Eli Lilly and Co., we recognized novel opportunities to tap into external global scientific talent, assets and resources from any locations around the globe. This presentation will highlight a new synthesis-based engagement model of scientific collaboration using the ASPL as a unique and common conduit to Drug Discovery paradigm

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Drug Discovery - Oral

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Eli Lilly

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**CONTROL ID:** 2257152

**TITLE:** [Using a Focused Small Molecule Library to Study Bacterial Quorum Sensing](#)

**CONTACT (NAME ONLY):** [Amy Danowitz](#)

**ABSTRACT STATUS:** re

**INSTITUTIONS (ALL):** 1. Chemistry, Mercyhurst University, Erie, PA, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Danowitz, Amy](#)<sup>1</sup>; Kuehne, Jessica<sup>1</sup>; Link, Connor<sup>1</sup>; Schneider, Ivonne<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The rise of antibiotic resistant bacteria is a growing global health concern. To combat this problem, it is essential to discover new routes to target bacterial growth and viability. One method that may show promise in this realm is perturbing bacterial quorum sensing. Quorum sensing (QS) is the process by which bacteria use small molecule signals to sense population density and trigger phenotypic responses. Many Gram negative bacteria species use *N*-acylated L-homoserine lactones (AHLs) as QS molecules. Previous work has demonstrated that synthetic AHLs are capable of modulating quorum sensing. Additionally, a number of other synthetic five-membered heterocycles have also been shown to perturb QS in Gram negative species. Along these lines, we have synthesized a focused isoxazoline library designed to mimic some of the natural functionalities of QS modulators. Herein, we report the synthesis and biological testing of these molecules for

their ability to alter QS in a variety of Gram negative bacteria species.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Research at Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Bradley Wile)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Mercyhurst University

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**CONTROL ID:** 2257358

**TITLE:** [Salt-Mediated Assembly of Bimetallic Nanoshells into Monolithic Aerogel Frameworks](#)

**CONTACT (NAME ONLY):** [Kulugammana Gedera Ranmohotti](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Governors State University, Steger, IL, United States.

2. Chemistry, Virginia Commonwealth University, Richmond, VA, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Ranmohotti, Kulugammana Gedera S.](#)<sup>1,2</sup>; Gao, Xiaonan<sup>2</sup>; Arachchige, Indika U.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** In recent years, galvanic replacement reactions have been successfully employed to produce bimetallic nanoshells of a range of shapes, yet to date very few efforts have been devoted to develop methods for the assembly of nanoshells into solid-state nanostructures for the generation of nanoparticle-based devices. Sol-gel method represents a facile yet powerful strategy for the self-assembly of metal oxides, chalcogenides, and metal-semiconductor hybrid nanoparticle systems into three-dimensionally connected porous nanostructures. In this study, preparation of bimetallic alloy aerogels (Au/Ag, Pd/Ag, Pt/Ag) from a novel approach that involves the salt-mediated self-assembly of metal nanoshells followed by supercritical drying will be presented. The attractive nature of this new strategy is the ability to increase the rate of self-assembly, which otherwise is an intrinsically sluggish process in the oxidation-induced NP assembly reported to date. In this presentation we will discuss how these materials can be prepared as large (centimeter to inch) self-supported monoliths within a day, and how the gelation kinetics can be tuned by engineering, the in-situ-generated ionic strength of the precursor colloids.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Call for Papers Inorganic Chemistry - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Brian Eklov)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Governors State University

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**CONTROL ID:** 2257372

**TITLE:** [New Methods for the Synthesis of \*N\*-Substituted 2-Pyridones](#)

**CONTACT (NAME ONLY):** [Carolyn Anderson](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry and Biochemistry, Calvin College, Grand Rapids, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Anderson, Carolyn E.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Due to the importance of *N*-alkylated heterocycles within both natural product and pharmacologically active structures, the synthesis of unique classes of *N*-alkylated aromatic imidate systems continues to be a major synthetic goal. Utilizing either lithium iodide or gold-catalysis, our group has discovered new methods for the synthesis of three distinct classes of *N*-substituted 2-pyridones. The scope of these methods for the preparation of functionalized frameworks bearing the desired *N*-substituted pyridone and the subsequent conversion of these intermediates into more complex targets will be presented.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Jay Wackerly)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Calvin College

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**CONTROL ID:** 2257464

**TITLE:** [Exploration into Rotationally Restricted \*N\*-Alkyl 2-Quinolones](#)

**CONTACT (NAME ONLY):** [Carolyn Anderson](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry and Biochemistry, Calvin College, Grand Rapids, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Bootsma, Andrea N.](#)<sup>1</sup>; Anderson, Carolyn E.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Axially chiral molecules are an interesting class of compounds whose chirality stems from restricted rotation around a central bond. As chiral agents, these species have potential uses as asymmetric ligands, chiral derivatizing agents, or as chiral building blocks for the preparation of more complex targets. We have identified a synthetically accessible *N*-alkyl 2-quinolone, which exhibits such slowed rotation. Using computational analysis, the rotational barriers for a series of more highly substituted analogues have been calculated, leading to the identification of a target that is predicted to be configurationally stable at room temperature. These results, along with efforts to prepare this candidate in the laboratory, will be presented.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Calvin College

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**CONTROL ID:** 2257416

**TITLE:** [Efforts Towards the Synthesis of  \$\beta\$ - and  \$\gamma\$ -Amino Acids Containing \*N\*-Alkyl Pyridones](#)

**CONTACT (NAME ONLY):** [Carolyn Anderson](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry and Biochemistry, Calvin College, Grand Rapids, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Christopher, Joy P.](#)<sup>1</sup>; [Heidmann, Brian J.](#)<sup>1</sup>; Anderson, Carolyn E.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** *N*-Alkyl pyridones are an interesting functional group found in a series of pharmacologically active and naturally occurring compounds. Due to their medicinal potential, incorporation of *N*-alkyl pyridones into interesting chemical motifs, such as unnatural  $\beta$ - and  $\gamma$ -amino acids, is an important synthetic goal. Utilizing a  $\beta$ -iodo *N*-alkenyl pyridone intermediate that was discovered in our laboratory, preparation of these unnatural amino acids is underway. Evaluation of a number of different protected propargylic amino alcohols in route to the required substrates will be presented, as will efforts to optimize the formation of the required nitrogen containing  $\beta$ -iodo *N*-alkenyl pyridones.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Calvin College

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**CONTROL ID:** 2257483

**TITLE:** [Enantioselective Photocatalytic Reactions](#)

**CONTACT (NAME ONLY):** [Tehshik Yoon](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry Department, Univ of Wisconsin Madison, Madison, WI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Yoon, Tehshik P.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The control of stereochemistry in photochemical reactions is a long-standing challenge with few general solutions. We have developed a robust dual-catalyst strategy that combines a photochemically active transition metal sensitizer with a chiral Lewis acid. The ability to apply the well-established principles of asymmetric Lewis acid catalysis to control the reactivity of photogenerated reactive intermediates provides a novel and potentially generalizable approach to stereocontrol in a wide range of photochemically initiated transformations.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Harnessing Radicals in Organic Synthesis - Oral

**SESSION HOST:** Organizer (David Nagib)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Univ of Wisconsin Madison

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**CONTROL ID:** 2257503

**TITLE:** [Synthesis and Evaluation of Chemical Probes for Delivering Antibody-Recruiting Small Molecules to Mycobacteria](#)

**CONTACT (NAME ONLY):** [Temitope Nathan](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry & Biochemistry, Central Michigan University, Mount Pleasant, MI, United States.

2. Department of Chemistry, Central Michigan University, Mt Pleasant, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Nathan, Temitope O.](#)<sup>1</sup>; Swarts, Benjamin<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** Tuberculosis, caused by bacterium *Mycobacterium tuberculosis*, is a devastating disease that results in approximately 1.5 million deaths per year. Administering antibiotic drugs has been a viable approach for treating tuberculosis, however, the course of treatment is lengthy, the availability of the drugs is limited in many countries, and drug resistance is on the rise. Immunotherapy may be an attractive adjunctive treatment for improving standard tuberculosis chemotherapy. We propose to develop a chemical approach to modifying the bacterial cell surface with antibody-recruiting small molecules, or ARMs. Here, we report the synthesis and evaluation of two chemical probes designed to deliver the ARM dinitrophenyl to the cell surface of *Mycobacterium smegmatis*, a model mycobacterium.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Central Michigan University

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**CONTROL ID:** 2257687

**TITLE:** [Hybrid Nanophotonic Materials for Enhanced Ultrafast Optical Response and Efficient Exciton Propagation](#)

**CONTACT (NAME ONLY):** [Gary Wiederrecht](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Wiederrecht, Gary P.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Future nanophotonic architectures for optical energy conversion and photocatalysis will require nanostructures with roles that work together cooperatively, such as structures with a large absorption cross section combined with features that enable guiding, propagating, and converting energy. Ultrafast optical responses in nanostructures are critical to understand for these applications. Although there is the potential for radiative and nonradiative energy losses, there is also the opportunity for accessing pathways for improved energy conversion, such as through the extraction of hot plasmonic electrons from metal nanoparticles. For propagation of energy in nanophotonic structures, nanostructured materials inspired by natural photosynthetic membranes represent an opportunity for efficient and directional energy transport. In natural photosystems, light harvesting complexes can transport excitons to the reaction center core with near unity conversion of absorbed photons to separated charge. A key to this process is the high rate of exciton hopping and the directionality of exciton flow due to an energy level waterfall effect of excitons in complexes as the reaction center core is approached. Efforts to induce similar behavior in biomimetically inspired nanostructures are described. Use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Nanophotonics for Energy and Catalysis - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Seth Rasmussen)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Argonne National Laboratory



**CONTROL ID:** 2258084

**TITLE:** [Photophysics of hybrid semiconductor nanowires in photocatalytic hydrogen generation applications](#)

**CONTACT (NAME ONLY):** [Masaru Kuno](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. University of Notre Dame, Notre Dame, IN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Kuno, Masaru K.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Semiconductor nanostructures possess a number of applications in solar energy conversion. This includes using colloidal quantum dots in solar cells and, more recently, using analogous nanostructures such as nanowires (NWs) in photocatalytic applications. Here we describe recent work to understand the photocatalytic response of solution-synthesized CdSe NWs within the context of hydrogen generation. Various CdSe NW-based systems such as core/shell structures and hybrid metal nanoparticle/semiconductor NW hybrid systems have been studied. In all cases, femtosecond transient differential absorption spectroscopy has been used to reveal relevant carrier relaxation processes in these materials as well as the flow of charges across the different heterointerfaces that are present. By correlating these transient absorption results to results from accompanying hydrogen generation efficiency measurements, we have, in turn, rationalized the response of these materials, clarifying the role that different heterojunctions play in establishing both charge separation and hydrogen generation efficiencies.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Nanophotonics for Energy and Catalysis - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Seth Rasmussen)

**PRESENTATION TYPE:** Oral Preferred

**CONTACT (INSTITUTION ONLY):** University of Notre Dame

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**CONTROL ID:** 2258265

**TITLE:** [Incorporation of hands-on gas chromatography-mass spectrometry into a one-year general chemistry curriculum](#)

**CONTACT (NAME ONLY):** [Bernard Liburd](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Grand Rapids Community College, Grand Rapids, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Liburd, Bernard](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Rarely are first-year general chemistry students exposed to or much less allowed to perform their own measurements on modern chemical instrumentation. This approach has changed at Grand Rapids Community College (GRCC) with the procurement of a gas chromatograph-mass spectrometer (GC-MS) through the National Science Foundation Grant DUE 1140509. The acquisition of the instrument has allowed GRCC science faculty to incorporate its' use across the general chemistry curriculum. The instrument was integrated into the general chemistry sequence to help students clarify the differences between an element and its isotopes, to introduce the science of chromatographic separation and mass spectrometry identification, and to provide students with hands-on experience in its use. With the goal of improving students' knowledge of, and providing a kinesthetic learning experience with GC-MS, experiments were developed and adapted to include the use of the instrument. This presentation will discuss the methods and outcomes of this work including curriculum development, student feedback, and assessment of student achievement.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** High School, Community College, and Undergraduate Education - Oral

**SESSION HOST:** Organizer (Thomas Higgins)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Grand Rapids Community College

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**CONTROL ID:** 2258623

**TITLE:** [General Chemistry for Engineering Students: Integrating the Results from Industrial Ecology Studies into the Curriculum](#)

**CONTACT (NAME ONLY):** [Craig Donahue](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Univ of Michigan, Dearborn, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Donahue, Craig J.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Engineers design and manufacture the buildings in which we live and work, the automobiles and aircraft in which we travel, and the electronic devices and appliances we depend on. Chemists, and many others, play an important role in supplying the materials (raw, refined, and new) and the energy systems upon which engineers rely on to produce and operate the aforementioned products. We, the chemistry educators, now encourage our students to embrace sustainable practices and green chemistry. The new, but rapidly expanding, field of industrial ecology provides us with a big picture and often a global view of key materials (e.g. steel, aluminum, copper) and how they are obtained, used, and recycled. These studies make clearer than ever before how energy-intensive, how environmentally friendly, and how sustainable our use of these materials really is. This presentation will provide a bibliography of some important industrial ecology studies, the vast majority of which have appeared in the last ten years. A short list of key observations/conclusions derived from these studies will also be provided.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Univ of Michigan

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**CONTROL ID:** 2258641

**TITLE:** [Electroless Deposition on Plastics](#)

**CONTACT (NAME ONLY):** [Craig Donahue](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Univ of Michigan-Dearborn, Dearborn, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Waldman, Zipporah](#)<sup>1</sup>; [Donahue, Craig J.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** A multi-faceted lab experiment that showcases electroless deposition on plastic is being developed. More specifically, a detailed protocol for depositing an electroless nickel coating on yellow Lego® bricks, made of ABS, has been worked out. Other metals have also been plated on the Lego® bricks by electroless deposition. The electroless nickel coating is actually an alloy of nickel and phosphorus assuming the

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hypophosphite anion ( $\text{H}_2\text{PO}_2^-$ ) is the reducing agent present in the nickel bath. The pH of the nickel bath determines the level of phosphorus in the nickel alloy coating. Several analytical methods, both destructive and non-destructive, are being developed to determine the nickel content of the electroless nickel coating. In an industrial setting, electroless deposition is often the first of several steps used to achieve the final product (e.g. a plastic automobile door handle that has a lustrous metallic surface coating). The appearance of the electroless nickel coating on the Lego® bricks has been further enhanced by performing one or more electroplating steps.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Univ of Michigan-Dearborn

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**CONTROL ID:** 2258636

**TITLE:** [General Chemistry for Engineering Students: Incorporating Results from Industrial Ecology Studies to Expand the Story of Aluminum](#)

**CONTACT (NAME ONLY):** [Craig Donahue](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Univ of Michigan, Dearborn, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Donahue, Craig J.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Aluminum is a relative newcomer to the array of metals/alloys available to the designer. Although it has been produced by the Hall-Héroult process for ~125 years, significant aluminum use did not take place until after WWII. However, since then end-user demand for aluminum has increased ~30-fold, a more dramatic increase than for any other metal. Out of a dozen end-use categories, the manufacture of the automobile uses more aluminum (17.5% of the total) than any other category. This dependence on aluminum by automakers is likely to increase given the recent announcement by Ford Motor Company that its 2015 model year F-150 pickup truck will shed 750 pounds compared to its predecessor by utilizing an all-aluminum body and cargo box. In this presentation, the results of several recent industrial ecology studies on aluminum will be drawn on to tell a more complete story of aluminum preparation, use, and recycling. This approach connects the world of chemistry to the world of engineering and vice versa.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Papers - Oral

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Univ of Michigan

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**CONTROL ID:** 2259136

**TITLE:** [The University of Michigan Vahlteich Medicinal Chemistry Core: Achieving Proof-of-Concept in Vivo for Novel Therapeutic Hypotheses](#)

**CONTACT (NAME ONLY):** [Scott Larsen](#)

**ABSTRACT STATUS:** re

**INSTITUTIONS (ALL):** 1. Medicinal Chemistry, University of Michigan, Ann Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Larsen, Scott D.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** The Vahlteich Medicinal Chemistry Core (VMCC) was established in the College of Pharmacy in 2007 to integrate pharmaceutical industry experience and expertise into early stage academic drug discovery at the University of Michigan. Our mission is to assist biomedical researchers in translating their novel therapeutic hypotheses into proof-of-concept in animal models of disease through design and synthesis of small molecule probes, regardless of therapeutic area. We also provide graduate students the opportunity to gain exposure to the process of drug discovery and development through both laboratory experience and classes on drug design. This talk will provide examples of projects where the VMCC has been successful at achieving in vivo activity starting with two different types of leads: high throughput screening hits and drugs optimized for other indications.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Upjohn, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Jed Fisher)|Organizer (Mike Barbachyn)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Michigan

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**CONTROL ID:** 2259198

**TITLE:** [Esterification of 2,2-dimethyl-1-propanol compared to banana flavoring](#)

**CONTACT (NAME ONLY):** [Elizabeth Sowers](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Spring Arbor, MI, United States.

2. Spring Arbor University, Spring Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Sowers, Elizabeth<sup>1</sup>; Baldwin, Bruce W.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** The goal of esterifying 2,2-dimethyl-1-propanol is to identify the ester that is used in the commercial banana flavoring, amyl acetate by Caravelle. The commercial banana flavoring ester, using gas chromatography, gave a peak at 7 minutes; this peak was compared to two similar esters that did not give the same peak. We will verify the two esters using Gas Chromatography and FTIR.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Spring Arbor University

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**CONTROL ID:** 2259403

**TITLE:** [Progress Toward the Synthesis of 5-Azido Inositol](#)

**CONTACT (NAME ONLY):** [Sarah Rundell](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Central Michigan University, Mount Pleasant, MI, United States.  
2. Department of Chemistry, Central Michigan University, Mt Pleasant, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Rundell, Sarah R.](#)<sup>1</sup>; Swarts, Benjamin<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** *Myo*-inositol is a carbohydrate that is found both in prokaryotes and eukaryotes which has functions in signal transduction pathways and is involved in anchoring proteins and other molecules to the cell surface. Chemically modified *myo*-inositol derivatives may be valuable in probing or inhibiting inositol-related metabolic pathways in various organisms. Unfortunately, *myo*-inositol derivatives can be challenging to synthesize due to inositol's internal plane of symmetry and the difficulty associated with distinguishing between its six secondary hydroxyl groups. Here, we report our efforts to produce 5-azido-inositol from a simple glucopyranoside starting material that bypasses these problems.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Central Michigan University

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**CONTROL ID:** 2259449

**TITLE:** [Green, highly efficient method for the protection of heterocyclic amino, hydroxyl, and thiol groups](#)

**CONTACT (NAME ONLY):** [Mia Jawor](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Western Michigan University, Kalamazoo, MI, United States.  
2. Chemistry, Western Michigan University, Steger, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Jawor, Mia](#)<sup>2</sup>; Mezei, Gellert<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** This project addresses the need for environmentally-friendly organic synthesis processes, by eliminating solvents, toxic/explosive reagents, purification steps, maximizing conversion/yield and minimizing waste production. Specifically, we propose a novel functional group protection method for heterocyclic amino, hydroxyl and thiol groups. This method is valuable for organic synthesis both at the laboratory and the industrial scales. Based on our preliminary results with pyrazole, we propose to extend the novel, green protection method discovered in our lab to a variety of substrates, including other heterocyclic amines, as well as hydroxyl- and thiol-functionalized compounds. To this end, we: 1) investigate the feasibility of the protection method and optimize the reaction conditions for number of different substrates, 2) test the hypothesis that the acidity of the substrate proton, which will be replaced by the protecting group, is directly correlated with the efficiency (conversion, reaction temperature, and time) of the process, and 3) test the hypothesis that heterocyclic amines can be selectively protected in the presence of primary amino (NH<sub>2</sub>) substituents.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Western Michigan University

**CONTROL ID:** 2259462

**TITLE:** [Alcohols, water, and hydrogen bonding: a simple set of experiments for the general chemistry lab](#)

**CONTACT (NAME ONLY):** [Mark Benvenuto](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, University of Detroit Mercy, Detroit, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Benvenuto, Mark A.](#)<sup>1</sup>; Paulsen, Bryan<sup>1</sup>; Lanigan, Katherine C.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Logic tells our students that if 25 mL of an alcohol and 25 mL of water are mixed that the resultant volume should be 50 mL. Yet this is not the case. For most other combined volumes the result is also less than the sum. This seminar will discuss how a series of alcohol and water mixtures can be made and their volumes graphed, so that students can see a real life example of hydrogen bonding and its macroscopic effects.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** High School, Community College, and Undergraduate Education - Oral

**SESSION HOST:** Organizer (Thomas Higgins)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Detroit Mercy

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**CONTROL ID:** 2259808

**TITLE:** [Cryptospirolepine: Revisiting and Revising the Structure Using Modern NMR Techniques, DFT Calculations, and CASE Program Capabilities](#)

**CONTACT (NAME ONLY):** [Gary Martin](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Process & Analytical Chemistry, NMR Structure Elucidation, Merck Research Laboratories, Rahway, NJ, United States.

2. Univ of Pittsburgh, Pittsburgh, PA, United States.

3. Molecule Apps, LLC, Wilmington, DE, United States.

4. American Herbal Products Association, Silver Spring, MD, United States.

5. Chemistry, University of Barcelona, Barcelona, Spain.

6. Bruker Biospin, GmbH, Rheinstetten, Germany.

**AUTHORS (LAST NAME, FIRST NAME):** Sauri, Josep<sup>1</sup>; Bermel, Wolfgang<sup>6</sup>; Blinov, Kirill<sup>3</sup>; Buevich, Alexei V.<sup>1</sup>; Sharaf, Maged H.<sup>4</sup>; Schiff, Paul L.<sup>2</sup>; Parella, Teodor<sup>5</sup>; Williamson, Thomas<sup>1</sup>; [Martin, Gary E.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Cryptospirolepine is a complex indoloquinoline alkaloid that was first isolated in late 1991 from extracts of the Ghanaian chewing stick, *Cryptolepis sanguinolenta*. The structure elucidation was reported in 1993<sup>1</sup> employing what were then state-of-the-art NMR methods and 3 mm micro NMR probe technology. Structure elucidation work done on the molecule preceded the development of <sup>1</sup>H-<sup>15</sup>N HMBC methods by several years. Using the NMR methods then available, no correlations were observed to the carbonyl in the HMBC data that could be acquired. The structure elucidation hinged on an ROE observed between a vinyl proton and one of the terminal resonances of a four-spin aromatic system and a putative <sup>4</sup>J<sub>CH</sub> correlation to a

quaternary carbon from the same aromatic proton. Computer-Assisted Structure Elucidation or CASE programs were then in their infancy and incapable of dealing with a molecule of the complexity of cryptospirolepine. In light of this history, we have interrogated a 700 µg voucher sample of cryptospirolepine using 1.7 mm MicroCryoProbe™ technology, 2 Hz optimized <sup>1</sup>H-<sup>13</sup>C and <sup>1</sup>H-<sup>15</sup>N LR-HSQMBC, and newly developed pure shift 1,1- and 1,n-ADEQUATE methods. Using this powerful ensemble of modern NMR experimental methods coupled with state-of-the-art DFT calculations and CASE methods, supplemented with the knowledge of the structure of a key degradant of cryptospirolepine whose structure was elucidated more than a decade ago using cryoprobe technology, we now wish to report the revision of the structure of cryptospirolepine.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Upjohn, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Jed Fisher)|Organizer (Mike Barbachyn)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Merck Research Laboratories

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**CONTROL ID:** 2259905

**TITLE:** [On the origin of 'synthetic metals': Herbert N. McCoy, Alfred René Ubbelohde, and the development of metals from nonmetallic elements](#)

**CONTACT (NAME ONLY):** [Seth Rasmussen](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, North Dakota State University, Fargo, ND, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Rasmussen, Seth C.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Organic materials that conduct electricity in the metallic range ( $>10^2 \text{ S cm}^{-1}$ ) are commonly called 'synthetic metals' and this term has become synonymous with doped conjugated organic polymers, as illustrated by the 2000 Nobel Lecture of Alan G MacDiarmid entitled "'Synthetic Metals': A Novel Role for Organic Polymers". While the origin of this term has been attributed to Alfred René Ubbelohde in the late 1960s, it can actually be traced further back to a 1911 paper in Science by Herbert N. McCoy. The origin and history of the term 'synthetic metals' will be presented, along with its growing use to describe organic conductors.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** History of Chemistry - Oral

**SESSION HOST:** Organizer (Seth Rasmussen)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** North Dakota State University

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**CONTROL ID:** 2259907

**TITLE:** [A Novel Approach to Generating Broad-Spectrum Antifungal Drug Candidates from the Natural Product Compound Aureobasidin A](#)

**CONTACT (NAME ONLY):** [Ake Elhammer](#)



**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. AureoGen Biosciences, Inc, Kalamazoo, MI, United States.  
2. Kalexsyn Inc, Kalamazoo, MI, United States.  
3. Kalexsyn, Inc., Kalamazoo, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Elhammer, Ake<sup>1</sup>; Wuts, Peter G.<sup>2</sup>; Simons, Lloyd J.<sup>3</sup>; Metzger, Brian<sup>1</sup>; Sterling, Rachel<sup>1</sup>; Slightom, Jerry<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** There is currently an immediate unmet need for new and better drugs to treat of systemic fungal infections. The natural product aureobasidin A (AbA) is a well-tolerated antifungal agent with robust efficacy in animals and a mode of action that is distinct from all drugs in current clinical use. However, although native AbA is active, and quite potent, against essentially all yeasts, as well a number of other fungi, it has little activity against the filamentous fungus *Aspergillus fumigatus*. *A. fumigatus* is an important human pathogen and attempts to improve AbA's activity this organism, by structural modifications, have to date involved chemistries too complex and costly for continued development. AureoGen has developed an entirely new, and much simpler, approach to modify the structure of AbA. The key step in the chemistry involves functionalization of the phenylalanine residues in the compound by iridium-catalyzed borylation. This is followed by displacement of the pinacol boron moiety to form the corresponding bromide or iodide and substitution by Suzuki biaryl coupling. The chemistry allows for synthesis of a truly wide range of derivatives and has to date produced compounds with *A. fumigatus* minimal inhibitory concentrations of < 0.12 µg/ml. The approach is also readily adaptable to large-scale synthesis and industrial production.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Upjohn, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Jed Fisher)|Organizer (Mike Barbachyn)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** AureoGen Biosciences, Inc

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**CONTROL ID:** 2259952

**TITLE:** [Consequences of chloromethane \(R40\) mixed in with tetrafluoroethane \(R134a\); production of trimethylaluminum, reactivity of TMA and various refrigerant oils and methods to deactivate trimethylaluminum](#)

**CONTACT (NAME ONLY):** [Zhichao Chen](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Michigan Tech, Houghton, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Chen, Zhichao<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Recently there have been reports of “fake refrigerants” and the dangers associated with these counterfeit refrigerants distributed as 1,1,1,2-tetrafluoroethane R134a. The substitution of chloromethane (R40) for R134a is likely produce pyrophoric trimethylaluminum (TMA) in the compressor. Reactions between Al containing materials and R40 were conducted and no sign of a reaction was observed until Mg was added to the mixture. The gas samples were analyzed by GC-MS which resulted in the detection of alkanes, indicating that trimethylaluminum (TMA) was produced in the reaction. A different study involving Al-foil, AlCl<sub>3</sub> and R40 resulted in a weight loss of 19% and cracks detected by SEM were found on the Al-foil. Methane was detected by GC-MS, suggesting formation of TMA. Several commercially available refrigerant oils were subjected to TMA. Only polyester oil resulted in a decrease in the theoretical quantity of methane released upon final deactivation with alcohol due to reactions between the methyl groups in TMA and reactive groups on the oil. Various chemicals were added to TMA in order to find which ones would react, and not produce methane. Ethyl acetate has a similar reductive effect to the polyester oil presumably

due to the reaction between TMA and the functional ester groups. Aldehydes and ketones were also found to react with TMA resulting in a reduction of the theoretical quantity of methane that could be released. Phthalaldehyde was determined to be the most efficient reagent by deactivating approximately 50% of the methyl groups on TMA resulting in a methylation product detected by GC-MS.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Michigan Tech

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**CONTROL ID:** 2260033

**TITLE:** [Spatial modulation spectroscopy for imaging single nano-objects](#)

**CONTACT (NAME ONLY):** [Mary Sajini Devadas](#)

**ABSTRACT STATUS:** re

**INSTITUTIONS (ALL):** 1. Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Devadas, Mary Sajini](#)<sup>1</sup>; Devkota, Tuphan<sup>1</sup>; Li, Zhongming<sup>1</sup>; Hartland, Gregory V.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Nano-structures, whether organic or metal based are characterized using optical spectroscopic techniques due to their signature properties like plasmon resonance as exhibited in Au metal nanostructures. Owing to sample heterogeneity, single optical spectroscopic techniques are being developed to unmask properties which allude to size and shape of the nano-object. The three most common techniques based on absorption are spatial modulation spectroscopy (SMS), photothermal heterodyne imaging (PHI) and transient absorption microscopy (TAM). These techniques are especially useful when the nanomaterials are (i) non-emissive and/or (ii) those that are much smaller than the wavelength of light. Out of these, SMS is the only method that gives the cross-section ( $\sigma$ ) of the particle directly. SMS can be performed by either moving the sample in-and-out of the laser focal spot using a piezo shaker (PS) or by moving the beam on-and-off of the particle using galvo-scanning mirrors (GSMs) with a fixed deflection distance ( $\delta$ ). Details of the SMS technique used to image and analyze metal and organic single nano-objects will be presented. Results of particles imaged on a surface, an optical trap and in fixed EMT6 cancer cells will be discussed along with its merits and limitations.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Nanophotonics for Energy and Catalysis - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Seth Rasmussen)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Notre Dame

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**CONTROL ID:** 2260049

**TITLE:** [Modeling interactions between PAI-1 and inhibitor: Combining molecular dynamics and density functional theory](#)

**CONTACT (NAME ONLY):** [Maria-Clelia Milletti](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Eastern Michigan University, Ypsilanti, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** Sadowsky, Mordechai<sup>1</sup>; Milletti, Maria-Clelia<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Human protein Plasminogen Activator Inhibitor 1 (PAI-1) is potentially a key regulatory target in the fibrinolysis pathway. Our group collaborates with researchers at EMU and the University of Michigan to explore potential small molecule inhibitors to PAI-1, a protein with no known endogenous inhibitors. This work focuses on the polyphenolic inhibitor CDE090 using a QM/MM computational approach. By using a molecular dynamics approach to inform a more likely initial conformation versus a *de novo* placement, the expense of density functional theory (DFT) calculations is reduced considerably. With significantly less expensive AMBER molecular dynamics methods, the protein-inhibitor complex is placed in a box flooded with water molecules, heated, and allowed to equilibrate over a 24 nsec period. Snapshots of low energy conformations are then taken and used as input for an ONIOM geometry optimization. Finally, the binding interaction between protein and inhibitor is analyzed using the NBO approach. When compared to that of two other polyphenolic inhibitors, the binding strength of CDE090 correlates well with IC<sub>50</sub>. Our results also point to the likely importance of interactions with specific amino acid residues within the binding site, particularly Glu<sup>222</sup>.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Eastern Michigan University

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**CONTROL ID:** 2260092

**TITLE:** [X-ray Crystallographic and Functional Characterization of BshC: The Third and Final Step of Bacillithiol Biosynthesis](#)

**CONTACT (NAME ONLY):** [Andrew VanDuinen](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Cell and Molecular Biology, Grand Valley State University, Allendale, MI, United States.

2. Department of Chemistry, Grand Valley State University, Allendale, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** VanDuinen, Andrew<sup>1</sup>; Cook, Paul D.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** Bacillithiol (BSH) is a low molecular weight thiol that reduces oxidative stress and regulates thiol homeostasis in some Gram-positive bacteria, including the pathogenic *Bacillus anthracis* and *Staphylococcus aureus*. It has recently been determined that bacillithiol plays a key role in resistance to the FDA-approved antibiotic fosfomycin. The biosynthesis of BSH is believed to occur via a three step pathway utilizing the enzymes BshA, BshB, and BshC. Although enzymes similar to BshA and BshB have been well-characterized, the structure and exact function of BshC was unknown. Presented here is the first ever structure of BshC from *Bacillus subtilis* containing three binding sites of interest. The active site is contained within a Rossmann fold domain and is highly conserved among across several Gram-positive species. BshC The enzyme forms a highly conserved tail-like projection that allows dimerization. An ADP molecule is bound within a pocket distinct from the active site. Among the species that produce bacillithiol, the amino acid residues of this ADP bound pocket are not highly conserved so the unique particular function of this site remains highly uncertain. Progress is reported toward a structure of BshC from the organism *S. aureus* to gain insight into the active site and ADP binding pocketse domains of interest in a different species. Functional analysis of BshC was also pursued to clue into the mechanism dictating its activity. Understanding how BshC functions will allow specific drug inhibitors to be designed to stop bacillithiol biosynthesis and re-

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establish fosfomycin as an effective antibiotic once again.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Grand Valley State University

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**CONTROL ID:** 2260098

**TITLE:** [The preparation of EDOT monomers for electrochemical sensing applications](#)

**CONTACT (NAME ONLY):** [Elizabeth Sanford](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Hope College, Holland, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Sanford, Elizabeth M.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Organic conducting polymers and redox polymers are important building blocks in the construction of electrochemical sensors and biosensors capable of detecting a broad range of analytes in a variety of environments. Using 3,4-ethylenedioxythiophene (EDOT) as the polymerizable moiety, we have prepared polymer films capable of mediating charge transfer between an electrode and analyte in solution. The preparation and characterization of monomers comprised of both a sensing and/or redox active moiety and EDOT is described. Monomers containing ferrocene, porphyrin, thymine, diketopyrrolopyrrole, Brooker's merocyanine and bipyridyl units have been prepared. The electrochemical polymerization of these monomers and the characterization of the resulting films will be described. Their use as sensors for both biological and environmental analytes will also be presented.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Jay Wackerly)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Hope College

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**CONTROL ID:** 2260129

**TITLE:** [Detecting Anaplastic Lymphoma Kinase activity by a time-resolved luminescence biosensor assay](#)

**CONTACT (NAME ONLY):** [Wei Cui](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University, West Lafayette, IN, United States.

2. Department of Biochemistry, Molecular Biology and Biophysics, University of Minnesota, Minneapolis, MN, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Cui, Wei](#)<sup>1, 2</sup>; Parker, Laurie<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** Abnormal kinase activity caused by genetic rearrangement of Anaplastic Lymphoma Kinase (ALK) is particularly prevalent in different types of cancer, such as non-small cell lung cancer, colorectal cancer, and anaplastic large-cell lymphoma. As next generation ALK inhibitors are being developed to overcome drug resistance of ALK, one key step to successful inhibitor development is efficient high-throughput screening (HTS) kinase assays with high sensitivity and specificity. Peptide-based biosensors provide an ideal platform for detecting kinase activity and inhibition with various readout method. Using ALK as a model kinase, we have shown that a set of customized mutation was sufficient to integrate lanthanide binding tag into kinase substrate peptide. Such peptide biosensors can chelate and sensitize Tb<sup>3+</sup> luminescence in a phosphorylation-dependent manner. This unique feature has allowed the direct detection of biosensor phosphorylation by ALK using a time-resolved lanthanide luminescence assay, without using any antibodies or special chemical labeling. This time-resolved luminescence biosensor assay has demonstrated HTS compatibility, and can be integrated with quantum dots to achieve multiplexed luminescence resonance energy transfer (LRET) kinase assay. The kinase assay strategy described in this research is an ideal option that could facilitate drug discovery efforts as well as kinase biology research.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Kinase Drug Discovery - Oral

**SESSION HOST:** Organizer (Mike Barbachyn)|Organizer (Jed Fisher)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Purdue University

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**CONTROL ID:** 2260127

**TITLE:** [Tekhelet, the evolution of an ancient dye molecule](#)

**CONTACT (NAME ONLY):** [Bruce Baldwin](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Spring Arbor University, Spring Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Baldwin, Bruce W.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Tekhelet is the Hebrew word for a specific blue dye commanded for use in tzitzit production in the Old Testament. The vast story of this molluscan derived dye spans approximately three millennia of human history. A modern understanding of this beautiful blueish dye has only recently been fully explained in the literature. A full telling of the story of Tekhelet requires examination of the biology, chemistry and nanotechnology of this precious dye molecule.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Preferred

**CONTACT (INSTITUTION ONLY):** Spring Arbor University

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**CONTROL ID:** 2260146

**TITLE:** [Photoactivatable Chemical Probes for Studying the Mycobacterial Outer Membrane](#)

**CONTACT (NAME ONLY):** [Jessica Stewart](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Central Michigan University, Mt Pleasant, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Stewart, Jessica A.](#)<sup>1</sup>; Swarts, Benjamin M.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:**

Tuberculosis, which is caused by *Mycobacterium tuberculosis* (*Mtb*), is one of the most widespread and lethal infectious diseases affecting humans. Mycobacteria possess a highly characteristic cell envelope that plays a crucial role in the infection process. It is for this reason that much of TB research is aimed toward the characterization of the mycobacterial cell envelope and its associated biosynthetic pathways. In this study, we propose a novel chemical approach for identifying and profiling proteins in the mycobacterial outer membrane. The ability to define the surface-exposed proteins of the outer membrane will provide a platform for exploring their contributions to various stages of *Mtb* pathogenesis. Traditional fractionation methods are not well suited for focused analyses of mycobacterial cell-wall subproteomes, especially the outer-membrane subproteome. We hypothesize that the outer membrane can be remodeled with reactive chemical tags that will allow us to capture and detect its associated proteins. In this work, we describe the synthesis and evaluation of novel chemical probes that are designed to exploit endogenous biosynthetic pathways in mycobacteria and ultimately incorporate unnatural functionalities into the outer membrane that should allow detection and analysis of proteins in this important layer of the cell wall.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Central Michigan University

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**CONTROL ID:** 2260158

**TITLE:** [Structural and functional studies of GDP-D-rhamnose and GDP-D-pneumose biosynthesis enzymes.](#)

**CONTACT (NAME ONLY):** [Benjamin Nicholson](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Grand Valley State University, Grand Rapids, MI, United States.

2. Department of Chemistry, Grand Valley State University, Allendale, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Nicholson, Benjamin](#)<sup>1</sup>; Cook, Paul D.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** GDP-D-rhamnose, produced by the enzyme RMD, is an unusual sugar found within the lipopolysaccharide of certain Gram-negative bacteria. We have determined an X-ray crystallographic structure of RMD from *Pseudomonas aeruginosa* to a resolution of 1.9 Å resolution. The model contains the cosubstrate NADPH within the active site displaying an ordered nicotinamide ring, which is not present in a previous structure of RMD from *Aneurinibacillus thermoaerophilus*. In addition, we report progress on the determination of steady-state kinetic parameters for RMD. The 4-epimer of GDP-D-rhamnose, GDP-D-pneumose, is produced using the same metabolic intermediate, and is produced via the enzyme GTS. Further studies of GTS and RMD will provide insight into the role of these enzymes, their products and the stereoselectivity that they provide. Characterization of RMD and GTS will allow for an understanding of how bacteria utilize these sugars and may give insight into the pathogenicity of certain Gram-negative bacteria. Furthermore, an understanding of the production of unusual sugars can allow for the derivitization of existing antibiotics in an effort to combat bacterial resistance.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Preferred

**CONTACT (INSTITUTION ONLY):** Grand Valley State University

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**CONTROL ID:** 2260193

**TITLE:**

[Diaminoacenaphthylene, a Key But Elusive Intermediate Toward Carbonyl-Substituted Perimidinespirohexadienone Photochromes.](#)

**CONTACT (NAME ONLY):** [Amber Prins](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Hope College, Holland, MI, United States.

2. Chemistry, Hope College, Holland, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Prins, Amber](#)<sup>2</sup>; Gillmore, Jason G.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:**

We are working to develop a new class of photooxidants based on organic photochromes that would add an additional level of gating to the process of photoinduced charge transfer (PICT) initiation of cation radical reactions with relevance to a variety of materials applications. Photochromes with long wavelength isomers (LW) capable of acting as photooxidants but with short wavelength isomers (SW) less capable of doing so are sought. This necessitates photochromes that revert only thermally and that have excited state reduction potentials that are more positive for LW than for SW. (As the difference in excitation energies is in the opposite direction, this requires a very large difference in ground state reduction potentials!)

The parent perimidinespirohexadienone (PSHD) photochrome meets these basic requirements, but with a very modest difference in excited state reduction potential between SW and LW, thus with minimal capacity for gating, and very modest photooxidizing power. Based on computationally predicted reduction potentials, carbonyl-substituted PSHDs are promising synthetic targets for increasing the difference in reduction potential between SW and LW and for making LW a far more potent photooxidant. Previous experimental results show that it is not possible to add carbonyls to the photochrome's naphthalene "bottom" before coupling. Thus, it will be necessary to prepare an acenaphthylene-bottomed PSHD. This requires the synthesis of diaminoacenaphthylene. This seemingly simple molecule has proved very difficult to make. After ruling out the most straightforward syntheses and the use of protecting groups, we now detail our current synthetic routes toward this challenging intermediate.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Hope College

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**CONTROL ID:** 2260191

**TITLE:** [New Modes of Initiating Cation Radical Cycloaddition Dimerization and Polymerization Reactions](#)

**CONTACT (NAME ONLY):** [Brianna Barbu](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Hope College, Midland, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Barbu, Brianna N.](#)<sup>1</sup>; Shin, Eun Jung<sup>1</sup>; Webb, Eric<sup>1</sup>; Green, David<sup>1</sup>; Gillmore, Jason G.<sup>1</sup>



**ABSTRACT BODY:**

**Abstract:** We are reinvestigating the work of Bauld and coworkers with respect to cation radical cycloaddition polymerization and dimerization. Bauld's most easily oxidized monomers provide suitable substrates for testing our group's novel photochromic photooxidants' abilities to gate sensitivity to photoinduced charge transfer initiation of cation radical reactions of materials interest. For instance, *N*-3-bis-(*trans*-1-propenyl)carbazole should be able to be photooxidized by the long-wavelength isomer of our quinazolinespirohexadienone photochrome. Revised synthesis of Bauld's monomers and a comparative study of their initiation by chemical oxidants, direct electrochemical oxidation, conventional photooxidants and our novel photochromic photooxidants will be reported.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Hope College

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**CONTROL ID:** 2260218

**TITLE:** [Drug Discovery at the University of Michigan](#)

**CONTACT (NAME ONLY):** [Martha Larsen](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Center for Chemical Genomics, University of Michigan, Ann Arbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Larsen, Martha J.](#)<sup>1</sup>; Groppi, Vincent E.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** University of Michigan's unique approach to academic drug discovery is best exemplified by the creation of the Center for the Discovery of New Medicines (CDNM). The center is a virtual institute that uses the pre-existing cores to coordinate, fund and mentor drug discovery efforts by UM researchers. The CDNM is comprised of the Center for Structural Biology, the Center for Chemical Genomics, the Vallteich Medicinal Chemistry Core and the Pharmacokinetics Core. The centers work in a coordinated, interactive environment to affordably provide academic investigators with the technology, informatics and expertise necessary for successful drug discovery. The CDNM has a leadership and administrative structure that provides support for early stage projects to advance them to translational projects with pharmaceutical potential. Peer-reviewed funding is available for both pilot initiatives as well as mature development projects to bridge the translational gap that stymies much of academic drug discovery. The center also connects biomedical researchers to resources available from labs and facilities outside of UM, as well as expertise at critical stages in drug development, such as clinical trials and intellectual property. Financial support from the Medical School, Life Sciences Institute, Office of Vice President for Research, the Comprehensive Cancer Center, the Provost and the College of Pharmacy underscores the significant shared investment by UM in academic drug discovery. Current therapeutic projects include new treatments for cancer, antibiotic-resistant bacteria, amphetamine addiction, breast cancer metastasis, schizophrenia, orphan diseases and other neurological afflictions. The CDNM represents a new academic model for advancing scientific discoveries to clinically relevant breakthroughs in the treatment of patients.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Upjohn, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Jed Fisher)|Organizer (Mike Barbachyn)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Michigan

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**CONTROL ID:** 2260313

**TITLE:** [Student research proposal projects in an advanced topics in environmental chemistry course](#)

**CONTACT (NAME ONLY):** [Anna Reinsel](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Thiel College, Greenville, PA, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Reinsel, Anna M.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** As part of an advanced topics in environmental chemistry course taken by upper level chemistry and environmental chemistry majors/minors, students designed, developed, wrote and presented a research proposal on an area of interest in the environmental chemistry field. The proposals consisted of introduction, method, references, personnel and budget sections. Smaller assignments leading up to the proposal included submitting journal article references as well as preparing short assignments for classmates which required researching and answering specific questions encountered during the student's literature research. Each student was then responsible for proving information and resources to fellow classmates to help answer the assigned questions. Informal presentations of this information as well as various sections of the students' proposals were done throughout the process and feedback was provided by classmates. Portions of these assignments as well as the students' proposals will be presented.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** General Posters - Posters

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Thiel College

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**CONTROL ID:** 2260401

**TITLE:** [Trifluoromethylation of Model Aryl Halides \(toward bistrifluoromethylquinazolinespirohexadienone\)](#)

**CONTACT (NAME ONLY):** [Jessica Scott](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemistry, Hope College, McMillan, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Scott, Jessica](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Our computational studies predict that replacing the methyl groups in our previous generation dimethylquinazolinespirohexadienone (QSHD) photochrome will make for a much more potent photochromic photooxidant. A previous group member determined that it is not possible to carry out the synthesis with trifluoromethyl groups present from the start as they completely inhibit a key nitration step. Meanwhile a current labmate has devised a synthesis of dihaloQSHD that could be amenable to installing the trifluoromethyls at a variety of points along the synthetic route. Five different options of when to perform this transformation are possible, replacing either a bromide or an iodide. I have undertaken model studies on four different aryl bromides and iodides to optimize trifluoromethylation conditions. The effects of competing

reactions and inhibitors were studied through competition experiments. Together these allow us to identify the most promising targets for trifluoromethylation in the synthesis of the desired bis(trifluoromethyl)QSHD.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** Hope College

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**CONTROL ID:** 2260501

**TITLE:** [Lanthanide and actinide coordination chemistry with multidentate CMPO compounds](#)

**CONTACT (NAME ONLY):** [Shannon Biros](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Grand Valley State University, Allendale, MI, United States.

2. The University of Tampa, Tampa, FL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Biros, Shannon M.](#)<sup>1</sup>; Werner, Eric J.<sup>2</sup>

**ABSTRACT BODY:**

**Abstract:** The synthesis of multitopic organic compounds containing the carbamoylmethylphosphine oxide (CMPO) motif will be described. The resultant *f*-element-ligand complexes have been characterized by IR, NMR and MS, and their ability to sensitize lanthanide luminescence has been demonstrated. We have also determined the ability of these compounds to extract lanthanide and actinide metals out of aqueous solution.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Organic Chemistry Research at Primarily Undergraduate Institutions - Oral

**SESSION HOST:** Organizer (Jay Wackerly)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Grand Valley State University

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**CONTROL ID:** 2260710

**TITLE:** [Oxidation reactions on the PdO\(101\) surface](#)

**CONTACT (NAME ONLY):** [Jason Weaver](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Chemical Engineering, University of Florida, Gainesville, FL, United States.

2. Chemical & Biomolecular Engineering, The Ohio State University, Columbus, OH, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Weaver, Jason F.](#)<sup>1</sup>; [Asthagiri, Aravind R.](#)<sup>2</sup>; [Zhang, Feng](#)<sup>1</sup>; [Pan, Li](#)<sup>2</sup>; [Choi, Juhee](#)<sup>1</sup>; [Li, Tao](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Interest in the surface chemistry of late transition-metal oxides has been stimulated by observations that the formation of metal oxide layers tends to dramatically alter the catalytic performance of transition metals in applications of oxidation catalysis. In this talk, I will discuss our investigations of the surface chemical properties of a PdO(101) thin film, focusing on the adsorption and activation of alkanes as well as

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the oxidation of CO. I will discuss characteristics of the binding and activation of alkane  $\sigma$ -complexes on PdO(101) as determined from both experiment and density functional theory calculations. I will also discuss elementary processes involved in the oxidation of CO on PdO(101) and the role that surface oxygen vacancies play in mediating reaction.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Catalysis and Surface Science to Advance Energy Efficiency - Oral

**SESSION HOST:** Organizer (Daniel Killelea)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** University of Florida

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**CONTROL ID:** 2260842

**TITLE:** [Discovery of an Allosteric JAK Inhibitor](#)

**CONTACT (NAME ONLY):** [Atli Thorarensen](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Medicinal Chemistry, Pfizer Global RD, Cambridge, MA, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Thorarensen, Atli](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Selective target inhibition is a fundamental goal of drug discovery in order to deliver efficacy while sparing potential adverse side effects from off-targets. This talk will outline the strategy and results from phenotypic screening strategies using primary cells and in cell binding experiments that identified active, non-ATP competitive modulators for JAK

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Upjohn, A Medicinal Chemistry Legacy in 2015 - Oral - INVITED ONLY

**SESSION HOST:** Organizer (Jed Fisher)|Organizer (Mike Barbachyn)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Pfizer Global RD

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**CONTROL ID:** 2260864

**TITLE:** [" High School, Community College, and Undergraduate Education: Issues of Dual Enrollment, Hybrid and Online Chemistry Courses"](#)

**CONTACT (NAME ONLY):** [Bal Barot](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Lake Michigan Colg, Benton Harbor, MI, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Barot, Bal](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Teaching in community college for high school students raises many issues, including opportunities and challenges. Offering hybrid and online chemistry classes for the community college students involve arranging on-campus lab meetings. To maintain quality and integrity is very important

aspect. We have addressed such issues with flipping classes, on-campus and in house testing as well as other innovative ways. A short survey of our pedagogy will be presented with summary of our evolved teaching innovation over three decades.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** High School, Community College, and Undergraduate Education - Oral

**SESSION HOST:** Organizer (Thomas Higgins)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Lake Michigan Colg

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**CONTROL ID:** 2260930

**TITLE:** [Ask Dr. Safety: Identification and control of reproductive hazards in the laboratory](#)

**CONTACT (NAME ONLY):** [Harry Elston](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. Midwest Chemical Safety, LLC, Dawson, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Elston, Harry J.](#)<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** Ask Dr. Safety is an open forum question-and-answer session for participants to get their environmental, health and safety questions answered. After a short presentation on the identification and control of reproductive hazards in the laboratory, the floor will be open to discuss any health and safety questions that may arise.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Current Issues in Chemical Lab Safety - Oral

**SESSION HOST:** Organizer (Kenneth Fivizzani)

**PRESENTATION TYPE:** Oral Only

**CONTACT (INSTITUTION ONLY):** Midwest Chemical Safety, LLC

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**CONTROL ID:** 2260949

**TITLE:** [Structure and behavior of alkylphenols in different chemical environments](#)

**CONTACT (NAME ONLY):** [Emily Mordan](#)

**ABSTRACT STATUS:**

**INSTITUTIONS (ALL):** 1. North Park University, Chicago, IL, United States.

**AUTHORS (LAST NAME, FIRST NAME):** [Mordan, Emily](#)<sup>1</sup>; Vazquez, Anne V.<sup>1</sup>

**ABSTRACT BODY:**

**Abstract:** A major concern in industrial chemistry is the management of potentially dangerous waste in the environment. One class of pollutants, called endocrine disruptors, is a class of compounds that are structurally similar to hormones. These compounds can alter normal endocrine function of animals exposed to them. This project is a study of the interactions between the suspected endocrine disruptors alkylphenols, and the soil component humic acid to understand how alkylphenols bind to soil using vibrational spectroscopy. Long chain alkylphenols have been shown to bind tightly to soil while other types of endocrine disruptors bind reversibly. The strength of endocrine disruptor-soil binding largely determines the bioavailability of the

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endocrine disruptor. Thus it is important to understand how different endocrine disruptors bind to soil to aid in the development of environmental remediation methods. Here, alkylphenols with different chain lengths are exposed to humic acid, and vibrational spectroscopy is used to determine how alkylphenol chain length impacts the binding to humic acid. Further, unexpected changes in the vibrational spectra of alkylphenols in different solvents are investigated to determine how solvent impacts alkylphenol structure, as these structural changes may impact the interpretation of vibrational spectra of these compounds.

**CONTACT (COUNTRY ONLY):** United States

**ABSTRACT SYMPOSIUM NAME:** Undergraduate Poster - Poster

**SESSION HOST:** Organizer (James Kiddle)|Organizer (Mark Thomson)

**PRESENTATION TYPE:** Poster Only

**CONTACT (INSTITUTION ONLY):** North Park University

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