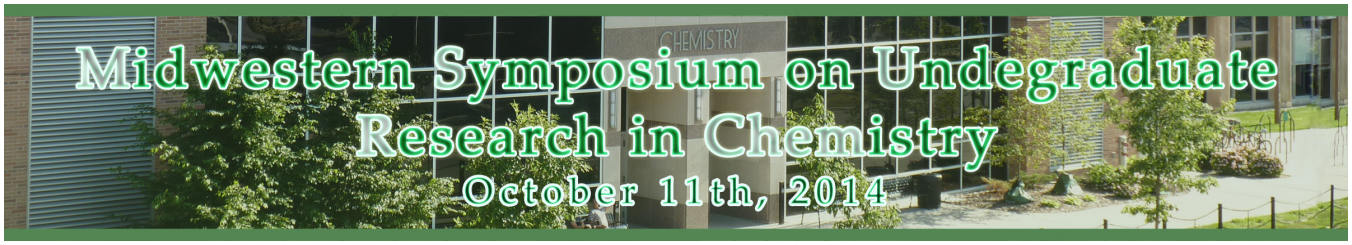
MICHIGAN STATE UNIVERSITY

Program & Abstract Book

Midwestern Symposium on Undergraduate Research in Chemistry

October 11, 2014



FOREWORD

Welcome to the Midwestern Symposium on Undergraduate Research in Chemistry! This symposium is an opportunity for undergraduate scientists, who have been working diligently in their labs, to get together, present their results for the first time, discuss science with other excited researchers, and get a glimpse of the broader scientific community. We have a busy weekend planned, with two poster sessions, a series of talks covering a range of cutting edge research, and tours of various research facilities on the MSU campus. We hope that you will leave this weekend with renewed enthusiasm for your work, fresh ideas, and a new network of friends in science.

ORGANIZING COMMITTEE

Viktor V. Poltavets
Assistant Professor
Department of Chemistry
Michigan State University
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Shannon Kraemer
Graduate Student
Department of Chemistry
Michigan State University

MSU-R:CHEM has been made possible by the generous support of our sponsors:

- **National Science Foundation (NSF DMR-1206718)**
- **Department of Chemistry at MSU**
- **College of Natural Science at MSU**
- **Office of the Vice President for Research and Graduate Studies**
- **Center of Research Excellence in Complex Materials**
- **MSU Local Section of the ACS**

EVENT LOCATION:

SATURDAY, OCTOBER 11, 2014

Registration: Atrium, BPS Building
Presentations: Room 1410 BPS Building
Poster sessions: Atrium, BPS Building
Lunch: The Vista at Shaw Hall
(500 ft north of the Chemistry Building)

SCHEDULE

SATURDAY, OCTOBER 11, 2014

If you are staying at Quality Inn University or Hampton Inn and Suites

- *a complimentary hot breakfast buffet is served beginning at 7:00 a.m.*
- *you need to check out in the morning due to the busy Symposium schedule*

9:00 - 9:30 am	Registration and Poster Set Up for Poster Session I
9:30 - 9:40 am	Welcome and Opening Remarks
9:40 - 10:00 am	Graduate Student Panel (Room 1410 BPS) *Faculty Gathering (Room 1400 BPS)*
10:00 - 11:20 am	**Poster Session I** **Undergraduate** posters in **Inorganic, Materials, Organic** areas; **Graduate** posters ~11:20 a.m. **Group photo**
11:20 - 12:30 am	Lunch
12:30 - 2:00 pm	**Poster Session II** **Undergraduate** posters in **Analytical, Biochemistry and Physical** areas **Graduate** posters
2:00 - 2:30 pm	**Dr. Brian Toby (Argonne National Laboratory – Advanced Photon Source)** *"100 years of Crystallography, 98 years of Powder Diffraction"*
2:30 - 2:50 pm	**Sarah Lockwood (MSU)** *"3D Printing as a Platform for* In Vitro *Pharmacokinetic Models"*
2:50 am - 3:20 pm	Tour of instruments/Coffee break
3:20 - 3:50 pm	**Prof. James Jackson (MSU)** *"Building block chemistry for the renewable refinery of the future: A path to organic reaction discovery?"*
3:50 - 4:00 pm	Presentation of Awards and Closing Words

REGISTRATION AND PARKING

The BPS Building and the Chemistry Building are connected. Enter the Chemistry Building and follow the signs to BPS.

Parking is available in Lot 41 and the Shaw Lane Parking Ramp, right across S. Shaw Lane from the Chemistry Building.
Parking permits are not needed after 6 pm, nor on weekends.

LIST OF PARTICIPANTS

Undergraduate Attendees

Name	Affiliation	Area	Poster Board
Alvarez, Jesus	Calumet College of St. Joseph	Biochemistry	**B1**
Ashby, Kristen	Calumet College of St. Josephs	Biochemistry	**B2**
Azeez, Zakee	Eastern Michigan University	Organic	**O1**
Baker, Andrew	Hillsdale College	Biochemistry	**B3**
Bannier, Sean	University of Wisconsin – Milwaukee	Biochemistry	**B4**
Banovetz, Joseph	Hillsdale College	Analytical	**A1**
Barbu, Brianna	Hope College	Organic	**O2**
Beaumier, Evan	Michigan State University	Inorganic	**I11**
Blackburn, Sean	Eastern Michigan University	Organic	**O1**
Bowers, Brittany	Calumet College of St. Joseph	Biochemistry	**B5**
Brunner, Michael	Grand Valley State University	Biochemistry	**B31**
Chavez, Martin	Calumet College of St. Joseph	Biochemistry	**B5**
Clark, Daniel	Hope College	Materials	**M1**
Coburn, Katherine	Grand Valley State University	Inorganic	**I1**
Compton, Jessica	Calumet College of St. Joseph	Organic	**O3**
Comstock-Reid, Brian	Eastern Michigan University	Materials	**M2**
Cortes, Elena	Calumet College of St. Joseph	Inorganic	**I2, O32**
Curtis, Ryan	Indiana-Purdue University, Fort Wayne	Organic	**O4**
Dang, Alexander	University of Notre Dame	Biochemistry	**B6**
Darr, David	Bowling Green State University	Organic	**O5**
DeGlopper, Kimberly	Hope College	Organic	**O6**
Dennis, Joseph	Hope College	Organic	**O7**
DeVries, Rachael	Valparaiso University	Biochemistry	**B7**
Diaz, Jennifer	Calumet College of St. Joseph	Biochemistry	**B8**
Diaz, Patricia	Calumet College of St. Joseph		
Dicken, Rachel	Ohio State University	Organic	**O8**
Dill, Rebecca	Calumet College of St. Joseph	Analytical	**A2**
Dood, John	Hope College	Physical	**P1**
Douglas, Shane	Ferris State University	Organic	**O9**
Duff, Lauren	Ohio State University	Biochemistry	**B9**
Eining, Colton	Calumet College of St. Jospeh	Biochemistry	**B10**
Eler, Jennifer	Northeastern Illinois University	Materials	**M3**
Ellsworth, Alyssa	Lake Superior State University	Organic	**O10**
Emaus, Miranda	Lake Superior State University		

Undergraduate Attendees (cont.)

Name	Affiliation	Area	Poster Board
Foley, Hannah	Central Michigan University	Biochemistry	**B11**
Fujiwara, Rina	Kalamazoo College	Biochemistry	**B12**
Gallimore, Jacob	Kalamazoo College	Biochemistry	**B21**
Gatson, Franqlin	Calumet College of St. Jospeh	Organic	**O11**
Gill, Nicole	Calumet College of St. Joseph	Biochemistry	**B5**
Gira, Matthew	Hope College	Materials	**M4**
Glass, Jacob	Calumet College of St. Jospeh	Biochemistry	**B13**
Gonzales, Moises	Calumet College of St. Jospeh	Biochemistry	**B1**
Hagerman, Thomas	DePaul University	Organic	**O12**
Hamann, Danielle	Lake Superior State University	Materials	**M5**
Harms, Katherine	Adrian College	Biochemistry	**B14**
Haskin, Chris	Eastern Michigan University	Analytical	**A3**
Hayes, Jake	Calumet College of St. Jospeh	Biochemistry	**B10**
Heim, Eric	Northern Michigan University	Organic	**O13**
Henry, Nicole	Calumet College of St. Joseph	Biochemistry	**B1**
Herrera, Annette	Calumet College of St. Joseph	Analytical	**A2**
Ho, Peter	McMaster University	Inorganic	**I3**
Hogue, Maxwell	Central Michigan University	Organic	**O14**
Hull, Brian	Ferris State University	Organic	**O15**
Jhangiani, Nikhyl	Case Western Reserve University	Organic	**O16**
Jones, Evan	Ball State University	Biochemistry	**B15**
Katz, Micah	University of Michigan, Ann Arbor	Biochemistry	**B16**
Kaur, Jagdeep	Kalamazoo College	Analytical	**A4**
Kemppainen, Cierra	Ferris State University	Organic	**O17**
Kenney, Sanna	DePaul University	Biochemistry	**B17**
Khobeir, Alexander	University of Michigan - Flint	Analytical	**A5**
La Roche, Elisse	University of Illinois at Chicago	Analytical	**A6**
Ladd, Nicole	Hope College	Biochemistry	**B18**
Lantis, Jeremy	Kalamazoo College	Physical	**P2**
Leander, Megan	University of Michigan	Biochemistry	**B19**
Li, Maxwell	University of Michigan	Physical	**P3**
Li, Qiuhan	University of Michigan	Organic	**O18**
Lopez, Hector	Calumet College of St. Joseph	Organic	**O19**
Lyza, Jessica	Valparaiso University	Biochemistry	**B7**

Undergraduate Attendees (cont.)

Name	Affiliation	Area	Poster Board
Maaieh, Haitham	University of Michigan, Ann Arbor	Materials	**M6**
Mahmood, Fariha	McMaster University	Physical	**P4**
Malonda, Roger	Calumet College of St. Jospeh	Biochemistry	**O19**
Malik, Zain	Northeastern Illinois University	Biochemistry	**B23**
Martinez, Jessica	Calumet College of St. Jospeh	Biochemistry	**B8**
Melero, Jorge	Calumet College of St. Jospeh	Biochemistry	**B1**
Messer, Lauren	Hope College	Organic	**O20**
Mizzi, Jessica	Michigan State University	Inorganic	**I4**
Mousseau, Matthew	Ferris State University	Biochemistry	**B20**
Murashova, Gabrielle	Adrian College	Biochemistry	**A10**
Narvaez, Sandra	Calumet College of St. Jospeh	Organic	**O19**
Navarro, Maya	DePaul University	Inorganic	**I5**
Newman, Jane	Lake Superior State University		
Nguyen, Jenny	Ball State University	Organic	**O21**
Nicholl, Michael	Ohio State University	Materials	**M8**
Nieto, Paula	Calumet College of St. Joseph	Biochemistry	**B5**
Nyawaga, Christine	Hillsdale College	Organic	**O22**
Patton, Erica	Valparaiso University	Materials	**M9**
Peecher, Benjamin	Hope College	Materials	**M10**
Peterson, Julia	Lake Superior State University	Inorganic	**I6**
Portela, Mariana	Calumet College of St. Jospeh	Biochemistry	**B13**
Prins, Amber	Hope College	Organic	**O23**
Prinzing, Brooke	Hillsdale College	Biochemistry	**B22**
Rawls, Brian	Grand Valley State University	Organic	**O24**
Rebiai, Rima	Northeastern Illinois University	Biochemistry	**B23**
Reeves, Emily	St. Olaf College	Inorganic	**I7**
Repak, Miroslava	Valparaiso University	Materials	**M11**
Rhodes, Ryan	Ball State University	Organic	**O25**
Rojas, Ramiro	Calumet College of St. Joseph	Biochemistry	**B8**
Saez, Julyssa	Calumet College of St. Jospeh	Biochemistry	**B2**
Salas, Maritza	Calumet College of St. Joseph	Organic	
Salczynski, Jennifer	Calumet College of St. Jospeh	Biochemistry	**B5**
Saleh, Ban	Wilfird Laurier University		
Siddiqi Abdullah	Eastern Michigan University		
Sosnofsky, Chris	Bowling Green State University	Inorganic	**I8**
Soto, Luis	Calumet College of St. Jospeh	Biochemistry	**B1**

Undergraduate Attendees (cont.)

Name	Affiliation	Area	Poster Board
Sportiello, Michael	University of Wisconsin-Milwaukee	Organic	**O26**
Stahl, James	Calumet College of St. Joseph	Organic	**O32, I2**
Steigerwald, Daniel	Ohio Northern University	Organic	**O27**
Stuart, Daniel	McMaster University	Inorganic	**I9**
Sullivan, Aaron	Ohio Northern University	Organic	**O27**
Swanson, Chelsea	Eastern Michigan University	Organic	**O28**
Szatkowski, Michael	Michigan Technological University	Physical	**P5**
Tamrakar, Shrasta	DePaul University	Biochemistry	**B17**
Tanygin, Vadim	University of Chicago	Inorganic	**I10**
Tran, Henry	Ohio State University	Physical	**P6**
Tuxford, Patricia	Calumet College of St. Jospeh	Biochemistry	**B5**
Urbanek, Bailey	Central Michigan University	Organic	**O29**
Utke, Elizabeth	Ferris State University	Biochemistry	**B20**
Utterbeck, Kimberly	University of Detroit Mercy	Physical	**P7**
Verdi, Christopher	Cleveland State University	Analytical	**A7**
Victor, Tim	Calumet College of St. Jospeh	Biochemistry	**B13**
Wagar, Zachary	Central Michigan University	Biochemistry	**B24**
Wampler, Katherine	Michigan State University	Materials	**M13**
Wang, Victor	University of Michigan, Ann Arbor	Materials	**M6**
Warsh, Jack	Michigan State University	Organic	**31**
Weidenbacher, Payton	University of Chicago	Biochemistry	**B25**
White, Alyssa	Calumet College of St. Joseph	Biochemistry	**B2**
White, Lilian	Heidelberg University	Analytical	**A8**
Woodcock, Lukas	Ferris State University	Biochemistry	**B26**
Woodhouse, Matt	Northern Michigan University	Organic	**O30**
Wyman, Leslie	Grand Valley State University	Biochemistry	**B27**
Yeung, Edith	University of Western Ontario	Materials	**M12**
Yorek, Tiffany	Calumet College of St. Joseph	Biochemistry	**B28**
Yousufzai, Hasib	Michigan State University	Analytical	**A9**
Zhou, Ning	University of Notre Dame	Biochemistry	**B29**
Zinn, Sarah	Ohio Northern University	Physical	**P8**
Zywot, Emilia	Ohio State University	Biochemistry	**B30**

Faculty Attendees

Name	Affiliation
Balanda, Peter	Ferris State University
Bartz, Jeff	Kalamazoo College
Brewer, Timothy	Eastern Michigan University
Chimon-Peszek, Sandra	Calumet College of St. Joseph
Colvert, Kim	Ferris State University
Hamilton, Christopher	Hillsdale College
Holt, Jennifer	Valparaiso University
Iretski, Alexei	Lake Superior State University
Janser, Ingo	Eastern Michigan University
Klosterman, Jeremy K.	Bowling Green State University
Lakhani, Ahmed	Calumet College of St. Joseph
Meyet, Courtney	Hillsdale College
Moorman, Veronica	Kettering University
Mosey, Robert	Lake Superior State University
Partigianoni, Colleen	Ferris State University
Powers, Rachel	Grand Valley State University
Sammelson, Robert	Ball State University
Srinivasan, Rekha	Case Western Reserve University
Stevens, Jonathan	University of Detroit Mercy
Tippmann, Eric	Indiana-Purdue University, Fort Wayne
Toby, Brian	Argonne National Laboratory
Zimmerman, Paul	University of Michigan

Plus many MSU faculty will be attending, as well.

Abstracts

A1

Differentiation and Identification of Smokeless Propellants by LC-CLND and LC-MS

Joseph Banovetz, Mark A. Nussbaum

Hillsdale College

According to the FBI's annual crime statistics, firearms were used in over eight 8,000 murders in the United States in 2012. Because firearms are so frequently used in the commission of crimes, techniques to gather information about firearms and ammunition have value as forensic tools. This research used high performance liquid chromatography combined with mass spectrometry and chemiluminescent nitrogen detection to characterize different brands of ammunition by the chemical characteristics of their respective gunpowders. Five different brands of ammunition and two different calibres were analyzed based on their nitroglycerin, nitrocellulose, 2,4- dinitrotoluene, diphenylamine, N-nitrosodiphenylamine and ethyl centralite content. Samples were analyzed both before and after being fired. Qualitative information was provided by MS chromatograms and quantitative concentration information was provided by the CLND. Each brand varied considerably by nitroglycerin, diphenylamine and ethyl centralite content.

A2

Measurements of O_2 and CO_2 While Learning About Metabolism Using New Leaf Device

Rebecca Dill, Annette Herrera, Dr. Ahmed Lakhani

Calumet College of St. Joseph

No abstract submitted.

A3

Characterization of a GC-TCD Instrument for Measurement of Atmospheric Methane

Chris Haskin, Gavin Edwards

Eastern Michigan University

The study of common greenhouse gases such as Carbon Dioxide (CO_2) and Methane (CH_4) is important because the concentration can be linked to added absorption of emitted terrestrial radiation, leading to warming of the atmosphere[1]. This research measures the concentrations of common greenhouse gases in the air surrounding Eastern Michigan University. Development of an auto-sampler system for long term use on the EMU campus will create a viable way to monitor greenhouse gas concentrations throughout the year. Samples were analyzed using an Agilent 6890 Gas Chromatograph and a Thermal Conductivity Detector fitted with a Restek 5A Molsieve column and a Varian poraPLOT column (part# CP7550) for proper molecular separation. Molecular data analysis is plotted using Peaksimple software by SRI Systems out of Torrance, Ca. Although the experiment is ongoing, preliminary data suggest this methodology could be used to detect atmospheric methane.

A4

Determining an Efficient Separation of 1-butyl-3-methylpyridinium Bromide, 2-butyl-2-hydroxy-N,N,N-trimethylhexan-1-aminium, and N,N,N-trimethylglycinium

Jagdeep Kaur, Jennifer Furchak

Kalamazoo College

Ionic liquids (ILs) are semi-organic compounds with attractive physical and chemical properties such as negligible vapor pressure, low melting points and feasible miscibility within a range of solvents. A key factor of ILs is the ability to design these solvents by manipulating the component anion or cation. This is a major reason why ILs are referred to as designer solvents and have been in keen interest in a range of scientific disciplines. This rise in interest has also led to the increased production of ILs, however the toxicity of these designer solvents is not well known. A major concern in utilizing ILs is to develop effective remediation methods in case of environmental contamination. A separation of 1-butyl-3-methylpyridinium bromide ([Bmpy][Br]), 2-butyl-2-hydroxy-N,N,N-trimethylhexan-1-aminium, and N,N,N-trimethylglycinium was determined to understand if various complex ILs can be separated from one another. Studies have indicated that potassium permanganate can be used to breakdown pyridinium based derivatives therefore 1-butyl-3-methylpyridinium bromide [Bmpy][Br] was studied and a separation technique was determined using 5 *mM* KH_2PO_4. Further research in the degradation of [Bmpy] [Br], 2-butyl-2-hydroxy-N,N,N-trimethylhexan-1-aminium, and N,N,N-trimethylglycinium may potentially exhibit an extraction method for environmental remediation.

A5

Development of Atmospheric Pressure Photoionization (APPI) Ion Source for GC-APPI-Orbitrap MS Setup

Alexander M. Khobeir, Kai Kroll, Hendrik Kersten, and Thorsten Benter

University of Michigan-Flint

Over the last century mass spectroscopy has continued to develop. There continues to be three distinct stages in mass spectrometers: (1) the inlet, (2) the ion source, and (3) the analyzer/detector. Several novel innovations in the second and third stages have occurred over the past decade. In 2000, Alexander Makarov built the Orbitrap mass spectrometer with a resolving power of over 150,000 FWHM. This cost effective, space saving, highly sensitive machine was the first of its kind. Thorsten Benter then combined the Orbitrap with atmospheric pressure photoionization ion sources to create a machine that is even more sensitive. Three prototypes were developed, with the third and final prototype yielding sensitivity in the femtogram range. With each new ion source, fluid dynamics and environmental factors within the source were considered before building the next one. This research poster details the results yielded by each prototype. In order to measure the success of each ion source, calibration curves were produced and limit of detection measurements were conducted. This was the first time that gas chromatography, atmospheric pressure photoionization, and Orbitrap mass spectrometry have been combined to yield sensitivity in the femtogram range.

A6

Corn Seedling Growth in 1.8×10^{-7} *M* core/shell Cadmium Selenide-Zinc Sulfide QD Solution.

Elisse La Roche, Preston T. Snee

University Of Illinois at Chicago

Quantum Dots (QDs) are highly fluorescent nanoparticles that have a wide range of technological applications, such as in biological imaging, solar panels, and LED display screens. There is growing demand for QD technology, resulting in an increase in production and availability. For example, quantum dot-based television sets recently became available from Sony and Samsung. As such, the potential for improper disposal of products containing QDs is increasing, and currently there is very little known about the environmental impact of quantum dots. Our experiments have been designed to evaluate the impact of nanomaterials in the environment. Specifically, we tested the effect of QDs on the growth of sweet corn (*Zea mays*) seedlings. Quantum dots were solubilized using a polyacrlyic acid to encapsulate them for dispersion into water and were subsequently purified with dialysis. Corn seeds were then germinated, and the seedlings were grown for 5 days in ~9 mL deionized water containing 1.8×10^{-7} *M* core/shell cadmium selenide-zinc sulfide QDs as well as pure water as a control. The seedlings were then freeze-dried, weighed, and separated into components of stems, seeds, and roots, then weighed. The initial results indicate that corn seedlings grow faster in water containing quantum dots as evident by the higher weight of the seedlings compared to control samples. However, the results are not statistically significant, most likely as more data need to be evaluated. Future research should determine how QD contamination might affect more advanced stages of corn growth, and examine the potential effects of other QD concentrations and solubilization processes, such as silica coating, on corn seedling growth.

A7

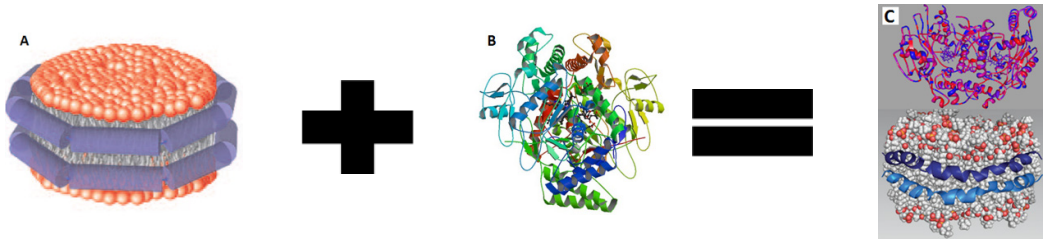
Calculating Specific Activity of Nitric Oxide Synthase with Nanodiscs

Chris Verdi, Ghaith Altawalbeh M.Sc., Mekki Bayachou Ph.D.

Cleveland State University

Nitric Oxide is an important bioregulator produced in various regions of the body by a family of isozymes referred to as Nitric Oxide Synthases (NOSs). Within vascular endothelial cells nitric oxide is generated from oxygen and the amino acid arginine by endothelial nitric oxide synthases (eNOSs). Nitric oxide is recognized to play several critical paracrine roles within the human vasculature, mainly antithrombotic and anti-atherosclerotic. This is accomplished through vessel dilation, inhibiting platelet function/aggregation and preventing leukocyte adhesion to the walls of the vasculature.

While the function of the enzyme is well understood, conditions or stimuli for induction or inhibition of the family of isozymes is poorly understood. To further understand the activity of the eNOS enzyme in vitro, we created “nanodiscs” to bind to the enzyme. Nanodiscs are small puck shaped complexes containing two components that self-assemble in solution. Nanodiscs contain a lipid POPC (1-palmitoyl-2-oleoylphosphadylcholine) and a membrane scaffold protein (MSP1E3D1) that wraps around the hydrophobic regions of the lipid like a belt.



The nanodisc provides a more accurate microenvironment to study the enzyme, mimicking the lipid bilayers of the endothelial cells lining our vasculature. Our experiments have so far shown consistently that a significant decrease in the activity of the enzyme (greater than 50% reduction), as calculated by production of nitrate through performing a griess assay, is witnessed when the enzyme is bound to the nanodisc.

To provide further elucidation about the activity of the eNOS enzyme within our bodies, further experiments will be performed with the eNOS/nanodisc complex. Further experiments are planned to include light scattering as well as electrochemical redox experiments to gather more information about the relationship of the enzyme with a lipid bilayer.

A8

Analysis of Ethanol in Hand Sanitizer

Lilian White

Heidelberg University

Ethanol is a commonly available active ingredient employed in retail hand sanitizers. This study investigated the concentration of ethanol in sealed and opened commercial products. The percentage (v/v) ethanol in water and hand sanitizer was measured via ^{1}H NMR over a period of two weeks. The concentration of ethanol was determined using a standard curve of the ratio of -OH to -CH_3 (obtained via integration of the spectra) vs. the theoretical concentration of the standards measured. The concentration of ethanol increased in the opened control samples and remained consistent in the closed control samples. The results suggest the ethanol concentration in the opened sanitizer sample bottles remains consistent with the ethanol concentration in the closed sanitizer sample bottles.

A9

Development of Carbon Fiber Electrodes for Exhaustive Electrolysis in a Bulk Cell with Thin Layer Behavior

Hasib Yousufzai, Julia Busik, Dr. Elahe Crockett, Denis A. Proshlyakov

Michigan State University

The use of electrodes is imperative in measuring activity of complex biological systems such as those in mitochondria. Planar glassy carbon has become the standard electrode material due to its biocompatibility, stability, and conductive properties. However, the two-dimensional surface area of glassy carbon electrodes limits their effectiveness and sensitivity requiring more concentrated samples and confines their use to thin-layer cells. In addition, planar electrodes are inefficient and time consuming in conducting exhaustive electrolysis. We have developed a mini-bulk electrode composed of carbon fiber bundles allowing for a three-dimensional effective surface area that is 1000 to 10,000 times larger than planar electrodes. Our design allows us to manipulate the analyte on the electrode in a bulk cell three to four orders of magnitude faster than with planar electrodes.

The electrodes were designed with bundles in a spiral geometry and each bundle had its fibers separated into smaller groupings to limit the diffusion distance between analyte and electrode. The diameter of each electrode was standardized to a 9 *mm* diameter and a length of 6 mm in a 1 *ml* cell. We chose the inorganic analyte, $Fe(CN)_6^{3-/2-}$ due to its stability and reversibility. The results from the mini-bulk electrodes were then compared to a glassy carbon electrode in bulk electrolysis and a thin layer cell with a planar electrode.

Our results showed a current response on the mini-bulk electrode that was two orders of magnitude greater than on the glassy carbon electrode. In addition, we were unable to notice exhaustive electrolysis using the glassy electrode after more than 1 hour. In comparison, the mini-bulk electrode completed electrolysis in less than 100 seconds. The results showed that mini-bulk electrodes could be utilized for exhaustive electrolysis in a bulk cell with thin layer behavior. We then further optimized the design by investigating bundle count and fiber density. Our results indicated that electrolysis was limited by the analyte's ability to access the effective surface and increasing the bundle count and density might be limiting this access.

The ability to conduct exhaustive electrolysis in a bulk cell allows us to manipulate the analyte at the electrode making it possible to characterize complicated biological systems while measuring its electrochemical activity. Future experiments will examine organic and protein analytes to investigate various applications of the electrode. Ultimately, we believe these electrodes will allow us to test more complex biochemical systems such as those in mitochondria.

A10

Glucose Reversibility and Glut1 Expression in Hyperglycemic and Normoglycemic Storage Solutions Cause Irreversible Effects on Red Blood Cells

Gabrielle A. Murashova[2], Kristen E. Entwistle[1], Dana M. Spence[1]

[1]Michigan State University, [2]Adrian College

Current protocols approved by the Food and Drug Administration (FDA) for the storage of donated red blood cells (RBCs) cause irreversible effects on the function as well as the proteins imbedded with in the plasma membrane of these cells. One of these storage solutions evaluated in this study is called Additive Solution-1 (AS-1). With a glucose concentration of 111 *mM*, this is approximately twenty times the glycemic level in normal blood. Using time-resolved fluorescence (TRF) and Western Blot Analysis glucose uptake data was collected and evaluated over a four-week storage period. Additional studies are currently underway in order to provide additional data to support these finding and conclusions. The evaluation of all the FDA approved storage solutions; AS-1, AS-3 and AS-5, needs to be conducted as well. This will increase the quality of transfused RBCs.

I1

Investigation of a Novel Multi-dentate Ligand for Extraction of *f*-elements

Katherine M. Coburn, Michael T. Perruzi, and Shannon M. Biros*

Grand Valley State University

A novel carbamoylmethylphosphine oxide (CMPO) derivative was investigated for its ability to extract f-elements. Spent nuclear fuel (SNF) rods containing *f*-elements are dissolved in nitric acid, the plutonium and uranium are removed, and the remaining *f*-elements in the SNF are deposited into environmental repositories as part of nuclear waste remediation. The required storage time is projected to be thousands of years. However, the storage time for the SNF could be greatly decreased if the remaining lanthanides and minor actinides in the SNF were separated. To identify new ligands with greater selectivity for minor actinides, the Biros group has investigated CMPOs with various R-groups. In particular, a CMPO derivative with phenyl groups was investigated for minor actinide selectivity. CMPOs have also been demonstrated to chelate to *f*-elements in a 3:1 ratio when used in current nuclear waste remediation techniques. To take advantage of the chelate effect, three CMPOs were coupled together with a cap molecule. This coupled phenyl CMPO (OTRAP CMPO Ph) derivative was thoroughly investigated for the extraction efficiency of *f*-element in varying concentrations of nitric acid.

I2

Echinacea Could be an Alzheimer's Disease Preventative

Elena Cortes, James Stahl, Amy Gasiorowski, and Dr. Sandra Chimon-Peszek

Calumet College of Saint Joseph

Large deposits of amyloid beta plaques have been found in brains affected with Alzheimer's disease. Studies have shown the amyloid beta peptide intermediate has higher neurotoxicity than the plaques, and if misfolding of the fibrils can be prevented then Alzheimer's can be prevented or slowed. In this study, we will increase the solubility of Echinacea by defatting it via extraction of seeds with a Soxhlet. These studies have shown that Echinacea has very promising potential to be used as a treatment for Alzheimer's disease. The current aims of our research are to further examine what possible effects that this compound has on the formation of fibrils that form in the brain in Alzheimer's patients, specifically looking at whether this compound has an effect of slowing or stopping the formation of the fibrils all together.

I3

Supramolecular chemistry of Iso-tellurazole N-oxides

Peter C. Ho, Jocelyn Sinclair, Patric Szydlowski, Philip J.W. Elder, Chris Gendy, Lucia M. Lee, Ignacio Vargas-Baca*

McMaster University

Molecules of the title compounds readily aggregate through strong Te-O secondary bonding interactions. In this way, a variety of supramolecular structures have been isolated and characterized by single-crystal X-ray diffraction, including polymers and macrocyclic tetra- and hexamers. Spectroscopic studies have demonstrated the existence of the cyclic structures in solution. These self-assembled macrocyclic supermolecules can act as ligands in coordination complexes and as fullerene receptors.

I4

Structural Chemistry and Magnetic Properties of Copper Pyromellitate Coordination Polymers Containing Pyridylnicotinamide Ligands

Jessica Mizzi

Michigan State University

A series of divalent copper pyromellitate (1,2,4,5-benzenetetracarboxylate, pyro) coordination polymers containing either 3-pyridylnicotinamide (3-pna) or 4-pyridylnicotinamide (4-pna) was hydrothermally prepared and structurally characterized by single-crystal X-ray diffraction. $[Cu_2(pyro)(pyroH_2)(3\text{-}pnaH)_2(H_2O)_2]_n$ (**1**) is a 2-D coordination polymer built from $\{Cu_2O_2(OCO)_2\}$ dimeric units, while $\{[Cu(pyro)(3\text{-}pnaH)_2(H_2O)_2]\bullet 4H_2O\}_n$ (**2**) possesses cationic 1-D chain motifs and unligated $pyroH_2$ dianions. $\{[Cu_2(pyroH_2)_3(4\text{-}pnaH)_2]\bullet 6H_2O\}_n$ (**3**) is also a 1-D coordination polymer, but built from the linkage of $\{Cu_2(pyroH_2)\}$ dimeric units. $\{[Cu_3(pyroH)_2(4\text{-}pna)_2(H_2O)_2]\bullet 2H_2O\}_n$ (**4**) manifests a 3-D coordination polymer network with rare frl topology, containing embedded $\{Cu_3(OCO)_2\}$ linear trimers. Moderately strong antiferromagnetic coupling (J = –76.4(3) cm^{-1}) was observed within the $\{Cu_2O_2(OCO)_2\}$ dimeric units in **1**, while very weak ferromagnetic coupling (J = 0.8(2) cm^{-1}) was observed within the $\{Cu_3(OCO)_2\}$ linear trimers in **4**.

I5

Studies of Steric and Electronic Behaviors of Palladium Compounds Bonded to Diphosphorus

Dr. Quinetta Shelby, Maya Navarro, Hetal Patel, Josh Smith, Stephanie Pacheco, and Darcy Velazquez,

DePaul University

The long-term research goal of the Shelby Group is to design palladium compounds bonded to negatively charged diphosphorus compounds and to test them for catalysis. We have explored two ways to synthesize these compounds. In the more promising method, the neutrally charged diphosphorus compound is bonded to palladium; then, while it is attached to palladium, the diphosphorus compound is converted to the negatively charged form. We have found that this procedure generally forms new palladium-diphosphine dimers in which symmetric diphosphines remain neutral. However, when an unsymmetric diphosphine compound was tested, the palladium complex contains negatively charged diphosphorus compounds. To our knowledge, this compound is the only zero valent palladium diphosphine dimer in which the ligands are unsymmetrical and in which the ligands are not neutral. As observed in our crystallographic data of this unique compound, if visually cut in half at an angle of ~20° off the vertical, the complex contains two of the target units in which each palladium atom is bonded to a negatively charged diphosphorus compound. Based on these results, we have narrowed our focus on unsymmetric diphosphine ligands that contain only aromatic substituents with different electronic and/or spatial character to further examine conditions that favor the diphosphine to become negatively charged. Currently we are working to improve its purity so that we can obtain better NMR spectra and elemental analysis data to complete our manuscript.

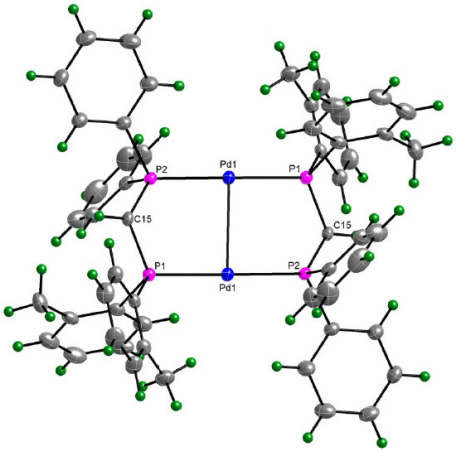


Figure 1: Crystal structure of the zero valent palladium diphosphine dimer

I6

Evaluating the Catalytic Properties of Mixed Metal Oxides for the Production of Biofuels

Julia D. Peterson, Megan A. Chui, Peter C. Ford

Lake Superior State University, University of California Santa Barbara

Alternative energy is a future necessity to society regarding the restricted supply of fossil fuel. Considering this, the formation of a liquid fuel product from the degradation of lignin, a component of biomasses and plentiful “biowaste”, would be a major advance. Previously it was shown that porous metal oxides (PMO) containing copper, aluminum, and magnesium were promising catalysts in the process of hydrodeoxygenation of lignin. It was proposed that the reactivity of these catalysts was enhanced by the addition of Lewis acidic elements. Thus, the selectivity of such new prepared mixed metal oxides was investigated. Each reaction was conducted at 300 °C with supercritical methanol as the media. Under these conditions it was found that copper gallium oxide fully converts dihydrobenzfuran (DHBF), a model compound of lignin, into ethylbenzene, an energy rich product, and 2-ethyl-cyclohexanol. Copper oxide and a mixture of copper oxide with titanium oxide showed good transformation of DHBF to ethylbenzene, cyclohexanol, methylcycolhexanol, 2-ethyl-cyclohexanol, and 2-ethyl-phenol. Furthermore, 5% copper alumina silica, copper praseodymium oxide and copper samarium oxide displayed favorable conversion of DHBF to phenol.

I7

Synthetic Methods for Hybrid PVP-Cysteine Coated Silver Nanowires

Emily Reeves, Douglas J. Beussman

St. Olaf College

Silver nanoparticles (Ag-NPs) have been proposed as potential drug delivery systems because of their effectiveness in combating HIV, MCF-7 (human breast cancer), and a number of bacterial species. Ag-NP cytotoxicity stems from particle dissolution to toxic silver ions in aqueous conditions, inducing apoptosis via cellular uptake or radical formation. While the development of nanosized drug delivery systems has gained extensive attention in the literature in recent years, tuning these materials for high target specificity and biocompatibility remains a major challenge.

Our work seeks to address these challenges by synthesizing silver nanorods and nanowires with hybrid PVP-cysteine surface coatings. The use of both materials provides both hard-soft and soft-soft interactions between silver cores and their coating, resulting in interactions of different strengths and consequential lability for controlling ion release. Incorporating an amino acid on the surface may also improve nanoparticle solubility and bioavailability in the target tissue. Surface design is explored through the lens of synthetic inorganic chemistry and utilizes characterization methods such as optical microscopy, NMR, UV-Vis, and IR spectroscopy.

I8

Designing Polysaccharide Beads for Photo-Responsive Drug Delivery

Christopher T. Sosnofsky, Giuseppe E. Giammanco, Dr. Alexis D. Ostrowski*

Bowling Green State University

It has been reported that alginate, a polysaccharide from brown algae, is able to form a gel after binding of Fe^{3+} in solution. We show that light irradiation of the Fe^{3+}-alginate gels leads to reduction of the Fe^{3+} to Fe^{2+}, oxidative decarboxylation of the polysaccharide, and dissolution of the gel. Another polysaccharide pectate, which is isolated from fruit and very similar in structure to alginate, was also able to form a photo-responsive hydrogel after coordination by Fe^{3+}. Fe^{3+}-pectate, like Fe^{3+}-alginate, undergoes the same photo reduction of Fe^{3+} to Fe^{2+} however the quantum yield was determined to be significantly lower for the Fe^{3+}-pectate. These two polysaccharides were altered and the quantum yield of the photoreaction was determined. The quantum yield for both carboxo-methylated and acetylated polysaccharides was significantly lower than for the native polysaccharides. From these results we hypothesize that these different quantum yields are due to the differences in stereochemistry in the binding of the Fe^{3+} with the alginate and pectate polysaccharides. These Fe-polysaccharide materials were used to create soft hydrogel beads. By irradiating with light and reducing Fe^{3+}, the beads break apart in solution. This has led us to move in the direction of trying to insert various drugs into these beads. The stability of the beads in the dark in biological solutions at 37 °C was determined for both polysaccharides alginate and pectate and pectate beads were more stable than alginate. Alginate beads were formed that hold epinephrine, a vasoconstrictor drug, inside of the polysaccharide network. With light irradiation of the beads, they release epinephrine into solution. The release of epinephrine was be quantified through a colorimetric assay and shows the increase in release of epinephrine with irradiation time. These experiments show that the release of epinephrine is dependent on the breaking down of the polysaccharide beads. Since the beads degrade in the presence of light, we are then able to control the amount of light that is being used and the time for which the beads are exposed to light. Our next step is to start testing the polysaccharide beads inside a biological system to determine the effectiveness of the drug delivery system. Future experiments will focus on testing the epinephrine release from the beads in pig coronary arteries by measuring vasoconstriction using a myograph.

I9

$[XeF_5]^+$ and $[Xe_2F_{11}]^+$ Salts of the $[Cr^{IV}F_6]^{2-}$, $[Cr^{V}OF_5]^{2-}$, and $[CrV_2O_2F_8]^{2-}$ Anions

Daniel G. Stuart, James T. Goettel, Hélène P. A. Mercier, Gary J. Schrobilgen
McMaster University

The known Cr(VI) oxide fluorides are represented by CrO_2F_2, $CrOF_4$, and $[CrOF_5]^-$. The latter anion has been characterized by means of vibrational spectroscopic studies of its $[NO]^+$ and Cs^+ salts. In the present work, the strong oxidative fluorinating agent, XeF_6, was reacted in varying molar ratios with $CrOF_4$, resulting in the formation of four new $[XeF_5]^+$ and $[Xe_2F_{11}]^+$ salts; $[Xe_2F_{11}]_2[CrF_6]$,$[XeF_5]_2[CrF_6]\cdot 2CrOF_4$ (see Figure), $[XeF_5]_2[Cr_2O_2F_8]$, and $[XeF_5][Xe_2F_{11}][CrOF_5]\cdot 2CrOF_4$. The salts were characterized by single-crystal X-ray diffraction and provide the first crystal structures of the known $[Cr^{IV}F_6]^{2-}$ anion and the previously unknown $[Cr^{V}OF_5]^{2-}$ and $[Cr^{V}_2O_2F_8]^{2-}$ anions. The formation of Cr(IV) and Cr(V) anions presumably result from reduction of Cr(VI) by elimination of O_2 and F_2, respectively.

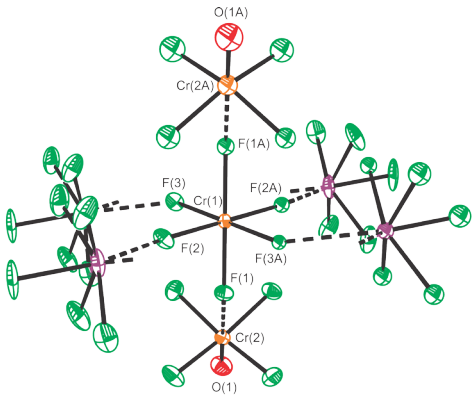


Figure. The crystal structure of $[XeF_5]_2[CrF_6]\cdot 2CrOF_4$; $P\bar{1}$, Z = 1, T = –173 °C, R_1 = 0.023.

I10

Improving the Contact at the ITO | CdTe Interface in Cadmium Telluride Solar Cells

Vadim Tanygin, Matt Kurley, Dmitri Talapin
University of Chicago

As awareness of the environmental impact and limited availability of conventional energy sources has grown, research into alternatives, including solar cells, has increased. However, high manufacturing costs, among other factors, have limited their commercialization. Thin-film solar cells have emerged as an alternative to crystalline silicon cells; in particular, solution-processed, thin-film solar cells consisting of successive indium tin oxide (ITO), cadmium telluride (CdTe), and zinc oxide (ZnO) layers have shown promise.

However, certain effects associated with the ITO|CdTe interface can impact the performance of these solar cells. The difference in work functions between the two materials creates an energy barrier that prevents holes from flowing into the ITO, reducing the short-circuit current of the cell. Additionally, the diffusion of indium, an n-type dopant, from the ITO into the CdTe layer, can reduce the current as well. The goal of our research is to test different materials that may be deposited onto the ITO to form a better contact with the CdTe, block indium diffusion, and increase the carrier concentration. Molybdenum(VI) oxide, aluminum oxide, and copper-doped CdTe were chosen as the interfacial materials based on these respective criteria. To prepare the control devices, solutions of CdTe nanocrystals were synthesized, washed, and spin-coated onto ITO-coated substrates via a layer-by-layer process, followed by a single ZnO layer. To prepare the first two types of test devices, aluminum oxide and molybdenum(VI) oxide were deposited onto the ITO by atomic layer deposition and thermal evaporation, respectively, before spin-coating the CdTe. To prepare the third set of devices, a single layer of copper-doped CdTe was spin-coated onto the substrates, followed by several layers of non-doped CdTe. Additionally, a layer of aluminum oxide was evaporated onto some of these devices after the Cu-doped solution was spin-coated, in order to prevent the Cu from diffusing away from the interface.

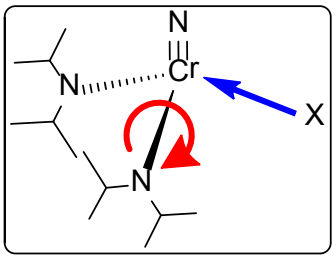
The devices with metal oxide layers showed lower short-circuit current vs the control device, indicating that the oxide layer may be too thick, causing increased series resistance. The devices with Cu-doped CdTe, but no aluminum oxide layer, showed similar performance compared to the control device, suggesting the Cu did diffuse away from the interface. Future experiments will focus on refining each approach; using thinner metal oxide layers should reduce resistance while still forming a good contact and blocking indium diffusion, while substituting CuTe for Cu-doped CdTe should reduce diffusion of the Cu away from the interface

I11

Investigating Donor Abilities of Ligands for High Valent Transition Metals and Synthesis and Reactivity of Chromium Complexes Bearing Nitrido, Imido, and Amido Ligands

Evan Beaumier, Ross Bemowski, Amrendra Singh, Bailey Bajorek, Richard Staples, Yvonne Deporre, Aaron Odom

Synthetic protocols have been developed for a wide variety of chromium(VI) nitrido compounds of the general formula $NCr(NPr^{i}_{2})_{2}X$, where X = anionic ligands varying from common Werner-type ligands (halides, CN, OCN, SCN, etc.) to common ancillaries for organometallic chemistry (heterocycles, NR_2, OR, OAr, etc.). These high valent metal complexes were then used as a method for experimental parameterization of ligand donor ability via ^{1}H NMR spin-saturation transfer.



The impetus for this study was to understand donor ability of ancillaries in our titanium-based multicomponent coupling chemistry, although we hope these methods will be applicable to a wide range of systems.

Additionally under current investigation is the synthesis and reactivity of chromium (VI) complexes bearing each of amido, imido, and nitrido ligands. We are looking to study potentially interesting reactivity with this novel complex, including cycloadditions, reactivity in presence of electrophiles, and reactivity in the presence of Brønsted acids. We also hope to potentially broaden the horizon of ligand donor parameterization in enabling the ability to test the known system for predicting imido donor ability.

In this poster, we will discuss what we have learned about how electronegativity, orbital overlap, and sterics conspire to give the overall donor ability of these ligands, as well as the synthesis and initial reactivity of the amido, imido, and nitrido chromium complexes.

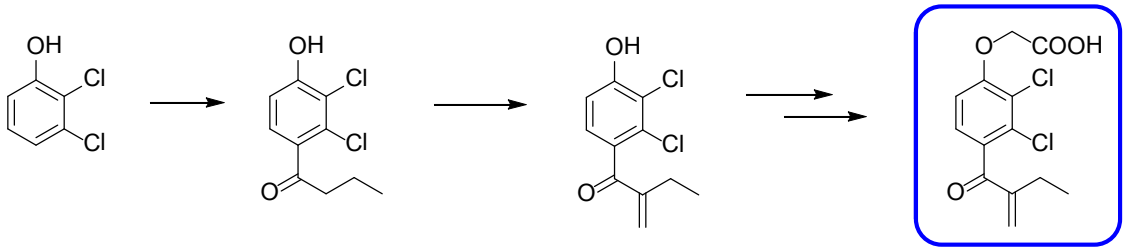
O1

Ethacrynic Acid as a Lead Structure for the Development of Potent Urease Inhibitors

Sean Blackburn, Zakee Azeez, Ingo Janser*

Eastern Michigan University

It is well known that Helicobacter pylori (H. pylori) produces urease, an enzyme that catalyzes the conversion of urea into ammonia and carbon dioxide. The production of ammonia makes it possible for H. pylori to inhabit the stomach. H. pylori urease has been identified as a potential therapeutic target for treatment of peptic ulcer. Recently we have synthesized ethacrynic acid and a series of its analogues and subsequently evaluated the compounds for their inhibitory effect on jack bean urease.



The synthesis was accomplished by a four-step reaction, including a Friedel-Crafts reaction, an S_N2 reaction, and an aldol condensation reaction. Efforts were made to optimize the reaction conditions in order to increase the yield of the C-acylated product versus the O-acylated product. The S_N2 reaction of the substituted phenols with an alkyl halide worked best if ethyl bromoacetate, instead of 2-cloro- or 2-iodocarboxylic acid, respectively, was used. In regards to the inhibition studies, the highest inhibitory activity was found for ethacrynic acid and its chain length analogue after a preincubation time of 4 hours at a concentration of 0.5 mM. Two other compounds, possessing one methoxy group at the aromatic system, were also able to significantly inhibit the enzyme. Due to the distinct inhibitory activities of the various compounds, it can be speculated that the substituents attached to the aromatic system have a great influence on the activity of the corresponding compound. The addition of sulfhydryl compounds reduces the activity of ethacrynic acid significantly. This is insofar not surprising since the sulphur of the sulfhydryl compound can attack the β-carbon of the α,β-unsaturated carbonyl unit, thereby preventing its reaction with cysteine residues in the active site of the jack bean urease. Testing precursors of our compounds which lack the α,β-unsaturated carbonyl unit for their inhibitory activity on urease reveals the importance of the α,β-unsaturated carbonyl unit because none of them show a measurable inhibition of the enzyme.

O2

New Modes of Initiating Cation Radical Cycloaddition Dimerization and Polymerization Reactions

Brianna N. Barbu, Eun Jung Shin, Eric W. Webb, David J. Green, and Jason G. Gillmore*

Hope College

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 syntheses of Bauld's monomers and a comparative study of their initiation by chemical oxidants, direct electrochemical oxidation, conventional photooxidants and our novel photochromic photooxidants is underway.

O3

Examining the Alzheimer's Prevention Potential of Almonds

Jessica Compton, Patricia Diaz, Danielle Burge

Calumet College of Saint Joseph

No abstract submitted.

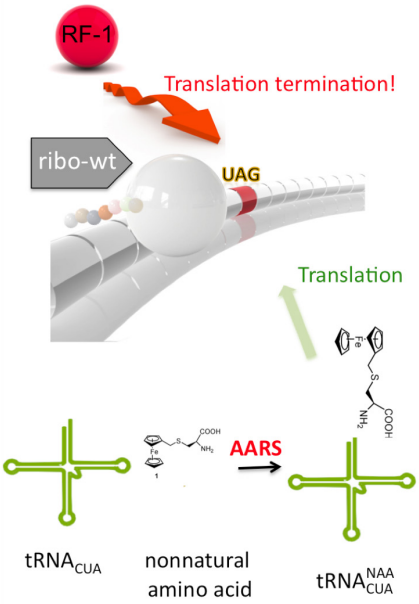
O4

Characterization of a Non-natural Amino Acid Encoding Enzyme

Curtis, Ryan; Culpepper, Seja; Tippmann, Eric

Indiana-Purdue University, Fort Wayne

Nearly all the proteins and enzymes that make life possible are formed from the same common 20 amino acids. This ubiquity of the common 20 amino acids extends to all known organisms, from bacteria and fungi to plants and people. The ability to incorporate non-natural amino acids into proteins by genetic or chemical methods allows one to introduce novel properties that do not exist in Nature. In this way, the structure or function of the protein may be altered without perturbing any of the other 20 common amino acids in the molecule. Here we describe the syntheses of an organometallic ferrocene non-natural amino acid and preliminary characterization its cognate aminoacyl tRNA synthetase (AARS).



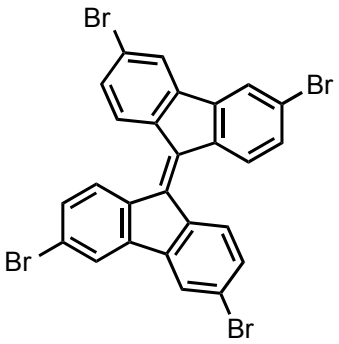
O5

Synthetic Progress towards 3,3′,6,6′-tetrabromobifluorenylidene

David Darr, Jeremy K. Klosterman*

Bowling Green State University

Bifluorenylidene is an intriguing compound due to the strained geometry of the central double bond. Clashing hydrogens force the two halves to take a nonplanar, anti-folded conformation. Altering the steric profile, by adding methyls or changing ring sizes, can induce a twisted conformation of higher energy. Alternatively, one could lock the molecule into a more planar geometry by tethering the two halves within a rigid framework. Here we report the synthetic progress towards making 3,3′,6,6′-tetrabromobifluorenylidene (**1**). This key intermediate enables further opportunities for structural modifications using modern palladium catalyzed cross-couplings. In particular, conversion to a tetra carboxylate bifluorenylidene derivative would be suitable for the construction of metal-organic frameworks.



3,3′,6,6′-tetrabromobifluorenylidene (**1**).

O6

Promoting Catalysis and Expanding the Scope of Organometallic Nucleophiles Utilized in the Nickel-Mediated Decarbonylative Cross-Coupling of Substituted Phthalimides

Kimberly S. DeGlopper, Megan R. Kwiatkowski, Jeffrey B. Johnson*

Hope College

A new method for synthesizing ortho-substituted benzamides has been developed through the nickel-mediated decarbonylative cross-coupling of substituted phthalimides with various diorganozinc reagents. This reaction demonstrates broad substrate scope, including both electron-rich and electron-poor aryl phthalimide substituents and a variety of commercially available and in situ generated diorganozinc reagents. However, this reaction suffers from two key limitations. First, it requires a stoichiometric equivalent of nickel, which limits its application in synthesis. Second, diorganozinc reagents are either pyrophoric or must be synthesized in situ. Efforts to promote catalysis include altering the phthalimide substituent, ligand, solvent, and catalyst used. Recent work has also focused on expanding the scope of nucleophiles to include boronic acids, which are safer and more commercially available, while optimizing reaction conditions of this new system.

O7

Incorporation of Boronic Acids in Cross-Coupling Reactions Proceeding through C-C Activation

Joseph M. Dennis, Chad T. Compagner, Connor D. McNeely, Jeffrey B. Johnson*

Hope College

Continued exploration of the rhodium-catalyzed intramolecular carboacylation of quinolinyl ketones and tethered alkenes has prompted the investigation into intermolecular cross-coupling reactions. Proceeding through a similar intermediate generated from C-C bond activation, a variety of rhodium catalysts, directing moieties, and boron transmetallating reagents were screened in pursuit of the selective activation and functionalization of substituted ketones. Apart from investigating the functional group tolerance of the reaction, current work is being done to optimize reaction conditions as well to develop facile sp^2-sp^3 cross-coupling pathways of ketones with alkyl boron reagents.

O8

Synthesis of Pyridine and Pyridinium Quinone Methide Precursors: Studies Towards the Realkylation of Aged Acetylcholinesterase

Rachel Dicken, Keegan Fitzpatrick, Ryan Yoder, Christopher M. Hadad, and Christopher S. Callam

The Ohio State University

Acetylcholinesterase (AChE) is an essential enzyme in the human body, which hydrolyzes acetylcholine into choline for biochemical processes. Organophosphorus (OP) nerve-agents such as Sarin, Soman and Tabun are covalent inhibitors of AChE. Following exposure to OPs, inhibited AChE undergoes a subsequent irreversible aging process in which the OP-AChE adduct is de-alkylated (aged) resulting in the accumulation of excess acetylcholine in the central nervous system. Current oxime based pharmaceuticals can only be used to treat the inhibited AChE and are ineffective on the aged AChE. Our research focuses on the design of small molecules that can be used to re-alkylate aged AChE. Previous studies have shown that high energy quinone methides (QM) could potentially reverse the damage done to the active site on aged AChE through a kinetically favored alkylation of a phosphodiester. We have used computational chemistry to guide our synthetic efforts. We have developed methods to synthesize various quinone methide precusors; including pyridine and pyridinium compounds. The synthesis of these compounds and testing of them will be discussed. Mechanistic understanding on the formation of high energy quinone methides and optimization of the reactions for their formation is currently still in progress.

O9

An Investigation of the Ability of Sulfisomidine to Form Cocrystals with Carboxylic acids.

Shane Douglas, Dr. Daniel Adsmond

Ferris State University

Cocrystals, defined as any multicomponent neutral molecular complex that forms a crystalline solid, are an important area of study due to various applications in industry, most notably pharmaceuticals. Sulfisomidine and sulfamethazine are anti-bacterial drugs with nearly identical structures; however, past cocrystallization experiments have shown sulfamethazine to form cocrystals readily when compared to sulfisomidine which generally does not form cocrystals. Later work with sulfamethazine has shown that by using an ideal solvent to decrease the solubility differences and by increasing the starting amount of the more soluble component; cocrystals formed that previously had not. In our research, these conditions were applied to sulfisomidine which was expected to enhance cocrystallization abilities. A starting ratio of 4:1 (acid:drug) with twenty-two mono-substituted benzoic acids in solutions of 80/20 methanol/water and 60/40 acetonitrile/water cocrystals systems was normally used. After several days of evaporation, these solutions usually produced crystalline solids. Solids were analyzed by infrared spectroscopy for shifts in the absorbance of functional groups, and by nuclear magnetic resonance spectroscopy to determine the ratios of components. Sulfisomidine formed cocrystals under these conditions with eleven of the twenty-two acids.

O10

Imidazoline Synthesis to Investigate the Extent of Heterocycle-Biomolecule Complex Formation

Alyssa Ellsworth , Robert A. Mosey

Lake Superior State University

2-imidazolines are heterocyclic scaffolds that are recognized for their wide variety of biological properties. Substantial efforts have been made in the way of synthesizing the 2-imidazoline core, yet single pot reactions to synthesize N-substituted 2-imidazolines from acyclic starting materials are scarce. Most commonly, syntheses of N-substituted 2-imidazolines utilize a 2-step procedures involving 2-imidazoline synthesis followed by either N-alkylation or metal-mediated N-arylation. The aim of our study was to develop a mild and efficient protocol by which N-alkyl and N-aryl substituted 2-imidazolines could both be prepared from similar acyclic starting materials. The development of such a protocol involving triflic anhydride-mediated dehydration of 2-(haloethyl)amides in the presence of amines will be discussed, as will be the scope of the reaction methodology and mechanistic insights.

O11

No Title

Franqlin Gatson

Calumet College of Saint Joseph

No abstract submitted.

O12

Coupling Reactions of 7-amino-4-methylcoumarin for Future Use as Caspase-1 Substrates

Thomas Hagerman, Caitlin E. Karver, Ph.D.

DePaul University

Inhibition of the cysteine dependent protease caspase-1 is a validated approach for the treatment of autoimmune disorders due to its regulation of levels of the pro-inflammatory cytokine interleukin 1-beta, but very few drugs targeting caspase-1 have reached the clinic. Our goal is to gain a more thorough understanding of the inhibition of caspase-1 by developing substrates for fluorescence activity studies. Caspase-1 cleaves its substrates after an aspartic acid residue to produce the active interleukin 1-beta. When caspase-1 cleaves the substrate it produces a free chromophore, which can be identified by spectrophotometric assays. Current peptide substrates make it difficult to analyze the effects of inhibitors because of slow enzyme kinetics of large peptide substrates. New small molecule substrates are therefore necessary. Before a new substrate containing an aspartic acid residue can be synthesized, the coupling conditions of the fluorescent molecule 7-amino-4-methylcoumarin (AMC) to the main substrate molecule must be better investigated. The synthesis of aspartic acid containing small molecules to which AMC can then be coupled has been successful. However, these syntheses have been stalled by the inability to couple AMC to the free acid. The problem in the coupling of AMC to acids such as cinnamic acid, acetylsalicylic acid, or 2-phenoxybenzoic acid appears to have been the activation of the nucleophilic nitrogen atom of AMC. Discussed herein are the syntheses involving peptide coupling reagents such as PyBOP, HCTU, DIC, and HOBT and bases such as pyridine, DMAP, DIPEA, and TEA. Acetic acid is now being used as a simple model system in the study of coupling reaction conditions, which will then be applied to reactions involving more complex substrates.

O13

Synthesis of Pyromellitic Diimide Flanked Co(II)-salen Complex and Its Application in the Supramolecular Catalyst Assembly Based on Aromatic Donor-Acceptor Interaction.

[2]Eric Heim, [1]Dr. Yu Liu

Northern Michigan University

Supramolecular catalysts, inspired by enzymes, imply multicomponent catalytic systems assembled through noncovalent interactions. The goal of this research is to explore aromatic donor-acceptor interaction as the driving force for the supramolecular catalyst assembly. Pyromellitic diimide as the aromatic acceptor moiety will be attached onto Co(II)-salen complex in this study. Currently, we are working on two synthesis routes, which will result in two final catalysts with different linker flexibility. The final catalysts will be compared in the catalysis of hydrolytic kinetic resolution of epoxides.

O14

Chemical Synthesis of Azido Inositols via Ferrier Rearrangement

Maxwell K. P. Hogue, Sarah R. Rundell, Cody J. Wilson, and Benjamin M. Swarts*

Central Michigan University

myo-Inositol is a carbohydrate that is widespread in nature, existing in both prokaryotes and eukaryotes and having notable functions related to signal transduction and anchoring of molecules to cell surfaces. Due to the challenge of studying carbohydrates using traditional molecular biology techniques, chemically modified *myo*-inositol analogs may have value as probes or inhibitors of inositol metabolic pathways and inositol-containing biomolecules. However, the synthesis of *myo*-inositol derivatives is quite challenging due to inositol's internal plane of symmetry and the requirement to differentiate six secondary hydroxyl groups. Here, we report on our efforts to use the Ferrier rearrangement to synthesize 4-azido inositol from a simple glucopyranoside starting material. We expect that this approach will be useful for accessing other azido inositols, which we plan to use to probe virulence-associated phosphatidylinositol mannosides (PIMs) in the global pathogen Mycobacterium tuberculosis.

O15

Towards the Synthesis of Bisbenzoxazoles from Resorcinol

Brian Hull, Dr. Peter Balanda

Ferris State University

In the current market, polymers are a commodity which is rising in both use and efficiency. The industrially made polymer Zylon® is a commonly used, highly conjugated, rigid-rod polymer with currently confined roles within the public markets. Its production relies on the classical process of nitration to produce an atmospherically unstable, intermediary species diaminodihydroxybenzene (DADHB) which must then be further processed. The goal of the research was primarily to create an alternative, less noxious method for the production of the intermediate through the use of amide functional groups. By using and combining existing methods, the process has been reduced to an unrefined, one-pot method synthesis of the more stable (4,6-dimethoxybenzene-1,3-diyl)-bisoctanamide. The process and mechanism of the amide formation were explored in depth to reveal and specify complications in the formation of the oxime intermediate which lead to a reduced capacity of output from the reaction. Upon production, routes were explored to modify and conform the material to the current polymer production process. Based upon the developed methodology, future explorations shall be made toward perfection of the method as well as to develop unique, benzoxazole materials and explore their uses or functionality.

O16

Treating Cancer with Curcumin: The Past, Present, and Future

Nikhyl Jhangiani, Dr. Rekha Srinivasan

Case Western Reserve University

This paper studies the role of Curcumin, a phytochemical compound in turmeric, and its transition from a being used in Ayurvedic Medicine to modern research that utilized nanoparticles and curcumin to target and treat cancer in vivo. Curcumin is a bis-α,β-unsaturated β-diketone and is relatively insoluble in water, but is able to dissolve in acetone, dimethylsulphoxide, and ethanol. When ingested by humans, the various analogues of curcumin have a variety of biological effects. This compound is known to exhibit antioxidant activity, ad can target multiple features in vivo; such as modulating various transcription factors, cytokines, growth factors, kinases, and other enzymes. Curcumin has also been proven to serve as a strong anti-inflammatory agent, since it suppresses the transcription factor NF-κB, which regulates pro-inflammatory gene products. Unlike other natural products, curcumin has not shown any toxic effects even when consumed daily, and, as such, is a key research component for a variety of cancer treatments. Studies have found that it can be both chemotherapeutic and chemopreventive, and this paper covers various studies showing the effects and potential uses of curcumin in treating cancer.

O17

An Investigation of the Ability of Dibenzyl Sulfoxide and Triphenylphosphine Oxide to Form Cocrystals with Carboxylic Acids and Phenols

Cierra Kemppainen and Dr. Dan Adsmond

Ferris State University

A cocrystal is a crystalline structure made up of two or more compounds in a definite ratio. The primary type of cocrystal is a binary cocrystal, which is a cocrystal composed of two different compounds in a definite ratio. My research was preliminary to explore the ability of carboxylic acids and phenols to form ternary cocrystals. Ternary cocrystals are cocrystals made up of three compounds in a definite ratio. I explored the ability of dibenzyl sulfoxide to form binary cocrystals with 10 different compounds that contain a carboxylic acid and a phenol. Data from over 85 experiments was collected and analyzed via infrared spectroscopy and nuclear magnetic resonance. From these experiments, one compound formed a cocrystal with dibenzyl sulfoxide. Experiments were conducted with triphenylphosphine oxide under the same conditions of dibenzyl sulfoxide, after it became apparent that dibenzyl sulfoxide was no longer a viable option for ternary cocrystals. Data from 78 experiments using triphenylphosphine oxide was collected and analyzed via infrared spectroscopy and nuclear magnetic resonance. In this talk we will discuss the history of dibenzyl sulfoxide, influence of solvents, and the ability of dibenzyl sulfoxide and triphenylphosphine oxide to form binary and ternary cocrystals in future experiments.

O18

New Avenues for Iron-Catalyzed Dehydrogenative Cross-Coupling Reactions

Qiuhan Li, Emilia Groso, Corinna S. Schindler

University of Michigan, Ann Arbor

The biaryl structural motif is an important feature found in many functional materials such as light-emitting diodes (LED) and liquid crystals. It is also present in many biologically active compounds. This motif is typically obtained via C-H activation and cross-coupling methods; however, these methods typically require the prefunctionalization of the coupling partners and subsequent removal of the activating groups. Inspired by the role of iron-containing P450 enzymes by which *M. tuberculosis* uses to catalyze oxidative coupling reactions, we aim to use transition metal complexes to catalyze the dehydrogenative cross-coupling reactions. This novel method will eliminate the need for lengthy prefunctionalization. Currently, the transition metals we are exploring are iron, chromium, manganese, copper, vanadium, and ruthenium. The ligands of interest are salen and salan ligands. Based on our preliminary phenol coupling catalyst evaluation results of 2,4-di-*tert*-butylphenol, iron-containing and vanadium-containing salen complexes give us a 60%-70% yield. After building up our ligand library and transition metal complex library, we are planning to conduct more comprehensive catalyst evaluation to test the ability of those complexes and to examine the substrate scope. Once we have viable transition metal catalysts, we can apply them to natural product synthesis. Specifically, we are interested in applying these catalysts towards the synthesis of mycocyclosin and similar substrates, which can potentially act as novel *M. tuberculosis* inhibitors.

O19

Effects of Soursop on Alzheimer's Disease

Sandra Narvaez, Hector Lopez, Roger Malonda, Dr. Sandra Chimon Peszek

Calumet College of St. Joseph

No abstract submitted.

O20

Next Generation Quinazolinespirohexadienone Photochromes for Application as Photochromic Photooxidants

Lauren E. Messer, Luke J. Peterson, and Jason G. Gillmore*

Hope College

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. 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. Replacing the naphthalene moiety of the PSHD's with a quinoline moiety gives the quinazolinespirohexadienone (QSHD) family of photochromes we have recently reported. In this presentation we describe recent efforts to develop even more electron deficient QSHD analogs capable of gating PICT and photooxidizing less reducible monomers of interest to materials applications.

O21

Synthesis of Quinolone-5,8-dione Analogues

Jenny Nguyen, Dr. Robert Sammelson

Ball State University

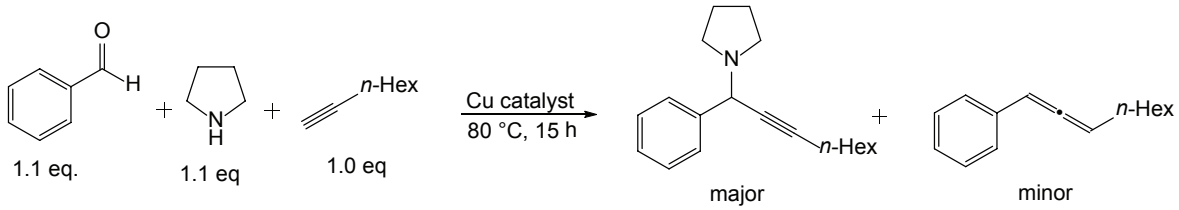
The substituents at the various positions on the quinone-5,8-dione determine its activation by NQ01, making the compound more toxic and specific towards NQ01-rich tumor cells. A series of reactions was conducted to synthesize 7-N-acetamido-2-formylquinoline-5,8-dione. The aldehyde group of this quinolone-5,8-dione was transformed into the corresponding oxime. The compound was further converted to the nitrile oxide and that created an isoxazoline or isoxazole through 1,3-dipolar cycloaddition with alkenes or alkynes, respectively. Recrystallization and column chromatography were performed to purify the products. The percent yields of oxime, isoxazoline and isoxazole are 51%, 71%, and 60%, respectively. Further tests will be conducted to study the toxicity and affinity of oxime, isoxazoline, and isoxazole for NQ01.

O22

Transition Metal Catalyzed Synthesis of 1,3 Disubstituted Allenes using an Amine Promoter

Christine Nyawaga, Dr. Courtney E. Meyet

Hillsdale College



The one-step copper-catalyzed three component coupling of pyrrolidine, aldehyde, and terminal alkyne to yield propargylamine results in a 1,3-disubstituted allene as a minor product. Work is underway to determine optimal conditions favoring allene over propargylamine. Pyrrolidine is suspected to act as a promoter in the formation of allene, perhaps going through a propargylamine intermediate. Although initial yields are low, and reaction times longer than 15 hours are necessary, preliminary results favor $Cu(OTf)_2$ as catalyst over CuI. Additionally, aryl aldehydes are found to result in the formation of allenes and propargylamines, where alkyl aldehydes produce solely propargylamine.

O23

Diaminoacenaphthylene, a key but elusive intermediate toward carbonyl-substituted perimidinespirohexadienone photochromes.

Amber J. Prins, Jason G. Gillmore

Hope College

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. This necessitates photochromes whose photogenerate long wavelength isomers (LW) revert to their stable short wavelength isomer (SW) only thermally and that have excited state reduction potentials that are more positive for LW than for SW. The parent perimidinespirehexadienone (PSHD) photochrome has 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 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.

O24

Nuclear Waste Reprocessing: The use of O and S-Donating Ligands for Selectivity toward Lanthanides and Actinides.

Dr. Biros, Paul Morse, Brian Rawls

Grand Valley State University

The goal of the Dr. Biros research group at GVSU is to analyze a class of organic molecules known to have high binding affinity toward specific metals in the lanthanide and actinide series. The molecules studied are derivatives to a class of compounds used in the TRUEX (TRans Uranium EXtraction) nuclear waste reprocessing, called CMPO (CarbomoylMethyl Phosphine Oxide) ligands. The molecules synthesized in this study were cdppeO (cis-diphenyl-phosphine ethylene oxide) and cdppeS (cis-diphenyl-phosphine ethylene Sulfide). Based off spectroscopic extraction studies using Arsenazo (III), these molecules showed high binding affinity toward the actinide metals (U, Th) and low binding affinity toward the lanthanide series.

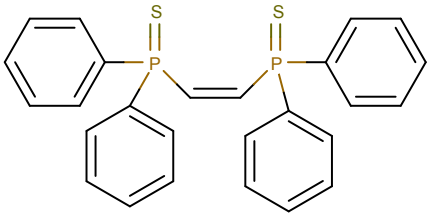


Figure 1: cdppeS

O25

Grignard and Aldol Condensation Reactions in the Synthesis of Compounds Containing Antidepressant Characteristics

Ryan Rhodes, Dr. Sammelson

Ball State University

Antidepressant pharmaceutical compounds, such as Prozac (fluoxetine, N-methyl-3-phenyl-3-[4-(trifluoromethyl)phenoxy]propan-1-amine), contain selective serotonin reuptake inhibiting (SSRI) properties, which is the main function by which these molecules act physiologically to reduce depression. Over recent years, these pharmaceutical products have been modified to act as dual inhibitors of serotonin and norepinephrine reuptake, which consequently increases their ability to reduce depression. The most famous of these new dual inhibition compounds is Cymbalta (duloxetine). Cymbalta's close resemblance in structure to Prozac suggests novel compounds containing similar functional groups and structures can have similar antidepressant qualities. The use of Grignard and Aldol condensation reactions has led to new synthetic routes that are capable of producing new compounds that are slight variations of the pharmaceutically available counterparts.

O26

Fluorescent Quinolones for β–Sheet Interception

Mike Sportiello, Alan Schwabacher Ph.D.

University of Wisconsin-Milwaukee

Much of antibiotic resistance results from membrane proteins that, through the process of active transport, remove antibiotics from within the membrane to outside the membrane, rendering said antibiotics useless. Many membrane proteins called efflux protein complexes responsible for this are, in part, folded by a different protein-complex called the β-barrel assembly machine (BAM). The structure of proteins folded by this machine is of the form of a β-barrel, composed of β-pleated sheets. Currently, a rigid quinolone structure with strategic hydrogen-bonding sites is being pursued as a molecular template that will hydrogen-bond small peptides by mimicking the interactions in a β-sheet, leading to potential studies of BAM inhibition. These templates will be used to study intramolecular forces in β-sheets and β-barrels.

O27

Inverse-Demand-Diels-Alder Reactions of 3-Formylchromones

Aaron J. Sullivan, Daniel C. Steigerwald, Benjamin Kasting, Olivia M. Johntony, Brian J. Myers, Jake R. Zimmerman

Ohio Northern University

The basic chromone structure has a variety of biological activities and has therefore been considered a privileged structure with regards to medicinal chemistry.[1] We have found that 3-formylchromones participate in an open air inverse demand-Diels-Alder reaction with a dienophile.[2,3] Various chromones were studied and their corresponding products were used to build a library of compounds to test for biologic activity. Apart from their medicinal interest, the products also fluoresce blue/green under long wave radiation.[4] This poster presents synthetic pathways for the creation of a small library of substituted 3-formylchromones, the medicinal capabilities of some of the products, and also UV-Vis data regarding the observed fluorescence.

1. Welsch, M. E.; Snyder, S.A.; Stockwell, B. R., *Curr. Opin. Chem. Biol.* **2010**, *14*, 1-15.
2. Duckert, H.; Khedkar, V.; Waldmann, H.; Kumar, K., *Chem. Eur. J*. **2011**, *17*, 5130-7.
3. Sosnovskikh, V. Y.; Khalymbadzha, I. A.; Irgashev, R. A.; Slepukhin, P.A., *Tetrahedron Lett*. **2008**, *64*, 10172-80.
4. Benedetti, E.; Kocsis, L. S.; Brummond, K. M., *J. Am. Chem. Soc*. **2012**, *134*, 12418-21.

O28

Cephalotaxine Analogues-Synthesis of Potential Anticancer Drugs

Chelsea Swanson, Reshmi Gopagani

Eastern Michigan University

Cephalotaxine, a natural organic compound is the parent member of the group of Chephalotaxus alkaloids and has been shown, in mice, to possess anti-leukemia properties. The goal of this research is to synthesize cephalotaxine analogues with reduced or no toxicity. The proposed methodology for manipulating the reactivity is to introduce a Michael system (an alpha, beta unsaturated carbonyl system) and later to change the substituents of the Michael system on the alpha position in order to manipulate the reactivity of the beta carbon and thereby the whole compound. The Michael system of the compound interacts with the sulfur-containing amino acids (cysteine) present in the active site of the Glutathione S-Transferase (GST) enzyme, thereby inhibition occurs. The normal function of GST is to mark compounds inside the cell for degradation; without this function cancer cells, as well as normal cells build up toxins and die. Cephalotaxine itself, however, is too toxic to be used in anticancer treatment. Our recent research has been focusing on the synthesis of benzazepines, a base structure of cephalotaxine with three major goals: (a) addition of a protecting group, (b) addition of a carbonyl group, and (c) ring closure. Various protecting group techniques have been employed in order to increase the yield of the synthesis and prevent an unwanted decarbonylation reaction from occurring, focusing on the use of the diisopropoxyphosphinyl group.

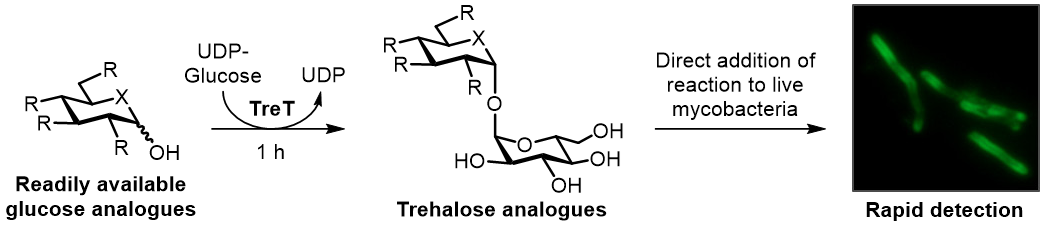
O29

Chemoenzymatic Synthesis of Trehalose Analogues: Rapid Access to Chemical Probes for Investigating Mycobacteria

Bailey L. Urbanek, Douglas C. Wing, Krystal S. Haislop, Chelsey J. Hamel, Rainer Kalscheuer, Peter J. Woodruff, Benjamin M. Swarts*

Central Michigan University

Trehalose analogues are emerging as valuable tools for investigating *Mycobacterium tuberculosis*, but progress in this area is slow due to the difficulty in synthesizing these compounds. Here, we report a chemoenzymatic synthesis of trehalose analagoues that employs the heat-stable enzyme trehalose synthase (TreT) from hyperthermophile *Thermoproteus tenax*. By using TreT, various trehalose analogues were prepared quickly (1 *h*) in high yield (up to > 99% by HPLC) in a single step from readily available glucose analogues. To demonstrate the utility of this method in mycobacteria research, we performed a simple "one-pot metabolic labelling" experiment that accomplished probe synthesis, metabolic labelling, and imaging of *M. smegmatis* in a single day with only TreT and commercially available materials.



O30

Synthesis of Aromatic Donor-Acceptor Interaction Based Supramolecular Catalyst and Its Application in Hydrolytic Kinetic Resolution of Epoxides

Matt Woodhouse, Dr. Yu Liu

Northern Michigan Univeristy

This research aims to develop aromatic donor-acceptor interaction based supramolecular catalysts and study their catalytic properties in hydrolytic kinetic resolution (HKR) of epoxides. In our design Co(II)-salen catalytic moiety will be flanked by two electron-deficient aromatic units. The interaction with electron-rich aromatic compound enables the assembly of the dinuclear Co(II)-salen supramolecular catalyst, which promotes of the bimetallic mechanism based HKR. The catalysts have been synthesized and characterized. Different HKR reaction conditions were also tested for catalysts. The preliminary results showed that an increasing reaction rate was observed when the electron-rich aromatic compound was added. It indicates the formation of the supramolecular catalyst by aromatic donor-acceptor interactions.

O31

The Effects of Nucleophiles in the Activation of PMHS During Palladium Catalyzed Hydrodehalogenation of Aromatic Boronic Esters

Jack H. Warsh, Chathurika R. K. Jayasundara, Monique Noel, Milton R. Smith, III, Robert E. Maleczka, Jr.

Michigan State University

Fluoro aromatic compounds are commonly used by the agrochemical, pharmaceutical, and related industries. The presence of sterically small fluoro group often allows drugs to act either agonistically or antagonistically to organism's receptors. Syntheses and/or elaboration of fluoro aromatic and aromatic compounds in general regularly involve cross-couplings of borylated compounds. As such the generation of aromatic molecules bearing both fluorine and boron substituents is a goal of many chemists working in the field. To the best of our knowledge, the fluorination of arylboronates is unknown. In contrast there are several ways to borylate fluorobenzenes. Unfortunately, traditional borylation methods typically demand the use of unattractive conditions (e.g. strong bases, cyrogenic conditions, high dilution, etc.). Ir-catalzed borylations have recently emerged as a new way to directly convert a C–H bond into a C–B bond. These reactions tolerate halogens, including fluorine. The regioselectivity of Ir-catalzed borylations is primarily driven by sterics, such that ortho borylations are rare. However with fluorobenzenes ortho borylations are common owing to the small size of fluorine. This can be favorable, but for fluorobenzenes where multiple positions are sterically accessible it can result in ortho, meta, and para products all being formed during the reaction

We have recently developed a two-step procedure to obtain a single product with the boron group ortho to fluorine. This alternative route uses substrates that containing a halide that in effect serves to block the meta and para positions from borylation. This new reaction scheme concludes with the halogen being removed under hydrodehalogenation conditions. My research has centered on the development of efficient methods for this hydrodehalogenation step. The outcomes of this research will be presented.

O32

Echinacea: A Possible Preventative for Alzheimer's Disease

James Stahl, Elena Cortes, Amy Gasiorowski, and Dr. Sandra Chimon-Peszek

Calumet College of St. Joseph

Beta-sheet fibril deposits are a crucial hallmark of Alzheimer's disease. Characterized by accumulations of highly toxic beta-sheet structures, fibril tangles disrupt synaptic function causing impaired memory. Amassing toxicity results in neuronal degradation and ultimately complete brain death. Beta-amyloid research focuses on one region of the 40-42 amino acid length beta-amyloid known as "KLVFFA"; this region, from residues 16-21, is believed to be the single, shortest, and most important contributor to beta-sheet formation. However, these theories overlook the crucial portion of the peptide, at residues 23-28, containing an ionic interaction inducing a hair pin turn. This potential rate limiting step in the folding of beta-amyloid provides new insight into the pathogenesis of Alzheimer's disease. Cleavage at residues 22 and 35 excludes the effect of "KLVFFA" and limits secondary folding interactions of the N-terminus after 35. Beta-sheet production occurs rapidly, but can be observed by the implementation of UV/Vis spectroscopy focusing on signature the pentamaric binding of multiple secondary beta structures to Congo-Red dye solution confirms the production of beta-sheets. Suppression of fibril formation by the addition of a concentrated orthomolecular compound, such as Echinacea, which is used to fight off various infections, could yield therapeutic techniques or possibly even a cure for Alzheimer's disease.

P1

Developing Ion Parameters Using Shared GPU Accelerator Hardware

John C. Dood and Brent P. Krueger

Hope College

Molecular dynamics (MD) simulations are used to model the structure and movement of macromolecules. The motion of finite particles is modeled by twice numerically integrating the forces on the atoms such as charge-charge interactions, van der Waals interactions using Lennard-Jones (LJ) potentials, Hookian bond length and angle interactions, and sinusoidal bond torsion interactions. Periodic boundary conditions (PBC) are used to approximate an infinite system of particles even though only a finite number are described. In many MD simulations water is simulated using a model with single van der Waals potential and mass. Additional detail is added through mass-less point charges that simulate the electrostatic properties (ESP) of the water molecule. Tip3p is the most popular simple water model. It includes a charge on the oxygen and the two hydrogens to give it a dipole moment. Tip4pew is a popular water model that is similar to TIP3P but instead of having a charge on the oxygen atom it places a charge where the lone pairs would be. Another style includes TIP5P which has a charge for each lone pair, and a charge for each hydrogen atom. Recently, a new water model, OPC, has been developed that uses the same style of charge distribution as TIP4P-Ew and has results that compare better to experiment than the TIP4P-Ew model. For this new water model to be useful, LJ parameters must be developed for at least a few monovalent ions. This study looks into developing these parameters using MD simulations running on a time sharing computer cluster and GPU accelerator hardware. MD simulations running on entry level GPU hardware run around 1.5 times faster than on high end traditional computing hardware. This has allowed us to produce preliminary results that show first peaks of RDFs for a variety of Na^+ and Cl^- LJ parameters within the OPC water model.

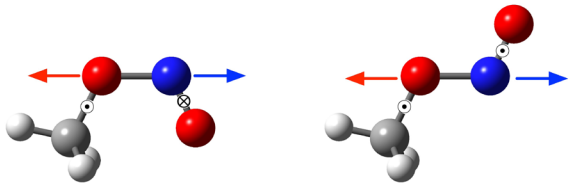
P2

Photodissociation of cis- and trans-CH_3ONO: Is Conformation Destiny?

Jeremy Lantis, Mara Birndorf, Marlon Gonzalez, and Jeffrey Bartz

Kalamazoo College

Methyl nitrite (CH_3ONO) is a molecule that has been studied extensively in chemical dynamics, by both theory and experiment, because of its small size, ease of synthesis, and excited state properties. CH_3ONO has two stable conformations, *cis* and *trans*, shown below. Laser excitation to the S_2 state causes prompt dissociation to methoxy and NO. Our hypothesis was that photodissociation will generate NO with different vector correlations, depending on the conformer excited. At longer wavelengths (280 nm), theory predicts that *trans*-CH_3ONO is excited, but at shorter wavelengths (230 *nm*), *cis*-CH_3ONO is excited. Using polarized lasers and velocity-mapped ion imaging, we determined the bipolar harmonics, including $\beta_0^2(20)$, corresponding to **μ-v** correlation, $\beta_0^2(02)$, corresponding to **μ-J** correlation, and $\beta_0^0(22)$, corresponding to **v-J** correlation in dissociating molecules to test the hypothesis. This contribution will present the results.



cis-CH_3ONO trans-CH_3ONO

P3

Hexagonal BCN Formation: From Ammonia Borane and CO_2 to an Oxygen Reduction Electrocatalyst

Maxwell Li, Ian Pendleton, Paul Zimmerman

University of Michigan

Carbon Dioxide (CO_2) is an abundant atmospheric gas that can function as a sustainable carbon source. Past research has shown that CO_2 can be converted into many useful materials, among which include boron nitrogen codoped graphene oxide (BCN). BCN is interesting because it can serve as an electrocatalyst for the oxygen reduction reaction in fuel cells, which is of high interest in the alternative energy economy[1]. Recent work has shown that BCN may be produced from the reaction of CO_2 and Ammonia-Borane (AB) through a two step process involving pyrolysis[2].

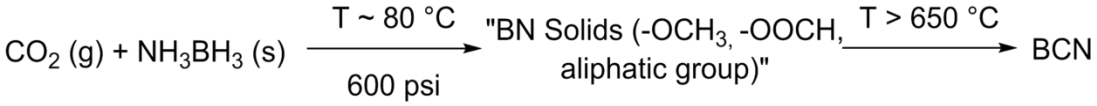


Figure 1: Formation of BCN[2]

However, the precise structure of BCN is difficult to identify and the full reaction mechanism is not clear. A better understanding of how the reaction of CO_2 and AB occurs would potentially reveal a more efficient and selective way to generate BCN, as well as providing more insight into the structure of BCN. This is important because more knowledge about BCN's structure, which is connected to its structure-activity relationships—namely the oxygen reduction reaction—could lead to improving the catalytic properties of BCN itself.

In this study, we focus on the mechanism by which AB and CO_2 react, including the transition states connecting the reactants to various products. Specifically, we detail the production of BCN-like ring structures and report several different pathways leading to six-membered rings. We also observe catalytic action between this BCN precursor and AB, which results in the release of H_2 from AB.

(1) Huang, X.; Qi, X.; Boey, F.; Zhang, H., *Chem. Soc. Rev*. **2012**, *41*, 666-686.
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P4

Rapid, Switchable Self-trapping of Laser Light in a Spiropyran-functionalized Hydrogel

Andy Tran[1,2], Ankita Shastri[2], Derek Morim[1], Fariha Mahmood[1], Joanna Aizenberg[2], Kalaichelvi Saravanamuttu[1*]

[1]McMaster University; [2]Harvard University

A continuous wave, visible laser beam (λ = 532 nm) reversibly self-traps and propagates without diverging in a spiropyran-functionalized hydrogel. Self-trapping was confirmed through changes in the spatial intensity profile of the beam at the exit face of the sample, which revealed a rapid, significant decrease in beam diameter (typically from 115 μm to 20 μm) with a corresponding increase in relative peak intensity (typically from 5% – 350%). Self-trapping originates from changes in refractive index associated with the laser-induced isomerization of spiropyran moieties from an open-chain to closed-ring conformation. When the optical field is removed, the units rapidly revert to their open-chain conformation and the system relaxes to its original state. Exploiting this property, we have demonstrated that self-trapped beams can be switched "on and off" in the medium at time-scales of 30 s over at least 45 trials (these parameters are limited only by our current experimental assembly). To elucidate the molecular-level origins of self-trapping, the effects of pH as well as the nature of the hydrogel backbone were examined in detail. This discovery of rapidly, switchable self-trapped beams in this soft-polymer system opens entirely new routes for designing light-activatable devices, photonics systems and the ability to perform logic operations by controlling the interactions of self-trapped beams.

P5

Action of a Broad Spectrum Antiviral Medication Against Human Herpes: a Quantum Chemical Investigation

Michael Szatkowski, Andrew Perla, Kapil Adhikari, Loredana Valenzano

Michigan Technological University

The *Herpesviridae* family encompasses many different double-stranded DNA viruses, of which only eight affect humans. As the current drugs on the market are only active against a few of the herpes viruses, there is strongly desirable to research, develop, and test a broader spectrum antiviral medication having a higher activity against most or perhaps even all of the strands of herpes capable of infecting humans. In this work, current quantum chemical computational approaches are employed to investigate the mechanism of action of a recently developed antiviral medication (PNU-183792, developed by Pharmacia Corp.) on single DNA bases, single base pairs, and corresponding intercalated configurations. While a previous computational study performed at molecular dynamics and docking levels hypothesized the inhibition mechanism of the drug with respect to the viral DNA polymerase, the knowledge gained from the current investigation performed at higher accuracy computational level will greatly aid in future works devoted to fully describe the mechanism of PNU-like molecules. Such a detailed investigation will allow comparing the proposed mechanisms to those of less efficient species in the attempt of guiding the development and engineering of novel drugs.

P6

Rovibronic Analysis of the A^2E'' State of NO_3 Radical

Henry Tran, Terrance Codd, Dmitry Melnik, Mourad Roudjane, Terry A. Miller.

The Ohio State University

The nitrate radical (NO_3) is a key reactant in atmospheric chemistry leading to the formation of acid rain and the oxidation of organic molecules. Analysis of the electronic spectrum has proved to be remarkably complex due to Jahn-Teller activity in the first (A^2E'') and second excited states. A recent vibronic analysis done by our group has shown moderate Jahn-Teller coupling in the A^2E'' state. Previously, the parallel vibronic bands were satisfactorily fit using an oblate symmetric top Hamiltonian. However, the perpendicular bands show more transitions than the model predicts. In this project, we have developed a modified rovibronic Hamiltonian for the rotational analysis which includes into the oblate symmetric top Hamiltonian spin-orbit, coriolis, spin-rotational, and Jahn-Teller coupling terms and we have added vibronic coupling terms to mix the different vibronic levels of the A^2E'' state. The nuclear spin statistics weights of the ground to first excited state transition ($A^2E''\leftarrow X^2A'_2$ transition) is also included. This Hamiltonian has shown to be capable of continuously transitioning between the limits of a symmetric top (D_{3h}) and an asymmetric top (C_{2v}) and will allow us to determine the molecular geometry of the A^2E'' state of NO_3. Initial analysis conducted on the 2^1_0 and $2^1_0 4^2_0$ vibronic bands has shown improved agreement between the simulation and experiment. The Hamiltonian, simulations, and parameters quantifying the Jahn-Teller distortions will be presented and discussed.

P7

Computational Study of Mechanisms of Fuel Cell Membrane Polymer Degradation

Kimberly D. Utterbeck*, Malcolm N. Spicer, Jonathan. E. Stevens

University of Detroit Mercy

PEMFCs, or Polymer Electrolyte Membrane Fuel Cells, or simply "Fuel Cells", are expected to continue to play a role in the ongoing development of applied alternative energy sources While the fluorinated polymer Nafion [1]is one proposed membrane material, For reasons of cost and environmental impact, nonfluorinated materials have also been proposed for polymer electrolyte membranes. Sulfonated polyether(ether) ketone, or sulfonated PEEK, or sPEEK membranes are one possible candidate for fuel cell membranes; Polyethersulfones (PSUs) can also be used to create proton-exchanging membranes. While studies suggest these materials are *physically* stable, questions remain over the *chemical* stability of such membranes, particularly in the presence of H and OH radicals.

Our group's research implements molecular orbital and density functional calculations to study the attack of OH and of H radicals on sPEEK polymers. Due to the large number of electrons to be modeled in the complete polymer, our group studies the chemistry of small model compounds of sPEEK and PSU used in previous studies [2]. Our density functional calculations show that H and OH radicals readily attach to the aryl rings of sPEEK and PSU polymers and that this addition weakens bonds from the ring to sulfonyl groups and to the backbone of the polymer.

1. Yu, T.H.; Sha, Y.; Liu, W-G.; Merinov, B.V.;Shirvanian, P; Goddard, W.A.; 'Mechanism for Degradation of Nafion in PEM Fuel Cells from Quantum Mechanics Calculations', *J. Am. Chem. Soc*. **2011**, *133*, 19857–19863
2. Panchenko, A.; 'DFT investigation of the polymer electrolyte membrane degradation caused by OH radicals in fuel cells', *Journal of Membrane Science*, **2005**, *278*, 269-278

P8

Effect of Basis Sets on Absorbance Spectra

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The ability to accurately and efficiently model realistic absorbance spectra remains a difficult task with today's theoretical models. In order to explore the extent of the accuracy and predictive qualities of today's theoretical models, Time-Dependent Density Functional Theory (TD-DFT) was used to explore the effect of basis set size on the accuracy of the calculated absorbance spectra. The effects of the Linear Response (LR) Random Phase Approximation (RPA) Pople and Dunning Basis sets 6-31G, 6-31G**, 6-311G**, 6-311G++, cc-pVTZ, cc-PVDZ, aug-cc-pVTZ, aug-cc-pVDZ, and aug-cc-pVQZ were explored and the LR Tamm-Dancoff Approximation (TDA) basis sets aug-cc-pVDZ, aug-cc-PVTZ, aug-cc-PVQZ, and 6-31G+ were also partially explored. On average, the error of all basis sets was acceptable and remained between 1% and 13%. The LR RPA basis sets explored had a general trend of aug-cc-pVTZ > 6-311G++ > aug-cc-pVDZ > cc-pVTZ > 6-311G** > cc-pVDZ > 6-31G** > 6-31G in order of decreasing agreement with experimental results.

B1

Can Tea Prevent Alzheimer diseases?

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After some researches we have found that beta peptide intermediate contains higher neurotoxicity than plaques, Alzheimer can be prevented or slowed if misfolding of the fibrils can be prevented also. After this research, the solubility of Echinacea was increased by defeating it when extracting the seeds with a solxlet. According to studies Echinacea has a great potential to treat Alzheimer's disease. The main purpose of this study is to find the possible effects that this compound has on the formation of fibrils in the brain of Alzheimer's patients, and find out if this compound can slowdown or stop the fibrils all together.

B2

Environmental Effects on Bacterial Growths

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Calumet College of St. Josephs

No abstract submitted.

B3

Enzymatic activity of Prolyl Oligopeptidases from *Spirosoma linquale* in Acidic Environments

Andrew Baker, Christopher Hamilton

Hillsdale College

Celiac Disease is an autoimmune disorder that is caused by the introduction of gliadin (a component of gluten) into the digestive system, it can result in damage to the villi of the small intestine if gluten is not eliminated from the diet. Certainly, the "gluten-free" food market provides some relief, but there is no present cure for the disease. Considering this disorder currently affects about 1 out of every 133 people, a therapeutic treatment is long overdue. The human digestive system does not contain any proline specific proteases (prolyl oligopeptidases) that are able cleave a proline-rich protein like gliadin. One current approach to therapy is an attempt to provide a supplemental enzyme. The proposed enzyme must maintain activity in the acidic environment of the stomach, and the overall focus of this research is to find enzymes that may work in these conditions. Previous work in our lab has shown that a prolyl oligopeptidase from the bacteria *Spirosoma linquale* is a promising enzyme, this research focused on testing the activity of the enzyme from this organism, as well as several variants containing mutations over a pH range. The activity was measured using a model substrate (H-Ala-Phe-Pro-pNA) and cleavage was observed by measuring the appearance of the pNA product on a UV-Vis spectrophotometer at a range of substrate concentrations. Several of the altered enzymes tested several had significant levels of activity between pH 5 – 8. Future work will focus on alterations to increase activity at lower pH.

B4

Glucose Oxidase as an Oxygen Scrubber

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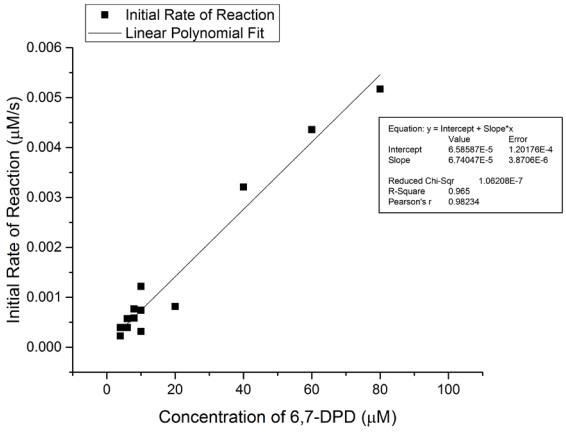
Glucose oxidase catalyses the oxidation of glucose by oxygen to yield gluconolactone and hydrogen peroxide via a ping-pong bi-bi mechanism. Glucose oxidase was shown to remove trace oxygen from solutions in experiments where rigorous anaerobic conditions are required. The glucose/glucose oxidase pair was used to exclude oxygen from solutions containing partially reduced enzymes that would be oxidized by the oxygen. However, in the absence of oxygen, glucose oxidase can begin to reduce other electron acceptors, such as (6,7-Dihydrodipyrido[1,2-a:2′,1′-c]pyrazinediium dibromide (6,7-DPD), which were used as a marker for when oxygen was thoroughly scrubbed from solution. Using steady-state kinetics and pseudo-first-order conditions, the cumulative results (Figure) show that the initial rate of reaction increased linearly as concentration of 6,7-DPD increased, showing that an increase in substrate led to a first-order increase in the rate of substrate disappearance. It can be concluded from kinetic data that the rate of 6,7-DPD reduction was a significantly slower process than the rate of oxygen reduction to hydrogen peroxide. An induction period of ~430 seconds, that persisted until the concentration of oxygen diminished significantly, was shown to be independent of the concentration of 6,7-DPD. Over extended time periods glucose oxidase catalyzed reduction of 6,7-DPD by glucose proceeded via two distinct exponential phases, showing that the rate-determining step changed over time. One proposed explanation is that as the product lactone accumulates it inhibits Gox due to tight binding at the active site (product inhibition).



B5

Using the Aromatic, Pungent, and Spicy Ginger as an Alzheimer's Preventative

Brittany Bowers, Nicole Gill, Jennifer Salczynski, Martin Chavez, Patricia Tuxford, Baula Nieto, Dr. Sandra Peszek

Calumet College of Saint Joseph

Alzheimer's Disease (AD) is a form of dementia that gradually gets worse over time. Alzheimer's Disease (AD) affects behaviour, thinking, and memory. Two abnormal structures called plaques and tangles are prime suspects in damaging and killing nerve cells in the brain. Plaques are a deposit of a protein fragment called beta amyloid. The beta amyloid builds up in the spaces between nerve cells. Another protein called Tau, twisted fibers which build up inside the cells, these proteins are the tangles that affect the brain. There are multiple experiments and trials to help prevent Alzheimer's Disease (AD) such as ginger. Ginger (Zingiber offinale) is a herbaceous plant found in southeast Asia. Ginger is a hot fragment spice made from the rhizome of a plant, ginger also resembles bamboo in appearance. Ginger has multiple uses for health and cooking. Ginger smooths pain, menstrual cramps, headaches, and inflammation. It also prevents nausea, cold, and flu. Ginger is also a great way to boost your immune system. Using ginger as a therapeutic way to prevent the progression of Alzheimer's Disease (AD). Using Ultraviolet Visible Spectroscopy, UV-Vis, results will be developed to identify and rank whether or not the mixture of flavonolignane diastereomers could inhibit aggregation on AB. To carry out this test, AB will be incubated with the test compound of ginger at a controlled temperature for a set amount of time, followed by ultrafiltration in order to separate the monomeric AB from its aggregates. Aliquots of the ultrafiltrate will be analysed for monomeric AB.

B6

Conantokin-G Attenuates Detrimental Effects of NMDAR Hyperactivity in an Ischemic Rat Model of Stroke

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Ischemic stroke is a global health problem and is a major cause of death and disability in developed countries. Excess glutamate release from ischemia leads to hyperactivation of the N-methyl-D-aspartate receptor (NMDAR), which is expressed throughout the central nervous system. Specifically, the GluN2B subunits of the active NMDAR channel are hyperactivated during the insult. Conantokin-G (con-G), a peptide with antagonistic properties towards the NMDAR and selectivity for the GluN2B subunit, was utilized in this study. The stroke model employed was the Middle Cerebral Artery Occlusion (MCAO), since >80% of stroke cases in humans are ischemic. Stroked rats were divided into two groups; one set of rats were left untreated, and the other set were intrathecally injected with 2 μM con-G. The rats were sacrificed after 4 or 26 hours of stroke induction. Then, their brains were harvested, sectioned, and stained with Tetrazolium chloride (TTC) and imaged to assess edema and infarct size. Con-G treated rats displayed improved neurological deficits compared to non-treated rats. Various histological analyses were performed to evaluate the therapeutic effect of con-G, such as hematoxylin and eosin, FluoroJade B, Von-Kossa, and Periodic acid-Schiff staining. Tissues treated with con-G showed a significant decrease in the number of degenerated neurons, calcium deposits, and cytoarchitecture damage in the peri-infarct region. Additionally, recovery of peri-infarct Microtubule Associated Protein (MAP2) staining and neuronal cytoarchitecture was observed in con-G treated rat brains at both timepoints. Con-G restored localization of GluN1 and GluN2B subunits, but not that of GluN2A, in the neuronal soma in the peri-infarct region at 4 hr and 24 hr. This suggests that molecular targeting of the GluN2B subunit has potential for reducing detrimental consequences of ischemia. Further studies will be performed to acquire data for post-ischemic redistribution of the GluN subunits at the synaptic level using immunoelectron microscopy. The purpose of this research is to utilize this data to develop safe and effective therapeutic agents that can specifically antagonize the NMDARs for treatment of ischemic stroke.

B7

The Activation of Biological Functions in Proteins by Gas Sensing Molecules

Jessica Lyza and Rachael DeVries

Valparaiso University

Heme proteins are a class of biological molecules that serve important roles throughout all forms of life. The protein studied in this research, CooA, is found in several bacteria such as *Rhodospirillum rubrum* (*Rr*) and *Carboxydothermus hydrogenoformans* (*Ch*). In nature, all forms of CooA sense a specific gas molecule, carbon monoxide, that allows the heme protein to bind DNA which activates the transcription process. Interestingly however, in the lab nitric oxide has also been found to activate DNA binding in *Ch* CooA, but it does not activate *Rr* CooA. It is hypothesized that a specific intermolecular interaction between amino acids within the heme environment is responsible for the different behavior of *Ch* CooA and *Rr* CooA. To test this hypothesis, the key amino acids that are proposed to be responsible for this interaction were mutated in both CooA proteins. Next, these variant CooA proteins will be reacted with carbon monoxide and nitric oxide, and the subsequent effects on DNA binding will be measured.

B8

Bacteria Growth and Change in Different Environments

Ramiro Rojas, Alfonso Hernandez, Jennifer Diaz, Jessica Martineza and Dr. Ahmed Lakhani

Calumet College of St. Joseph

Bacteria are part of a large genome of microorganisms found almost everywhere around the world. Some bacteria are harmful, while many can be extremely useful for human survival. Nonetheless, all bacteria need sufficient nutrients to grow, and depending on their environment this factor can change very much. Through the use of microscopes one can identify certain structures of bacteria and gain a broad understanding on how they function and grow. The bacteria that was being analyzed for the following experiment was gram negative and this allowed for consistent observations of cell wall structure. Can bacteria grow in a negative control has been the main topic of study in the experiment. Then once the bacteria grows in a controlled environment can bacteria continue to sustain growth if the environment is altered with a negative control. These manipulated situations have become the independent variables of choice and have created essentially a biological experiment, while continuing research in the biochemical aspect of bacteria growth and structure manipulated through environmental change.

B9

Substrate Recognition by the $tRNA^{His}$-guanylyltransferase: A Kinetic Investigation with Model RNA Substrates

Duff, Lauren

The Ohio State University

All tRNAs undergo post-transcriptional modifications before being aminoacylated with their specific amino acid. In the case of $tRNA^{His}$, this modification includes the addition of a required guanosine at the –1 position (G-1) in order for histidyl-tRNA synthetase (HisRS) to recognize the tRNA and charge it with histidine. The $tRNA^{His}$ guanylyltransferase (Thg1) enzyme, with family members found in all domains of life, completes this reaction via its novel ability to add nucleotides in the 3′ to 5′ direction in a reaction that is chemically similar to that of canonical 5′ to 3′ polymerases. Eukaryotic Thg1 enzymes selectively recognize $tRNA^{His}$ for modification with G-1, however the molecular basis for this observed substrate selectivity is not completely understood. Therefore, the long-term goal of this project is to elucidate the molecular features that participate in recognition of tRNA substrates by Thg1.

Insight into tRNA recognition by HisRS has been achieved by using small RNA stem-loop substrates and a similar approach is applied here to probe tRNA recognition by Thg1. The first substrate (micro-His) mimics the 7 base pair acceptor stem of $tRNA^{His}$, and the second substrate (mini-His) mimics the acceptor stem and 5 base pair T stem, which coaxially stack in full-length tRNA. The three Thg1 enzymes being tested for activity with these model RNAs are from *Methanobrevibacter smithii*, an archaeal species, *Bacillus thuringiensis*, a bacterial species, and *Saccharomyces cerevisiae*, an eukaryote. Here we report the results of the kinetic assays with each of these purified enzymes and 5′-triphosphorylated substrates, all of which analyze using previously described single-turnover assays and evaluate 3′-5′ addition. The data from these assays will be used to evaluate the dependence of diverse Thg1 family enzymes on the length of the model RNA stem and the potential for forming Watson-Crick vs. non-Watson-Crick base pairs during the 3′-5′ addition reaction.

B10

The Effects of pH on Bacterial Growth

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Calumet College of St. Joseph

No abstract submitted.

Different species of bacteria grow within certain pH ranges, most falling within the neutral range. Most bacteria cannot live outside of their normal pH range and will die off, while others halophiles can adapt to the new environment. This phenomenon can be observed by plating the cell cultures and then subjecting the established colonies to different pH conditions by placing filter paper saturated with different pH solutions on the established growths. The death of the bacteria outside of their normal pH range results in a “ring of death” in the area surrounding where the environmental change occurred, whereas bacteria that can adapt will survive and show no die-off. Bacteria that can adapt to the new environment may have undergone physical or chemical changes. in order to survive, Gram staining can be used to differentiate between cell wall components. The thickness of the peptidoglycan layer that is present within the cell wall determines whether or not that cell is gram positive or gram negative. If the layer is thick the cell will be gram positive due to the crystal violet dye bonding with the peptidoglycan and persisting through the alcohol decolorization step. If this layer is thin the crystal violet dye will be able to bond due to the lack of peptidoglycan present and will instead be washed away during decolorization and replaced with safranin counterstain.

B11

A Chemical Reporter for Extracellular Mycolylation in Mycobacteria

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Central Michigan University

Mycobacterium tuberculosis (*Mtb*), the causative agent of tuberculosis, currently infects 2 billion people worldwide and kills 2 million people per year. The complex cell wall of *Mtb* presents a formidable barrier to antibiotics and harbours various components that are involved in pathogenesis, prompting the development of new tools to better understand and therapeutically target this essential structure. In particular, the unique mycobacterial outer membrane, or "mycomembrane," appears to be a valuable target for drug development, but many aspects of its biosynthesis, structure, and dynamics are still not well understood. Here, we present the development of a chemical reporter strategy for investigating biosynthesis of the mycomembrane in live mycobacterial cells.

B12

SCH66712 and EMTPP are the First Mechanism Based Inactivators of Both Human CYP2D6 and CYP3A4

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Kalamazoo College

Cytochrome P450s (CYPs) are heme-containing enzymes that metabolize small organic molecules including drugs. CYP3A4 and CYP2D6 are responsible for more than 70% of pharmaceutical drug metabolism and inactivation of these enzymes can lead to drug-drug interactions. The substituted imidazole compounds, 5-fluoro-2-[4-[(2-phenyl-1H-imidazol-5-yl)methyl]-1-piperazinyl]pyrimidine (SCH66712) and 1-[(2-ethyl-4-methyl-1H-imidazol-5-yl)methyl]-4-[4-(trifluoromethyl)-2-pyridinyl]piperazine (EMTPP), have been previously identified as mechanism-based inactivators (MBIs) of CYP2D6. The current study shows SCH66712 and EMTPP are also MBIs of CYP3A4. The partition ratios for SCH66712 and EMTPP were 11 and 94, respectively. The rates of inactivation, k_{inact}, and inhibition constant, K_i, were 0.21 min^{-1} and 1.6 μM for SCH66712, and 0.046 min^{-1} and 11.7 μM for EMTPP, respectively. Whole protein MS analysis was consistent with a binding stoichiometry of 1:1 for both MBIs on CYP3A4 apoprotein. MS analysis of digested peptides of inactivated enzymes was not able to show the site of protein adduction due to low sequence coverage (~65%). Studies of SCH66712 and EMTPP metabolites formed by CYP3A4 showed four mono-oxygenated SCH66712 metabolites and eight mono-oxygenated EMTPP metabolites. Further analysis with MS^n coupled with $TiCl_3$ treatments suggested that one mono-oxygenated product of SCH66712 and one of EMTPP were the result of *N*-hydroxylation. Additionally, inactivation mechanisms of enzymes by possible electrophiles of SCH66712 and EMTPP are proposed. SCH66712 and EMTPP are the first MBIs to be shown to be potent inactivators of both CYP2D6 and CYP3A4.

B13

Going Green for Alzheimer's

Jacob Glass, Tony Rubino, Timothy Victory, Alyssa Bogolin, Mariana Portela, Dr. Peszek

Calumet College of St. Joseph

It is commonly known that there have been large amounts of amyloid beta plaques inside of brains that are currently affected with Alzheimer's disease. This has a higher neurotoxicity than plaque does, and if this can be prevented by our plant, then Alzheimer's can be prevented as well.

B14

Acute and Chronic Effects of Somatostatin on Fast and Slow Calcium Oscillations in the Pancreatic β-Cell

Katherine Harms[1], Benjamin Thompson[2], Eric Glynn[2], Leslie Satin[2]

[1]Adrian College, [2]University of Michigan

It is known that insulin secretion oscillates in the presence of glucose. There have been two types of calcium oscillations observed: fast and slow. It is known that somatostatin (SST) inhibits insulin secretion but we found that it had differential effects on fast vs. slow oscillations. We hypothesized that chronic SST would increase the glucose sensitivity of islets by inhibiting insulin release overnight and thus cause the internalization of K_{ATP} channels from the plasma membrane of the beta cell. To test this, calcium imaging was used to compare the effects of SST treated vs. untreated cells while varying acute concentrations of glucose. When islets were acutely exposed to SST, it was found that slow oscillations and fast oscillations were differently effected. These results indicate that the mechanism of the fast and the slow oscillations is different. Understanding pancreatic oscillations is critical because patients with type 2 diabetes show irregular Ca and insulin oscillations.

B15

Using the ykkCD Riboswitch as a Caging Compound for Targeted Drug Delivery

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Ball State University

Riboswitches are aptamers of RNA that are folded in a specific shape and undergo changes when exposed to a specific molecule and regulate expression of the downstream gene. The ykkCD riboswitch in the presence of tetracycline allows the downstream translation of a multidrug efflux pump in *Bacillus subtillis*. Our goal is to use this riboswitch as a transport mechanism for targeted drug delivery. We present fluorescent binding assays and thermal melting studies to show that the ykkCD riboswitch is stable under a variety of conditions expected to be encountered in mammalian cells.

B16

Identifying Protein-Protein Interactions at the DNA Promoter Using Photoactivatable Amino Acids

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University of Michigan

Misregulated transcription results in a multitude of disease states, including diabetes and many forms of cancer. The development of novel therapies for these diseases thus requires a detailed understanding of the mechanisms of eukaryotic transcription. However, efforts toward this goal have been hampered by limitations with the tools that are currently available to study the moderate affinity and transient protein-protein interactions (PPIs) that comprise transcription initiation. Recently, the genetic incorporation of photoactivatable amino acids into transcriptional activators has proven a powerful tool in covalently capturing transcriptional PPIs *in vivo*. Furthermore, when combined with formaldehyde cross-linking (termed tandem reversible irreversible cross-linking (TRIC)), this novel technique enabled the identification of directly interacting PPIs at a specific promoter. Herein, we describe the use of TRIC to identify direct partners of the transcriptional activators VP16 and Gal4 at the *GAL1* promoter in live *Saccharomyces cerevisiae*. We have identified TATA-binding protein (TBP), an integral component of the RNA Polymerase II preinitiation complex, as a direct binding partner of both VP16 and Gal4 at this promoter. Furthermore, we have investigated the role of the histone acetyl-transferase complex, SAGA, in the recruitment of TBP to the *GAL1* promoter. This work provides invaluable insight into the recruitment model of the eukaryotic transcriptional machinery and so unlocks new potential sites for therapeutic intervention in transcription originating diseases.

B17

Isothermal Titration Calorimetric Study of Mpp10 and Imp3 Interaction

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DePaul University

Eukaryotic ribosome biogenesis (eRB) is a process in the cell that regulates cell growth. It is hypothesized that dysfunction in this system leads to diseases like cancer, and the growth of tumors. The heterotrimeric complex of Mpp10 binding with Imp3 and Imp4 independently is known to be essential for eRB to function properly, thus information of the protein-protein interactions and the ideal conditions is critical in understanding this system. The thermodynamic binding parameters were determined using the isothermal titration calorimetry in a buffer mixture, injecting Mpp10 into the sample cell containing Imp3. It was determined through the analysis of binding at 15 °C, 25 °C, and 37 °C, that the interaction is exothermic, enthalpically driven, and had the greatest binding affinity at 15°C, with a molar ratio of 1:1. However, supplemental experiments need to be completed in order to verify the results, and demonstrate that the data is reproducible.

B18

Exploring the Role of xCT in Neuroregeneration through Laser Ablation of Zebrafish Neurons

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[1]Hope College, [2]Whitworth University

System x_c^- is a heterodimeric amino acid transporter comprised of a light chain unit, xCT, which confers the transport specificity, and a heavy chain unit, 4F2HC. System x_c^- has been shown to facilitate the exchange of intracellular glutamate for extracellular cystine. Within the cell, cystine is rapidly reduced to cysteine, the rate limiting reagent for glutathione (GSH) production. GSH is an endogenous reducing reagent that is important in mitigating the oxidative stress that can develop within cells which, untreated, can trigger cell death. It has been shown that system x_c^- is strongly expressed in the central nervous system, particularly in activated neuroprotective cells such as astrocytes and glia. It is believed that relief of oxidative stress in the environment of neurons and their protective counterparts is critical in processes such as neuroregeneration, an ability unique to teleost fish, including zebrafish. Using this information, the thrust of the current study is to identify the role that xCT plays in neuroregeneration *in vivo*. To initiate neuroregeneration, we will use a femtosecond laser to perform ablation on zebrafish neurons. Confocal microscopy will be used to observe the trafficking of an xCT:GFP fusion protein during the neuroregeneration process.

B19

Cardiac Contractility: The Discovery of Unique and Novel Molecular Switches in Myosuppressin Signaling

Megan Leander and Ruthann Nichols

University of Michigan

Ligand-receptor interactions are critical in a mechanism underlying receptor activation and peptidergic control of physiology. Myosuppressin decreases cardiac contractility; thus its signaling pathway is a target to influence physiology. To investigate the mechanisms involved in cardiac contractility, the interactions between *Drosophila melanogaster* myosuppressin (DrmMS; TDVDHVFLRF-NH_2) and its receptors, DrmMS-R1 and -R2 (DrmMS-Rs), were predicted through docking. Our hypothesis was MS ligand-receptor contact sites are consistent with structure-activity relationship data. Further, we predicted that contact sites of inactive DrmMS analogs, which may act as antagonists, would differ from DrmMS and agonists.

To determine if mechanisms involved in the activation of the DrmMS signaling pathway were applicable to other species, the MS receptor (MS-R) of the disease vector *Rhodnius prolixus* was identified and modeled; it shared high sequence identity to DrmMS-Rs. *R. prolixus* myosuppressin (RhpMS; pQDIDHVFMRF-NH2) was docked to RhpMS-R to identify receptor contacts. Docking of N-terminal RhpMS truncations led to the predictions of an active core and antagonist which were confirmed in a heart rate assay.

Finally, examination of MS-Rs for molecular switches common to family A rhodopsin-like receptors identified a unique ionic lock and a novel 3-6 lock stabilizing the inactive state of the receptor. Our results proved the hypotheses and set the basis for a project to design mimetics targeting switches and receptor contacts involved in activation.

B20

Kinetic Characterization of Mutant Beta-Glycosidase from *Sulfolobus Solfataricus* Chemically Rescued by Indol

Jacob Hare, Matthew Mousseau, Elizabeth Utke and Dr. Kim Colvert

Ferris State University

The β-glycosidase from the thermophilic bacterium *Sulfolobus solfataricus* has been engineered to exhibit ligand-dependent activity by replacing a buried tryptophan residue with a glycine, resulting in a loss of structural integrity in the active site and an inactive enzyme. The enzyme has been shown to be “rescued” by the inclusion of indole. In this work we examine the effect of temperature on the rescued activity and compare the results to the native enzyme. The rescued activity is not as resistant to temperature effects as the native, suggesting the mutant was more susceptible to denaturation without the indole structure of tryptophan. The Arrhenius plot for the mutant was not as distinctly biphasic as that of the native enzyme possibly due to the loss of a thermal conformation transition.

B21

Effect of Acid Sphingomyelinase on Membrane Fluidity in Circulating Angiogenic Cells: Implications for Diabetic Retinopathy

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Diabetic hyperglycemia and dyslipidemia affect the retinal blood vessels in diabetic patients, causing 65% of patients to develop diabetic retinopathy. The diabetic metabolic insult leading to retinal vascular degeneration is proposed to involve retinal endothelial cell damage, that is then inadequately repaired due to compromised availability and functionality of circulating angiogenic cells (CACs). CACs become "trapped" in the diabetic bone marrow due to reduced deformability and are unable to migrate to, extravasate and home to the retinal sight of injury. The central hypothesis of this work is that migration, extravasation and homing depend on high membrane fluidity in CACs.

Acid sphingomyelinase (ASM) is an enzyme responsible for the conversion of sphingomyelin to ceramide and is upregulated in diabetic patients. We propose that an increased level of ASM in diabetic patients increases ceramide levels, thus decreasing fluidity in the cell membrane, which in turn leads to reduced deformability of diabetic CACs. To measure the effect of ASM on membrane fluidity, CACs from ASM–/–, wild type (WT), and diabetic mice were examined. A novel approach for measuring membrane fluidity was developed by utilizing time-resolved fluorescence decay measurements of the chromophore, perylene in live cells. Fluidity is related to the measured viscosity, or resistance to flow. A higher viscosity value indicates a less fluid membrane. ASM WT mice displayed a statistically significant decrease in membrane fluidity compared to the ASM–/– ($p < 0.05$) and diabetic mice had a significantly less fluid membrane than WT mice ($p < 0.05$). This provides support for the hypothesis that upregulation of ASM in diabetic cells could contribute to the deformability seen in diabetic CACs and provide potential areas of focus for diabetes retinopathy research. Future work will focus on measuring membrane fluidity in healthy and diabetic human CACs.

B22

Analyzing Kumamolisin-As as a Therapeutic Enzyme for Celiac Disease

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Celiac Disease is a genetic disorder characterized by an immune response to undigested gluten proteins that results in the destruction of intestinal villi. Many have turned to enzyme therapy in the hopes of finding one capable of breaking down the proline-rich (and therefore degradation-resistant) gluten molecules either in the stomach or the small intestine. Kumamolisin-As, a serine protease with a modified catalytic triad, and an engineered form of the enzyme, KumaMax, were tested for their peptidase activity in conditions mirroring those of the stomach. Spectrophotometric kinetic assays showed that the enzymes had no activity on small p-nitroaniline linked di- and tri-peptides. LC-MS showed that KumaWT had no activity and KumaMax had very minimal activity on gliadorphin, a 7-mer of α–gliadin. However, an ELISA showed that both KumaWT and KumaMax are capable of breaking down gluten. We therefore conclude that KumaWT and KumaMax are specific for proteins larger than 7 residues, and must be mutated to work on smaller peptides before they can be used as enzyme therapeutics for people with Celiac Disease.

B23

Domain Structure of Bacterial Red Light Photoreceptors as Revealed by Atomic Force Microscopy

Rima Rebiai,[1] Zain Malik,[1] Marie E. Kroeger,[2] Emina A. Stojković,[2] Stefan Tsonchev,[1] and Kenneth T. Nicholson[1]

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Atomic Force Microscopy (AFM) has been used to analyze a wide variety of samples to provide insights into material functionality at the nanoscale. This technique uses a mechanical probe to magnify surface features in order to produce three-dimensional images of samples at high resolution. In this particular study, AFM has been employed to characterize the structure of intact bacteriophytochromes (BphPs) in biologically relevant media. BphPs are red light photoreceptors found in both photosynthetic and non-photosynthetic bacteria. These photoreceptors are responsible for perceiving light and initiating an important physiological response to optimize growth and development. Structural characterization of these proteins may also play an essential role in the engineering of infrared fluorescent tissue markers. Intact BphPs are very challenging to crystallize, especially in the light-adapted state for X-ray crystallography and are too large for analysis by nuclear magnetic resonance. Using AFM, we have collected images of intact BphPs found in non-photosynthetic *Stigmatella aurantiaca* (SaBphP2) and photosynthetic *Rhodopseudomonas palustris* (RpBphP3) in their respective light-adapted states. Both P2 and P3 contain a light sensing module, which has a covalently bound biliverdin chromophore, a chemical moiety that is responsible for absorbing light. For both photoreceptors, global conformational changes are anticipated to occur upon light exposure. As a result, multiple orientations of P2 and P3 have been observed on mica and compared to models of intact BphPs generated using PyMOL software and X-ray crystallographic structures of related BphPs in the dark-adapted states. The cross-sectional analysis and total volume measurements of the proteins are in close agreement with the models. Our future goals include characterization of intact BphPs in their dark-adapted states and visualizing dynamics of receptor–ligand interactions in live bacterial cells using AFM.

B24

Uptake of Fluorinated Trehalose in *Mycobacterium smegmatis*

Zachary Wagar, Benjamin M. Swarts

Central Michigan University

Mycobacteria, in particular the tuberculosis-causing pathogen *Mycobacterium tuberculosis*, continue to have a dire impact on human life around the world, infecting 2 billion people and killing 1.5 million per year. Mycobacteria possess a protein complex called SugABC-LpqY that imports the non-mammalian sugar trehalose. In the present study, we asked whether the SugABC-LpqY pathway could be exploited to transport synthetic trehalose analogs, specifically fluorinated trehalose (FluoroTre) analogs, into the cell. To address this question, we evaluated SugABC-LpqY-dependent uptake of four regioisomeric FluoroTre analogs in M. smegmatis wild type, a mutant lacking a functional SugABC-LpqY transporter (ΔsugC), and its complement (ΔsugC::sugC). Using GC-MS analysis of derivativitized cellular extracts from these experiments, it was found that all four FluoroTre analogs were taken up into *M. smegmatis* in a SugABC-LpqY-dependent manner. This study, in combination with the absence of trehalose in humans, suggests that radioactive ^{18}F-modified trehalose analogs could potentially be used as positron emission tomography (PET) imaging agents to specifically and non-invasively visualize tuberculosis infection within the human host.

B25

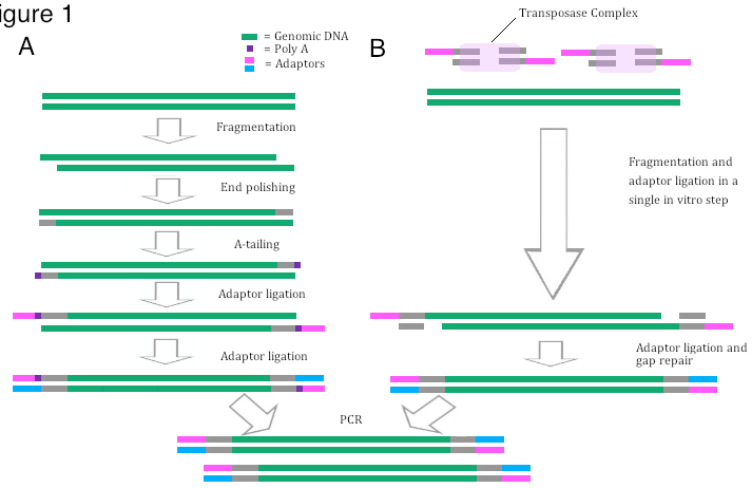
Low Input 5-Hydroxymethylcytosine Mapping Using Transposase.

Payton Weidenbacher, Xingyu Lu, Dali Han, Boxuan Simon Zhao, Chuan He,

The University of Chicago

Cytosine methylation and further oxidative modifications resulting from TET family proteins may explain an active demethylation pathway or regulatory elements within the genome. To understand the methylation and hydroxymethylation patterns in the genome mapping of these modified bases is becoming increasingly important. The opportunities to better understand DNA modifications hinge on our ability to locate cytosine modifications in low input systems, allowing for an understanding in an idealized single cell limit. The conventional method of shotgun library construction (Figure 1A) is usually done purely in vitro and requires an immense amount of purification steps. Transposase mediated integration of sequencing adaptors (Figure 1B) has been shown to reduce the amount of required DNA through reduction of steps and greater efficiency. This integration can be followed by a bisulfite reaction. The assimilation into this conventional laboratory method suggested that a similar integration of transposons could replace the library preparation steps in 5-hydroxymethylcytosine (5hmC) profiling and mapping techniques. Detection of 5hmC on low input samples has proven difficult due to the amount of DNA required to examine methylation and hydoxymethylation patterns. The 5hmC profiling method (hmC-Seal), developed by our group enriches strands of DNA containing 5hmC via a selective chemical labelling and pull down of 5hmC. The 5hmC mapping technique — a modified bisulfite technique — (Tab-Seq), also developed by our group, allows realization of the whole genome single-base detection of 5hmC. By coupling these reactions with transposase mediated library preparation one was able to reduce the DNA required and allowed for examination of hydroxymethylation patterns in less prevalent samples.

Figure 1



B26

Role of Putrescine Oxidase His 432 in Substrate Interaction

Lukas Woodcock and Dr. Kim Colvert

Ferris State University

The active site of the enzyme putrescine oxidase positions the putrescine amine group close to the FAD prosthetic group. Modeling shows that a histidine residue is close to the amine but is proposed to aid in stabilizing the substrate rather than participating in catalysis. Two mutants were modelled and prepared by site-directed mutagenesis where this histidine is replaced by alanine or by glutamic acid (H432A and H432E). The kinetics of overexpressed proteins were determined. The catalytic efficiencies for both mutants were lower than for wild type as would be expected. The K_M for H432A was higher and for H432E lower than the wild type K_M suggesting that putrescine binds less effectively when the smaller alanine is present and that the negative charge of the glutamic acid binds the positive amine of putrescine more tightly.

B27

Discovery of Lead-like Inhibitors of OXA-1 β-lactamase

Leslie A. Wyman, Josh M. Mitchell, and Rachel A. Powers

Grand Valley State University

β-lactams, like penicillin, are the most clinically prescribed antibiotics. However, due to their overuse, resistance has developed.β-lactamase enzymes are the most common resistance mechanism used by bacteria to combat the effects of these drugs. These enzymes efficiently hydrolyze the β-lactam ring that defines this class of antibiotics. In response, β-lactamase inhibitors were created to disrupt this type of bacterial resistance. Alone, β-lactamase inhibitors have minimal antibiotic activity, but when given in combination with a partner β-lactam, they enable the antibiotic to work by inhibiting the β-lactamase enzymes produced by resistant bacteria. Unfortunately, the structures of the inhibitors also contain a β-lactam ring. The chemical similarity has allowed for resistance to develop against the inhibitors as well. Additionally, these compounds do not inhibit members of the class D β-lactamases. Therefore, there is an urgent need for the discovery of novel β-lactamase inhibitors that do not resemble β-lactams. A structure-based approach was used to discover possibilities for potential novel β-lactamase inhibitors of the class D β-lactamase OXA-1, a key clinical resistance target. The program DOCK was used to screen the ZINC database of commercially available compounds. So far, twenty-one compounds from the lead-like subset have been ordered and tested experimentally for inhibition of OXA-1. Of the compounds tested, seven inhibited OXA-1 with K_i values < 1 *mM*. Further work is currently underway to obtain X-ray crystal structures of OXA-1 in complexes with these novel DOCK-predicted inhibitors to aid in optimization efforts.

B28

Environmental Effects on Microbiological Growth

Tiffany Yorek, Kristen Ashby, Julyssa Saez, Alyssa White, Dr. Ahmed Lakhani

Calumet College of St. Joseph

No abstract submitted.

B29

Effect of Antagonists on the Heteromerization of the NMDA Receptor Ligand Binding Domains

Ning Zhou, John Cheriyan, and Francis. J. Castellino

University of Notre Dame

The N-methyl-D-aspartate receptor (NMDAR) is a glutamate- and voltage-gated cation channel expressed throughout the central nervous system. NMDAR exists prevalently as a hetero- tetramer composed of two glycine binding GluN1 subunits and two glutamate binding GluN2 subunits. NMDAR plays a crucial role in neuroplasticity, learning, and memory. Although structure based understanding of ligand binding to GluN1 and GluN2A has been reported, their inter-subunit associations and the role of ligands in modulating the functional behavior of these domains needs better understanding. Here we studied the interaction between the ligand binding domains (LBDs) of GluN1 and GluN2A subunits and how they are affected by two potent antagonists of NMDAR namely, DCKA and AP-5. We expressed the LBDs in Drosophila S2 cell expression system and purified them to homogeneity for our studies. Using analytical ultracentrifugation, we show that DCKA negatively affected the heteromer formation of GluN1 and GluN2A while AP-5 did not. We are also exploring how NMDAR specific peptide antagonists affect the heterodimerization potential. Our findings provide new detail to the mechanism of action of the NMDAR antagonists with respect to hetero-oligomerization of the receptor domains. Our studies on the inter-subunit associations and the role of antagonists in modulating the functional behavior of NMDAR will ultimately help towards devising methods to counter its dysregulation in several neuropathies like stroke and epilepsy.

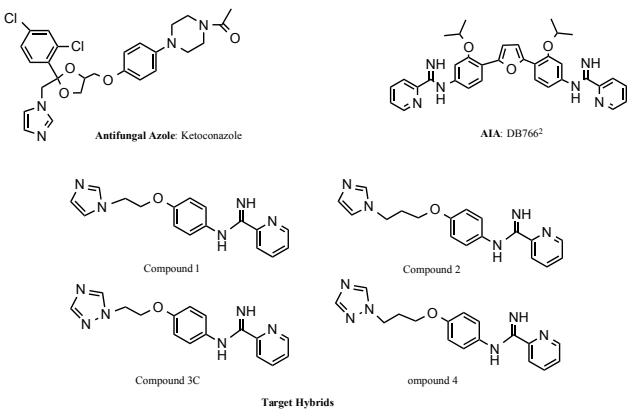
B30

Synthesis and Testing of Novel Compounds to Fight the Parasitic Disease Leishmaniasis

Emilia Zywot[a], Abdelbasset Farahat[b], David Boykin[b], Karl Werbovetz[a]

[a]Ohio State University; [b]Georgia State University

Leishmania parasites cause up to one million cases of leishmaniasis annually, which appears in two forms. The visceral form lowers the immune system and often leads to fatality, while the cutaneous form causes sores along the body. The fact that the disease is widely spread in developing parts of the world exacerbates issues with ineffective treatment. Since the current drugs suffer from several weaknesses in treating leishmanaisis in an efficient and effective manner, research to find new drugs is necessary. The compound DB766, an arylimidamide (AIA), was found to be highly effective against multiple species of *Leishmania* in vitro, with an IC_{50} value of 0.036 μM, but was not effective enough in *Leishmania*-infected animals to continue to clinical studies. Recently, antifungal azole drugs and DB766 were found to be synergistic against *Leishmania* in vitro. Thus, compounds possessing structural characteristics of both AIAs and azoles may be highly effective against *Leishmania*. Preliminary data indicate that such compounds show promising efficacy against *Leishmania* (e.g., DB2340 and DB2342, synthesized at Georgia State University, both display IC_{50} values of 1.8 μM against *L. amazonensis* in vitro), although the compounds are not as effective as DB766. AIA-azole hybrids that are structurally distinct from the Georgia State compounds are also being synthesized at Ohio State. The comparison of the results of the in vitro antileishmanial evaluation of these hybrids with the Georgia State hybrids will allow for the elucidation of a structure-activity relationship. Future studies will involve testing active compounds in *Leishmania* infected mice. Long-term benefits of this project may include the discovery and development of an effective oral medication against leishmaniasis.



B31

Investigating the Potential of Arylboronic Acids as OXA-1 β-Lactamase Inhibitors

Michael R. Brunner and Rachel A. Powers

Grand Valley State University

β-lactam antibiotics, such as penicillin and carbapenems, have been used within the medical community to battle bacterial infections for several decades. However, due to years of overuse, widespread resistance has developed within bacteria. β-lactam resistance is obtained through many different means, yet perhaps the most effective is the production of β-lactamase enzymes. These enzymes hydrolyze the lactam ring of these drugs, which renders them inactive. To overcome this obstacle, β-lactamase inhibitors were developed. However, these inhibitors mimic the classic β-lactam antibiotic structure, which results in bacteria developing resistance to these inhibitors as well. This presents an urgent need to develop novel inhibitors for the four classes of β-lactamases. Class D β-lactamases are some of the least understood and most clinically dangerous enzymes, and are capable of hydrolyzing last resort antibiotics, such as carbapenems. They are also not inhibited by clinically available β-lactamase inhibitors, like clavulanic acid and sulbactam. Boronic acids are known transition-state-analog inhibitors of both class A and C β-lactamases and provide a novel means to inhibit class D β-lactamases. Twenty-three different arylboronic acids were tested for inhibition of the class D β-lactamase OXA-1. Several compounds offered encouraging leads, with the best arylboronic acid having a K_i value of 110 μM. The development of an analog database, the determination of low Ki inhibitors, and use of X-ray crystallography to map a structure of the enzyme-boronic acid inhibitor complex provides an excellent platform from which to further optimize and explore the use of these potential drugs. Optimization of these boronic acids may lead to the discovery of a new novel clinical class D β-lactamase inhibitor.

M1

Utilizing Scanning Electron Microscopy to Characterize Conductive AFM Tip Degradation and Microsphere Deposition

Daniel E. Clark, Dr. Jennifer R. Hampton and Dr. Joshua P. Veazey

Hope College

Scanning Electron Microscopy (SEM) is a method by which the morphology of a sample can be determined. Energy Dispersive X-ray Spectroscopy (EDS) can determine the elemental composition of the sample. This project examined two microsystems using these techniques. The first microsystem examined the quality of the coating on Atomic Force Microscopy (AFM) tips. In contact AFM, a tip is physically dragged across the surface to determine the topography of the sample. The SCM model tips have a conductive coating, which can be damaged due to the dragging required to make the measurement. In the second microsystem, the SEM was used to examine the results of depositing polystyrene microspheres on gold substrates to determine what parameters lead to a close-packed monolayer.

M2

Phase Transfer of Gold-Silver Alloy Nanoparticles

Brian Comstock-Reid

Eastern Michigan University

Nanoparticles observable properties change with variation in shape, composition, size and the medium in which they are dissolved. Changing any of these factors influences the catalytic ability as well as the absorbance spectra of the nanoparticle. The project's aim was to transfer gold-silver alloy nanoparticles from an aqueous medium into a variety of nonpolar solvents. Small spherical nanoparticles were made with varying composition of gold and silver and then transferred from water into chloroform, dichloromethane, and toluene using various phase transfer catalysts. Absorbance spectra taken before and after transfer were compared to prove the transfer. The UV-VIS spectra showed a linear correlation of the maximum absorbance peak with the refractive index. Modeling using Mie theory was also performed to investigate the predictability of the shift in spectra with respect to alloy and solvent composition.

M3

Encapsulation of a Model Compound Delays its Release From a Biobased Polymer

Dr. Victoria Finkenstadt[1] and Jennifer Eler[2]

[1]National Center for Agricultural Utilization Research, [2]Northeastern Illinois University,

Biobased polymers have several advantages over petroleum-based polymers such as polystyrene or polyethylene in that they can be less expensive and more environmentally friendly while retaining functional properties such as controlled release of biologically active compounds. The food-contact tray was originally designed with a biobased polymer infused with an anti-microbial agent such as Nisaplin™; however, caffeine was substituted as the model compound in our preliminary investigations. This composite was then extruded with thermoplastic starch for preliminary investigations in constructing a food contact tray. Caffeine was then combined with pectin and then extruded with thermoplastic starch to form a composite suitable for food-contact trays. Pectin is a cell-wall polysaccharide with unique functionality that makes it ideal for controlled release systems using encapsulation. Starch is the main energy storage polysaccharide for several cereal crops. Both starch and pectin can be processed into a thermoplastic material. Caffeine was physically mixed or encapsulated through dissolution and freeze-drying with pectin. UV-VIS spectroscopy (λ = 273 *nm*) was utilized to measure the release of caffeine from the composite submerged in water. A spike standard curve was used to compensate for any UV absorption by the polysaccharide in the region of interest. Encapsulation did delay the release of the caffeine. The release rate was delayed by at least one hour when the model compound was encapsulated before extrusion. The three types of starch were normal, high-amylose, and waxy corn starch with different amounts of amylose and amylopectin. The type of starch did not affect the release profiles in a significant manner.

M4

Capacitance and HER Characterization of Electrodeposited Nickel Alloy Thin Films

Matthew Gira, Dr. Jennifer Hampton

Hope College

With the global energy demand growing, there is greater need for production of energy. One of the ways of producing this energy is creation of hydrogen gas to store energy, however, this technique is not yet economically favorable compared to many other energy sources. One reason for this is the current use of platinum in hydrogen production. As a result, we are exploring other less costly metals for use as hydrogen producing catalysts. With the technique of electrodeposition, different nickel alloy thin films were created to characterize their structure, composition, and hydrogen production capabilities. Characterization was completed using atomic force microscopy (AFM) to measure roughness, scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDS) to measure composition, and cyclic voltammetry to measure electrochemical capacitance. Linear sweep voltammetry was used to perform the hydrogen evolution reaction (HER), a reaction that produces hydrogen gas as a product. The use of these characterization techniques and HER measurements could help further understanding of the production of hydrogen and help fuel cells become more economically favorable using these earth-abundant metals.

M5

Characterization of Perovskite Thin Films for Use in Solar Cells

Danielle M. Hamann*, D. Westley Miller, Dr. Mark C. Lonergan

***Lake Superior State University, University of Oregon**

Solar photovoltaic cells have proven potential as a major source of energy. Polycrystalline silicon currently dominates production of solar cells, however, perovskite thin film devices are potentially more efficient and less expensive making them a potential competitor. The methyl ammonium lead halide perovskites, with the ABX_3 crystal structure, have recently emerged as very efficient thin film absorbers in solar cells, though the material is still poorly understood. In order to get working devices and study the properties of the pervoskite solar cells, pinhole free perovskite layers need to be deposited via spin coating in a nitrogen atmosphere. By varying the solvents and concentrations of the perovskite solutions, and manipulating spin coating conditions a pinhole free film was developed. The films were analyzed using UV-VIS spectrometry, optical profilometry, and X-ray diffraction. The film deposited from the 0.88 *M* perovskite solution in DMSO and γ-butyrolactone was the smoothest film, with an RMS roughness of 15.2 *nm*. Devices made with the 0.88 molar perovskite films were the only devices to show diode like behavior with the other films appeared to only act as resistors.

M6

The Effects of Thiol-modified Hyaluronan in Poly(ethylene glycol) on Hydrogel Mechanics

Haitham Maaieh, Victor T. Wang, Rhima M. Coleman, PhD.

University of Michigan, Ann Arbor

The use of hydrogels as scaffolds for tissue engineering has expanded rapidly in the last decade due to its regenerative applications. When designing hydrogels for tissue regeneration, differences in network properties and mechanics can affect cellular behavior. Studies have shown that the introduction of hyaluronic acid (HA) to hydrogels can greatly improve chondrogenic differentiation and proliferation; however, they are known to significantly reduce the mechanical properties of gels and can be removed by digestion and diffusion over time. In this study, HA was thiol-modified (HA-SH) to study the effects of covalently attached HA to PEG via Michael-type reaction on gel mechanics. Ten percent 4-arm poly(ethylene glycol) (PEG) acrylate was UV photo-polymerized with varying concentrations of HA or HA-SH to form hydrogels through free-radical polymerization and were swelled overnight for 24 hours. Mechanical testing was conducted on 1%, 1.25%, 2%, 2.5%, 5%, and 7.5% HA or HA-SH using 0.1% Irgacure. There was a significant negative correlation between % HA and the shear modulus ($p < 0.001$). Furthermore, HA-SH in PEG significantly increased the shear modulus of the PEG hydrogels compared with similar concentrations of unmodified HA in PEG ($p < 0.001$) at concentrations greater than 2%. In future studies, the effect of thiol-modification of hyaluronan and gel mechanical properties on chondrocyte behavior will be assessed.

M7

Quantitative Characterization of Methanol Oxidation Catalysis on Dealloyed NiCu Films

Matthew A. Milliken, Jennifer R. Hampton

Hope College

The topic of catalytic nanoporous materials has seen a surge of interest in the past decade. With Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Spectroscopy (EDS), the surface area, topography, and composition of these nanostructures can be characterized. The accessibility of these instruments has generated interest involving the interactive effects of surface topography and catalytic activity of binary alloys. The research conducted involved electrodepositing, dealloying, and characterizing various nickel-copper binary alloys on a Au substrate for methanol oxidation applications. By dealloying copper out of a NiCu alloy using Controlled Potential Electrolysis (CPE), a high-surface area nanoporous material was fabricated. The composition and capacitance of the NiCu alloys (before and after the dealloying step) were characterized via SEM/EDS, and Cyclic Voltammetry (CV) respectively. Utilizing Chronoamperometry (CA), the oxidation of methanol was analyzed before and after dealloying to determine whether porosity enhanced the catalytic efficiency.

M8

Engineering Self-Assembling Peptide Amphiphiles for Cancer Imaging

Michael J. Nicholl, Arijit Ghosh, Christian Buettner, Joshua E. Goldberger

The Ohio State University

The design of new self-assembling biomaterials that change morphology under precise stimuli can lead to much advancement that includes sensors, imaging agents and therapeutics. For example, we are designing a new class of peptide materials that transform from spherical micelles to nanofibers in the slightly acidic environment of cancerous tissue. However, designing a vehicle that transforms under a specific pH value in vivo requires a more detailed understanding on balancing the attractive hydrophobic forces and the repulsive electrostatic forces of these surfactant-like molecules. To these ends, we studied how balancing the alkyl chain length and the number of anionic amino acids in the charged region affect the sphere to nanofiber transition pH, starting from C_{16}-$Y_2A_2E_4K$(DO3A:Gd)-NH_2. In general, increasing the alkyl chain length promotes nanofiber formation at a given set of conditions, while increasing the number of charged amino acids promotes micelle formation. However simultaneously increasing the alkyl chain length by one methyl unit and the number of charged amino acids by one glutamic acid, gives a system that undergoes a sphere to nanofiber transition at close to the same pH and concentration values though the micelle morphology is slightly preferred. Consequently, this work shows that balancing the attractive and repulsive forces of the molecule is a powerful avenue for fine-tuning the self-assembling properties of next generation stimuli responsive materials.

M9

Spectroscopic Determination of the Binding Constant and Thermodynamic Values of a Host-Guest System

Erica Patton, Jennifer S. Holt

Valparaiso University

A host-guest system occurs when a guest molecule, in this case Brooker's merocyanine (BM), enters the host molecule, beta-cyclodextrin (β-CD), to form a complex. The equilibrium of a host-guest system becomes established through weak intermolecular interactions when the guest molecule binds to the host. The strength of the interactions can be studied using the equilibrium binding constant. By altering the structure of the β-CD through modifications of the chemical substituents along the outer rims of the β-CD cavity, we can better understand the different types of interactions between host and guest, such as hydrogen bonding and van der Waals forces. The determination of the binding constant at different temperatures allows for further understanding of these complexes. To determine the binding constant, the Benesi-Hildebrand equation can be used to analyze data collected using fluorescence spectroscopy. The binding constant of β-CD complex does appear to be temperature dependent, so the thermodynamic values of ΔG, ΔH, and ΔS were calculated. However, the binding constants for some of the modified β-CD complexes do not appear to exhibit a strong temperature dependence, so these thermodynamic values were not determined. Determining the temperature dependence of these complexes allows better insight into how strong the modified β-CDs will bind to a guest molecule, which allows for better predictions of their behaviors under different conditions.

M10

Electrodeposition and Dealloying of Nickel-Cobalt and Nickel-Cobalt-Copper Thin Films

Benjamin Peecher, Dr. Jennifer Hampton

Hope College

This project focuses on characterizing nickel-cobalt and nickel-cobalt-copper electrodeposited thin films. These films can be engineered to have high surface areas, giving them fuel cell and capacitance-related applications. Using a three-electrode electrochemical cell, metal alloys are deposited from solution onto a gold substrate. These films are then studied in a scanning electron microscope (SEM) with an energy dispersive x-ray spectroscopy (EDS) attachment to determine their structures and compositions. It was found that when nickel and cobalt are deposited together, there is consistently a higher ratio of cobalt in the film than in the solution. When nickel, cobalt, and copper are deposited together, the ratios in the film are generally closer to those in the solution, but there is more nickel in the film than in the solution. The nickel-cobalt and nickel-cobalt-copper films are then electrochemically dealloyed. To dealloy the films, a steadily increasing potential is placed between the working and counter electrodes, re-oxidizing the metals and pulling them off of the substrate. Different metals re-oxidize at different potentials, so depending on when one stops the potential, it is possible to pull out certain metals, leaving others behind. When dealloying the nickel-cobalt films, nickel and cobalt strip out of the film in nearly equal amounts, despite cobalt reacting at a lower potential. When dealloying nickel-cobalt-copper, nickel and cobalt are kinetically stabilized, and the copper pulls out, leaving a porous nickel-cobalt film behind. Preliminary results also suggest that dealloying the nickel-cobalt-copper films increases their capacitances.

M11

Spectroscopic Study of Dye Isomerization in a Host-Guest Complex

Miroslava Repak, Jennifer S. Holt

Valparaiso University

Host-guest complexes are systems in which a guest molecule binds to a host molecule through weak intermolecular interactions, such as van der Waals interactions or hydrogen bonding. β-cyclodextrin, the host molecule, is a seven-membered ring with a hydrophobic inner cavity and a hydrophilic outer surface. Brooker's merocyanine, the guest, is a dye molecule with a photo-induced isomerization cycle. The isomerization of Brooker's merocyanine was analyzed using UV-Vis spectroscopy to understand differences in the behavior of the dye in the solution and in modified cyclodextrin cavities. The molecule in solution cannot be isomerized directly from the trans to cis configuration unless energy in the form of UV light is added. However, when the dye is complexed with β-CD, it undergoes isomerization without UV light exposure. It appears the dye molecule changes conformation within the cyclodextrin to relieve the strain inflicted by the cavity. Different modifications to the outer surface of the cyclodextrin have been studied to see how these modifications might affect this unique isomerization behavior. By understanding guest behavior in the cavity, a molecular level understanding of host-guest chemistry will help to improve practical applications of materials.

M12

Adhesion of Proteinogenic Amino Acids on Thin Layers of Graphene

Edith Yeung, Faranak Sharifi and Giovanni Fanchini

University of Western Ontario

Large-area, solution-processed graphene thin films are of interest in several applications in which their biocompatibility is essential. In order to demonstrate the biocompatibility and bioactivity of graphene, tests of adhesion of proteinogenic amino acids are a critical step. Theoretical studies predicted that these amino acids bind to graphene with Van der Waals forces proportional to their molecular weight. In order to corroborate these findings we tested seven different amino acids, including: tryptophan, arginine, phenylalanine, lysine, aspartic acid, asparagine and alanine with Kelvin Probe Fore microscopy and solid-state ultraviolet-visible spectrophotometry using ninhydrin as a marker. The first technique probes the adhesion strength of the specific amino acid on graphene, while the second technique is able to quantify the total amount of molecules situated on the surface. We find that surface treatments of graphene are important in improving the adhesion of specific amino acids, specifically alanine and asparagine. Our results corroborated the theoretical predictions and confirmed recent conclusions that clean graphene is hydrophobic, as previously assumed.

M13

Creating a More Efficient Thermoelectric Material

Katherine Wampler, Shannon Kraemer, Viktor Poltavets

Michigan State University

The project is focusing on quantum confined nanostructures. Ideally the project will be able to increase the Seebeck coefficient in the figure of merit equation which is used to determine the efficiency of thermoelectric materials. The idea is to create nanoparticles of lead telluride and cadmium telluride p-doped with sodium, using the co-precipitation reaction method. The doping will introduce holes into the material, which will allow the material to conduct. The PbTe and CdTe have varying band gaps which allows for more movement of the holes. These things along with the use of nanoparticles should increase the Seebeck coefficient, ultimately leading to a better thermoelectric material.

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Logan Plath (Adrian College)

Inorganic Chemistry
Chad Tenbusch (Michigan State University)

Organic Chemistry
Mitchell Groenenboom (Calvin College)

Physical Chemistry
Courtney Talicska (University of Michigan)

2013

Analytical Chemistry
Tarick El-Baba (Wayne State University)

Inorganic Chemistry
Alex Mayo (University of Guelph, Canada)

Organic Chemistry
Kelsey Longe and Michaelyn Lux (Michigan State University)

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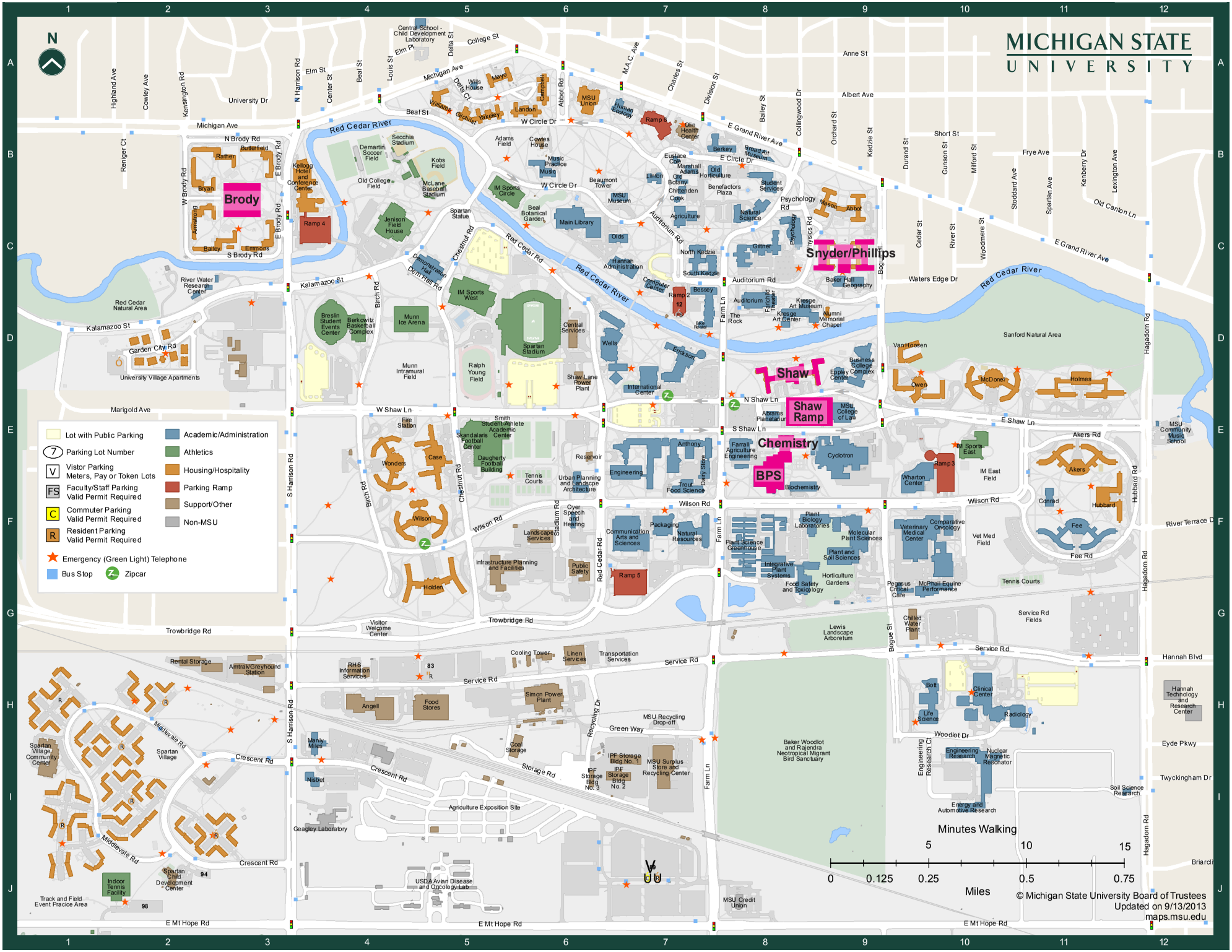
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