The Twelfth Annual

Undergraduate Research Symposium

Sponsored by the Western New York Section
of the American Chemical Society

Saturday April 27, 2019

D'Youville College

D'Youville

Welcome Message from the Organizing Committee

Welcome to the 12th annual Undergraduate Research Symposium sponsored by the Western New York Section of the American Chemical Society! This year's exciting Symposium will highlight some of the stimulating research being performed by undergraduates and their mentors from institutions throughout Western New York and the surrounding areas, including Southern Ontario.

I hope all participants will get the chance to engage one another in active discussions about the chemistry being presented. Please use this meeting as an opportunity to develop professionally by networking with scientific peers and faculty mentors in a relaxed scientific atmosphere. And of course, have fun!

Thank you to all of our student presenters and especially to our keynote speaker, Dr. Pablo Guzman, Department of the Army. I would also like to extend my appreciation to our generous sponsors and to the members of the Organizing Committee, without whom this Symposium would not be possible.

Sincerely,

Dominic L. Ventura, Ph.D.
Chair, 2019 Symposium Committee

2019 Symposium Organizing Committee

Chair: Dr. Dominic L. Ventura
Dr. Kacie Liwosz
Dr. Christopher Patridge
Dr. Greg Soja
Department of Chemistry, D'Youville College

Dr. Timothy M. Gregg
Department of Chemistry and Biochemistry, Canisius College

Dr. Valerie A. Frerichs
Dr. Rachel S. Ventura
Department of Chemistry, University at Buffalo SUNY

Dr. Robyn Goacher
Department of Biochemistry, Chemistry and Physics, Niagara University

Thank you for attending the 12th Annual Western New York ACS Undergraduate Research Symposium

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Interim Dean – School of Arts, Sciences and Education, D'Youville College

Our Keynote Speaker

Dr. **Pablo E. Guzmán** is a research chemist for the Energetic Technology Branch, Lethality Division, Weapons and Materials Research Directorate of the U.S. Combat Capabilities Development Command Army Research Laboratory (CCDC ARL) at Aberdeen Proving Ground, MD. His team leads the design, synthesis and characterization of novel energetic materials. He is currently performing a detail assignment as Technical Assistant to the Director at the Vehicle Technology Directorate (VTD) at CCDC ARL. VTD explores fundamental and early applied research efforts associated with autonomy, mobility, aeromechanics, propulsion, reliability, and vehicle component technology. Prior to CCDC ARL, Guzmán earned his B.Sc. in Chemistry from Chicago State University, M.A in Chemistry from University at Buffalo, and a Ph.D. in Chemistry from Emory University. After a postdoctoral fellowship at California Institute of Technology, Guzmán accepted a position serving the Department of the Army in 2015 as a Distinguished Hire.

Serving the Current and Future Warfighter

Dr. Pablo E. Guzmán

U.S. Army Combat Capabilities Development Command Army Research Laboratory, APG, MD

As the nation's premier laboratory for land forces, the U.S. Combat Capabilities Development Command Army Research Laboratory (CCDC ARL) has the mission to lead in the discovery, development and delivery of the technology-based capabilities required to enable Soldiers to win our Nation's wars and come home safely. CCDC ARL conducts research focused on the development of novel materials for military applications. In this presentation, three topics will be discussed: I. organic chemistry and its relationship with energetic materials II. synthesis and characterization of energetic materials and III. pathways towards the doctorate and opportunities for scientists in the federal government.

Schedule of Events

April 27, 2019

D'Youville Academic Center (DAC)

8:00 am-8:45 am Registration (DAC room 512)

8:45 am-9:00 am Introductory Remarks: **Prof. Dominic Ventura**

9:00 am-10:15 am Student Oral Presentations: Moderator **Prof. Kacie Liwosz**

- 9:00 am-9:15 am **Cole W. Tower**, Allegheny College
- 9:15 am-9:30 am **Jared Thomson**, Brock University
- 9:30 am-9:45 am **Gregory O'Brien**, Buffalo State College
- 9:45 am-10:00 am **Zackary C. Putney**, The College at Brockport
- 10:00 am-10:15 am **Alexander R. Green**, SUNY Fredonia

10:15 am-11:45 am Student Poster Presentations (DAC sixth floor)

11:45 am-12:45 pm **Lunch** (DAC sixth floor)

12:45 pm-1:45 pm **Keynote presentation:** (DAC room 512)

Dr. Pablo Guzmán, Department of the Army

"Serving the Current and Future Warfighter"

1:45 pm-2:00 pm Symposium Awards and Closing remarks: **Prof. Dominic Ventura**

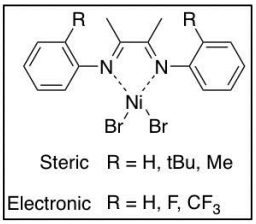
Talk 1.

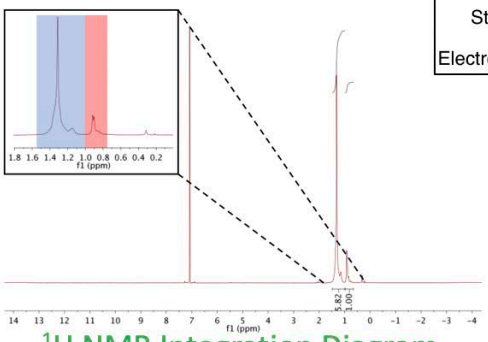
Temperature, Steric, and Electronic Effects on Microstructure and Average Molecular Weight of Poly(1-hexene) Synthesized by Chain Walking Polymerization

***Cole W. Tower**, Dana O'Connor, Alexandra Metzger and Timothy Chapp**

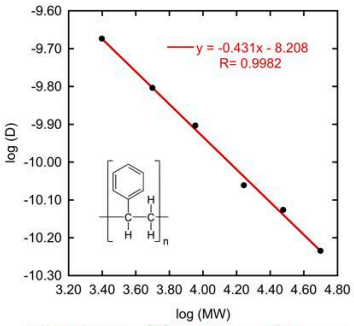
Department of Chemistry, Allegheny College, Meadville, PA

Poly(1-hexene) can be produced by a chain walking mechanism if an α-diimine nickel catalyst is used. The mechanism can be exploited to produce poly(1-hexene) with a tunable degree of branching (by favoring a 1,2-insertion or a 2,1-insertion) by altering the steric and electronic properties of the catalyst. Much of the current research is performed at high temperatures (T > RT), so subzero temperatures were used in this study. Understanding the microstructure and average molecular weight of a polymer is important for understanding and tuning the properties of a bulk polymer. 1H NMR was used to determine branching degree (methyl groups per 1000 carbons) in each produced polymer. 2D Diffusion ordered NMR spectroscopy (DOSY) was used to calculate the average molecular weight of each polymer sample without the need for a chromatographic method.





^{1}H NMR Integration Diagram



DOSY Calibration Curve

R Substitution	Branching, 0 °C (#Me/1000C)	Branching, -10 °C (#Me/1000C)	MW, 0 °C (g/mol)	MW, -10 °C (g/mol)
H	138	187		
Me	133	147	601.5	309.5
tBu	99	97	7381.2	26304.3
CF_3	133	142		

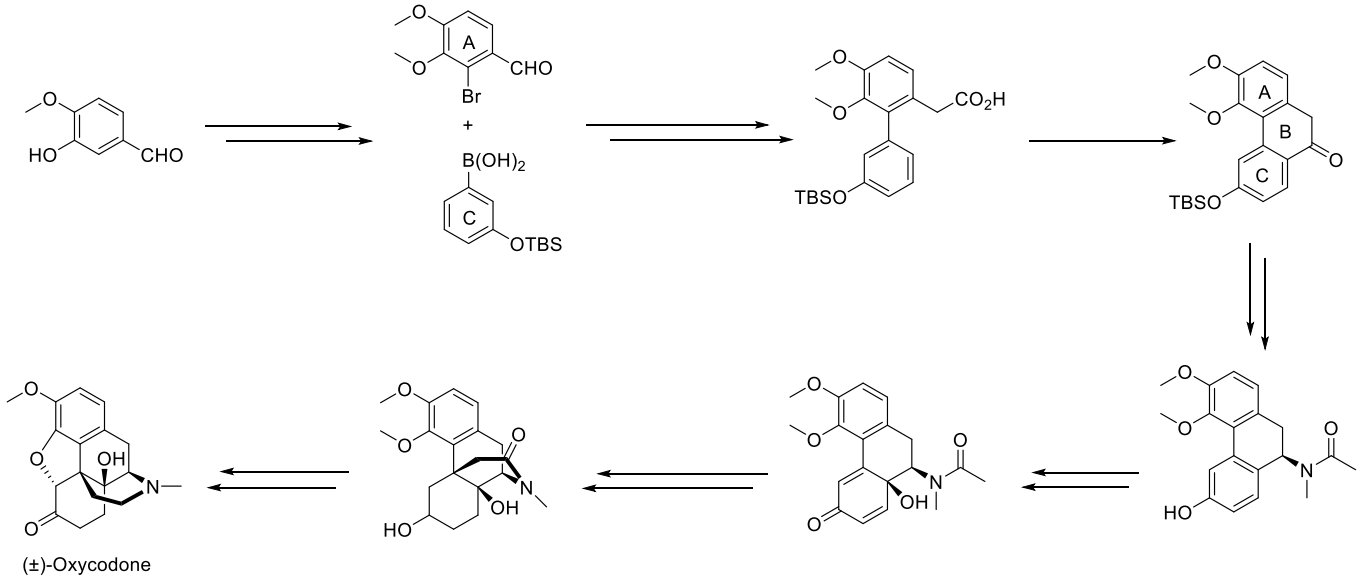
Talk 2.

Total Synthesis of (±)-Oxycodone

***Jared Thomson**, Tyler Bissett and Tomas Hudlicky**

Department of Chemistry, Brock University, St. Catharines, ON

An approach toward the total synthesis of (±)-oxycodone will be presented. Key steps include a Suzuki cross coupling of A- and C-ring fragments, an Arndt-Eistert homologation, an intramolecular Friedel-Crafts cyclization and an oxidative dearomatization step, inspired by a previous synthesis[1], to install the key C-14 hydroxyl group. The aim of the project is to provide a shorter, more efficient synthetic pathway toward (±)-oxycodone. The progress toward this goal will be reported.



(1) Kimishima, A.; Umihara, H.; Mizoguchi, A.; Yokoshima, S.; Fukuyama, T. *Org. Lett*., **2014**, *16*, 6244-6247.

Talk 3.

Peptidomimetics that Contain Amino Acid Surrogates, Synthesized Using Buchwald-Hartwig Amination

***Gregory O'Brien**, Mahmuda Rahman, Elifnur Yeldez Victoire-Grace Karambizi and Sujit Suwal**

Department of Chemistry, SUNY Buffalo State College, Buffalo, NY

Buchwald–Hartwig amination (BHA) is palladium-catalyzed coupling of amines and aryl halides. Synthetic utility of BHA stems primarily due to the shortcomings of other aromatic C-N bond formation methods, that often suffers limited substrate scope and functional group tolerance. BHA is widely used in organic synthesis to create a variety of molecules that have medicinal and pharmaceutical essence. With this prospect, we explored BHA towards restructuring several heterocyclic halides into highly functionalized amino acid surrogates that could fuel syntheses of novel peptidomimetics having better pharmaceutical indices. Most importantly, these building blocks allow us designing conformationally constrained oligomers that are cell permeable, proteolytically stable and potentially offer high-affinity protein ligands. To date, we are successful in synthesizing more than a dozen of amino acid surrogates. Currently, we are optimizing solid phase syntheses of hybrid peptides/peptoids that contain surrogate amino acids. Also, we are exploring MS-based sequencing method that can deconvolute subunits within the oligomers.

Talk 4.

Solvation of Phosphonium Ionic Liquids in Supercritical Carbon Dioxide

Zackary C. Putney *and Mark P. Heitz**

Department of Chemistry, The College at Brockport, SUNY, Brockport, NY

We present steady-state and time-resolved fluorescence spectroscopic data derived from coumarin 153 (C153) in a binary solution comprised of trihexyltetradecylphosphonium bis(trifluoromethylsulfonyl)imide ($[P_{6,6,6,14}]^+$ Tf_2N^-) and supercritical CO_2 ($scCO_2$). Steady-state fluorescence of C153 was measured in neat $scCO_2$ and ionic liquid (IL)-modified $scCO_2$ solutions. The steady-state excitation and emission peak frequency data in neat $scCO_2$ and IL/$scCO_2$ diverge at low fluid density ($\rho_r = \rho/\rho_c < 1$). The prominent spectral differences at low fluid density provided clear evidence that C153 reports different microenvironments, and suggested that the IL is solubilized in the bulk $scCO_2$ and heterogeneity of the C153 microenvironment is readily controlled by $scCO_2$ density. C153 dimers have been reported in the literature, and this formed the basis of the hypothesis that dimerization is occurring in $scCO_2$. Time-dependent density functional theory (TD-DFT) electronic structure calculations yielded transition energies that were consistent with excitation spectra and provided supporting evidence for the dimer hypothesis. Time-resolved fluorescence measurements yielded double exponential decays with time constants that further supported dimer formation. The associated fractional contributions showed that the dominant contribution to the intensity decay was from C153 monomers, and that in high density $scCO_2$ there was minimal contribution from C153 dimers.

Talk 5.

Synthesis and Characterization of a Novel Nitrosamine, an NO and HNO Donor

***Alexander R. Green**, Timothy H. Warren and Allan Jay P. Cardenas**

Department of Chemistry and Biochemistry, SUNY Fredonia, Fredonia, NY

Nitrosamines are known to release nitric oxide (NO), a molecule that is involved for a variety of biological functions, such as vasodilation and neurotransmission. A related molecule nitroxyl (HNO, or NO-), which is a reduced form of nitric oxide, offers a different pharmaceutical benefit by acting as a myocardial contractor. Recently, there are very few medicinal sources of nitroxyl such as Angeli's salt or Piloty's acid. This synthesized novel nitrosamine demonstrates the release of nitroxyl as well as nitric oxide in the presence of an oxidant. This presentation will feature the synthesis and structural characterization of nitrosamine that gives insight to its reactivity. Furthermore, proposed mechanism will be discussed, supported by kinetic studies.

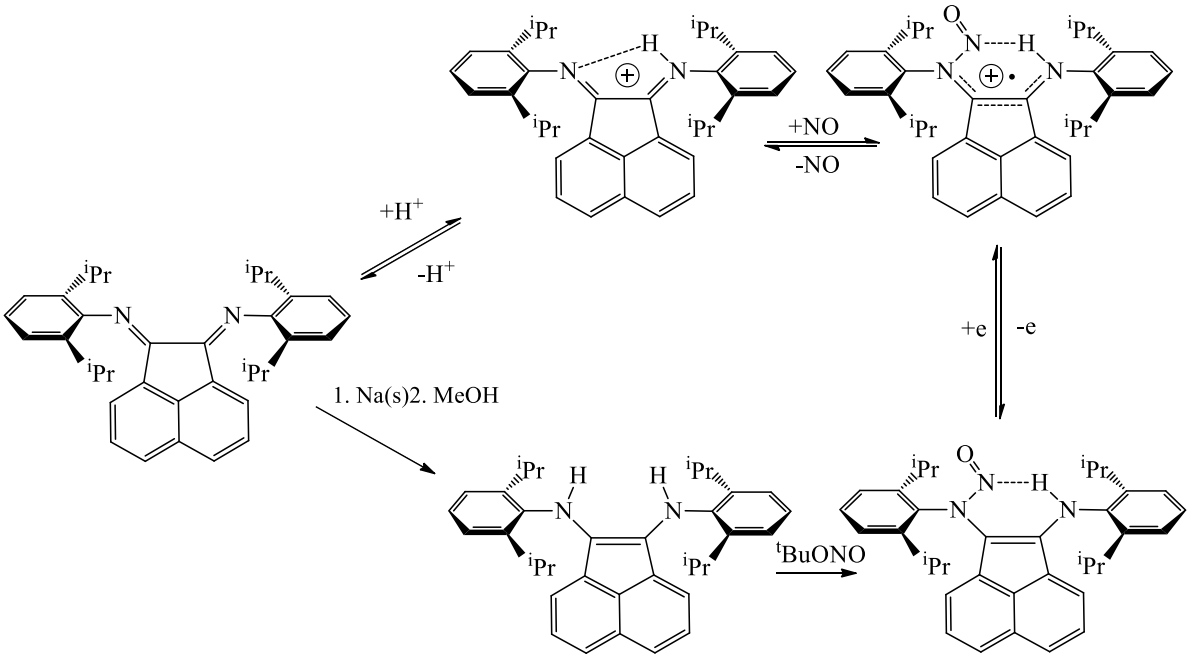


Figure 1. Diimines as scaffolds for NO and HNO capture and redox interconversion

Student Poster Presentations

Time: 10:15 - 11:45 AM (DAC Sixth Floor)

Poster 1. **Sean Lewis**, Xinbei Liu, Zachary Ward, Ciara LaClair and Lea Vacca Michel*
School of Material Science, Rochester Institute of Technology, Rochester, NY

Investigating Pal's Interaction with Peptidoglycan

Poster 2. **Nolan Nardangeli** and Tomas Hudlicky*
Department of Chemistry, Brock University, St. Catharines, ON

Program in Chemoenzymatic Synthesis in the Hudlicky Group

Poster 3. **Filippo Gentile**, **Matthew Berardi** and Timothy M. Gregg*
Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY

Synthesis of Pyran-2-one Compounds with Anti-Fungal and Antibiotic Properties

Poster 4. **Hyein Kwon, Jessica Levine,** Kaitlin Ordiway and Joseph A. Gardella, Jr.*
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

ToF-SIMS Analysis of Polycyclic Aromatic Hydrocarbons for Source Apportionment in the Tonawanda Coke Soil Study

Poster 5. **Molly M. LaRocca** and Mark P. Heitz*
Department of Chemistry, The College at Brockport, SUNY, Brockport, NY

Solvation Dynamics in Deep Eutectic Solvents

Poster 6. **Dylan A. DiGrazia**, **Christina T. Scalzo**, **Lauren N. Scott** and Fehmi Damkaci*
Department of Chemistry, SUNY Oswego, Oswego, NY

Multicomponent Synthesis of 1,4-Disubstituted-1,2,3-Triazoles Using *N*-Picolinamides as Ligands

Poster 7. **Rachel Smolinski**, Didar Asik, Joseph Spernyak and Janet Morrow*
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Iron(III) MRI Contrast Agents: From Laboratory Hood to Mouse Imaging

Poster 8. **Swar Dakein**, Brianne M. Weichbrodt and Allan Jay P. Cardenas*
Department of Chemistry and Biochemistry, SUNY Fredonia, Fredonia, NY

Synthesis and Reactivity of a New Class of Boron-Sulfur Frustrated Lewis Pairs

Poster 9. **Elizabeth R. Hinterberger** and Gregory R. Soja*
Department of Chemistry, D'Youville College, Buffalo, NY

Adsorption and Surface Coverage of Mercaptohexadecanoic Acid on SnO_2 Thin Films

Poster 10. **Daoyang Zhang**, Matthew R. Crawley and Timothy R. Cook*
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Self-Assembled Cofacial Prisms and Their Applications Towards O_2 Catalytic Reduction

Poster 11. **Maham Alamgir**, Brent Boleslav and Robyn E. Goacher*
Department of Biochemistry, Chemistry and Physics, Niagara University, NY

Metformin and Metformin-Related Compounds: Stability and Quantification

Poster 12. **Timeka Snead**, David T.R. Stewart and Dominic L. Ventura*
Department of Chemistry, D'Youville College, Buffalo, NY

Identification of Products of Metallophthalocyanine (MPc) Catalyzed 2,3-Sigmatropic Rearrangements

Poster 13. **Anxhela Nezha,** Shohini San-Britain and Joseph A. Gardella Jr*
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Explaining Common Fragmentation Patterns in HEMA via Quantum Molecular Dynamics Calculations

Poster 14. **Rachel I. Riga** and Mark P. Heitz*
Department of Chemistry, The College at Brockport, SUNY, Brockport, NY

Molecular Solvation in Phosphonium Ionic Liquids

Poster 15. **Justin A. Maxwell**, Zachery Schmidt, David F. Watson* and Kacie R. Liwosz*
Department of Chemistry, D'Youville College, Buffalo, NY

Effect of Chalcogenoxanthene Dye Chain Length on Electron Injection and Recombination on Zirconium Dioxide and Titanium Dioxide

Poster 16. **Nicholas Nordblum-Sinclair**, Akanksha Patel and Janet R. Morrow*
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

FeTOB and Its Uses as a CEST MRI Contrast Dye

Poster 17. **Jennifer Sescil** and Timothy M. Gregg*
Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY

Synthesis and Analysis of Novel Compounds for Spectroscopy Lab

Poster 18. **Victoire-Grace Karambizi**, Mahmuda Rahman, Elifnur Yeldez, Greg O'Brien, Julianna Du-Hart and Sujit Suwal*
Department of Chemistry, SUNY Buffalo State College, Buffalo, NY

Syntheses of Piperazine Derivatives Through Reductive Amination

Poster 19. **Taiylor Q. Cristman** and Theodore S. Dibble*
Department of Chemistry, SUNY ESF, Syracuse, NY

Production of Organo-Mercury Compounds in the Atmosphere

Poster 20. **Ronald T. Jerozal**, Travis B. Mitchell and Jason B. Benedict*
Department of Chemistry, University at Buffalo, SUNY, Buffalo NY

Engineering (?) Photoactive Crystalline Solids

Poster 21. **Catherine C. Lincourt**, Dhvani Patel, Peter Cao, Yasser Heakal* and Dominic L. Ventura*
Department of Chemistry, D'Youville College, Buffalo, NY

Synthesis and Evaluation of Chloroquine Analogs in Breast Cancer Cells

Poster 22. **Jenna Schlosser**, Julia Freemire, Kaitlin Schreader and Robyn E. Goacher*
Department of Biochemistry, Chemistry and Physics, Niagara University, NY

Distributed Pharmaceutical Analysis Laboratory (DPAL): Developing an HPLC method for Ampicillin and Cloxacillin Quantitation in Ampiclox Pills

Poster 23. **Mahmuda Rahman**, **Elifnur Yildiz**, Greg O'Brien, Victoire-Grace Karambizi and Sujit Suwal*
Department of Chemistry, SUNY Buffalo State College, Buffalo, NY

Towards the Synthesis of a Library of Foldamers Using Amino Acid Surrogates

Poster 24. **Tyler Johnston** and Mark P. Heitz*
Department of Chemistry and Biochemistry, The College at Brockport, SUNY, Brockport, NY

Interference of Ionic Liquids on the Bradford Assay: A Spectroscopic Study

Poster 25. **Caitlin M. Massimi**, Connor Gould and David T.R. Stewart*
Department of Chemistry, D'Youville College, Buffalo, NY

Selection of an Extraction Method for Nonpolar Organic Compounds from Silicone Wristbands

Poster 26. **Jonathan M. DeMaria** and Allan Jay P. Cardenas*
Department of Chemistry and Biochemistry, SUNY Fredonia, Fredonia, NY

Synthesis and Characterization of a Biomimetic Copper Complex of CuZnSOD

Poster 27. **Connor Gould,** CeDrice B. Howard and David T.R. Stewart*
Department of Chemistry, D'Youville College, Buffalo, NY

Work Towards the Use of Silicone Wristbands as Personal Passive Sampling Devices for Environmental Contaminants

Poster 28. **Kaycie R. Malyk** and Mark Janik*
Department of Chemistry and Biochemistry, SUNY Fredonia, Fredonia, NY

Synthesis and Characterization of Modified Anticancer Chalcone Analogues

Poster Abstracts

Poster 1.

Investigating Pal's Interaction with Peptidoglycan

***Sean Lewis**, Xinbei Liu, Zachary Ward, Ciara LaClair and Lea Vacca Michel**

School of Material Science, Rochester Institute of Technology, Rochester, NY

Peptidoglycan associated lipoprotein (Pal) has been shown to exhibit a unique dual orientation in *Escherichia coli* (*E. coli*). That is, Pal has two subpopulations, one surface exposed subpopulation and one periplasmic subpopulation. The periplasmic Pal subpopulation binds tightly (but noncovalently) to peptidoglycan. Both subpopulations of Pal are thought to be released from *E. coli* under certain conditions, and released Pal has been shown to be implicated in the clinical condition of sepsis. This study uses site-directed mutagenesis and ultracentrifugation to elucidate the detailed structural interaction between Pal and peptidoglycan, with the long-term goal of understanding the role of that interaction in Pal's release from *E. coli.* Preliminary data suggest several key residues in Pal dictate the Pal-peptidoglycan interaction.

Poster 2.

Program in Chemoenzymatic Synthesis in the Hudlicky Group

Nolan Nardangeli *and Tomas Hudlicky**

Department of Chemistry, Brock University, St. Catharines, ON

Current Projects in the Hudlicky research group involve the use of enzymatic metabolites produced by the stereocontrolled dihydroxylation of aromatic compounds by a recombinant strain of *E. Coli* JM 109 (pDTG601A) and by *R. eutrophus* B9. Enzymatic metabolites derived from substituted aromatics are utilized as chiral building blocks in the total synthesis of various natural products, such as *Amaryllidaceae* alkaloids, morphine alkaloids, as well as in studies toward the recent total syntheses of tetrodotoxin and (+)-oxycodone.

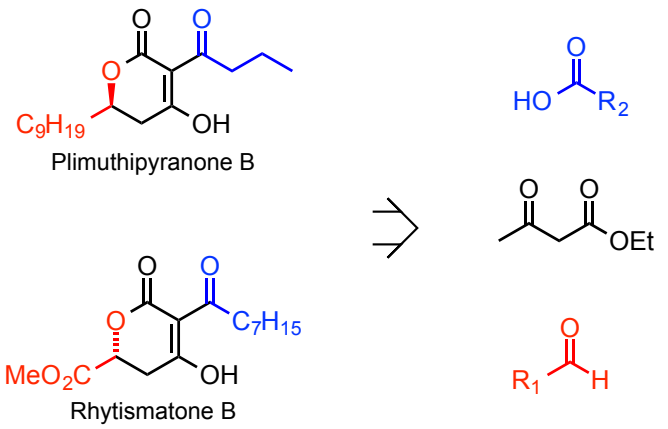
Poster 3.

Synthesis of Pyran-2-one Compounds with Anti-Fungal and Antibiotic Properties

Filippo Gentile, Matthew Berardi *and Timothy M. Gregg**

Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY

5,6-dihydro-2*H*-pyran-2-ones are a family of chiral natural products with a common structural core, but with biological activities that vary widely, including anti-fungal and antibiotic activity. We have begun efforts to synthesize pyran-2-ones in both racemic and enantiomerically enriched form. Aldol addition of a dienolate anion provides the pyran-2-one core, and C-acylation has provided a racemic route to Plimuthipyranone B. We are in the process of exploring several enantioselective routes that can also provide diverse structural analogs, including Rhytismatone B.



Poster 4.

ToF-SIMS Analysis of Polycyclic Aromatic Hydrocarbons for Source Apportionment in the Tonawanda Coke Soil Study

Hyein Kwon, Jessica Levine, *Kaitlin Ordiway and Joseph A. Gardella, Jr.**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Polycyclic aromatic hydrocarbons (PAHs) are a class of compound composed of a series of fused aromatic rings. This aromaticity stabilizes the compounds making them resistant to degradation and susceptible to local and long-range deposition. Combustion and industrial emissions are primary sources of PAHs in the environment. PAHs are of particular concern due to the carcinogenicity. PAHs have been used as indicators of specific sources of pollution. The correlation between emission source and the PAHs produced make it possible to attribute emission source based on the PAHs present in the area of interest. Time of flight secondary ion mass spectrometry (ToF-SIMS) was utilized to analyze PAH standards. ToF-SIMS allows us to look at a high mass range in order assess the higher mass fragments that are often excluded from traditional mass spectrometry methods. Higher mass fragments allow for more accurate tracking of the source of the PAHs. Lower mass fragments run a higher chance of being located at other emission sources, rather than just the target source. PAH standards were solution casted (50 mg/L) onto silicon wafers and then analyzed using ToF-SIMS. Based on the data that we acquire from the mass spectra of the different standards; we can compare the fragmentation pattern from the standards to soil samples acquired from the Tonawanda Coke soil study.

Poster 5.

Solvation Dynamics in Deep Eutectic Solvents

Molly M. LaRocca *and Mark P. Heitz**

Department of Chemistry, The College at Brockport, SUNY, Brockport, NY

Deep eutectic solvents (DESs) are important, novel solvents with application toward replacing, or at least reducing the amount of, hazardous organic solvents that are widely used in chemical industry. DESs are typically viscous making the solvent more difficult to work with, so the addition of modifiers such as cosolvents can significantly improve solution fluidity. In this work we are determining the physical properties of DES + cosolvent binary solvent systems and the subsequent interactions in neat and cosolvent-modified DESs. The physical properties measured in this work are primarily based on density and viscosity. In addition to physical properties characterization, we used steady-state and picosecond time-resolved fluorescence spectroscopy to determine the solvation dynamics in the DES + cosolvent binary mixtures. Coumarin 153 (c153) and coumarin 343 (c343) are the fluorescent probes used to describe the solvation behavior in DESs. We will contribute to the chemical literature on environmentally friendly alternative solvents.

Poster 6.

Multicomponent Synthesis of 1,4-Disubstituted-1,2,3-Triazoles Using *N*-Picolinamides as Ligands

Dylan A. DiGrazia, Christina T. Scalzo, Lauren N. Scott *and Fehmi Damkaci**

Department of Chemistry, SUNY Oswego, Oswego, NY

The heterocyclic compounds 1,2,3-triazoles have many useful properties, including those in the fields of medicinal chemistry, biological, and material science. It has been shown that 1,4-disubstituted-1,2,3-triazoles can be synthesized via a one-pot reaction containing a terminal alkene, a benzyl halide, and an azide under room temperature. The hope is to improve the yield using *N*-Picolinamide ligands, while altering the conditions. One factor this research explores is adjusting the solvent to determine its effect on the reaction. The time the reaction occurs at is being modified in order to see if the reaction could perform at an equal yield in a shorter amount of time. Lastly, the temperature is being tailored to suit the solvent's boiling point and to see the effects on the resulting yield. The outcome of the research is to see if the highest yields occur when using *N*-Picolinamides as ligands under the most effective conditions.

Poster 7.

Iron(III) MRI Contrast Agents: From Laboratory Hood to Mouse Imaging

***Rachel Smolinski**, Didar Asik, Joseph Spernyak and Janet Morrow**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Magnetic resonance imaging (MRI) is a widely used non-invasive diagnostic imaging tool. Clinically used MRI contrast agents (CAs) contain gadolinium, however there are concerns of potential toxicity when using Gd(III) based CAs. The purpose of this project is to synthesize and characterize potential alternative T1 contrast agents using Fe(III) macrocyclic complexes. High spin Fe(III) agents show promise as they show good T1 water proton relaxivity and are exceptionally inert towards release of the metal ion. The design of the Fe(III)TASO complex includes a triazacyclononane (TACN) ligand with one sulfonate and two alcohol donors. Fe(III)TASO has been characterized by mass spectroscopy, magnetic susceptibility and inner sphere water interactions were studied by ^{17}O NMR spectroscopy. Electrochemical studies were carried out by using cyclic voltammetry. In vitro and in vivo experiments of T1 relaxivity were performed on a 4.7 T MRI scanner. The results are promising and encouraging in the development of alternative CAs that contain Fe(III).

Poster 8.

Synthesis and Reactivity of a New Class of Boron-Sulfur Frustrated Lewis Pairs

***Swar Dakein**, Brianne M. Weichbrodt and Allan Jay P. Cardenas**

Department of Chemistry and Biochemistry, SUNY Fredonia, Fredonia, NY

The Chemistry Frustrated Lewis pairs (FLPs) has been an interest in field in the last decade. Frustrated Lewis pairs has been in metal-free catalysis as well as activating small molecules. The most common FLPs as phosphorus and boron, this study aims to synthesize a Boron-Sulfur frustrated Lewis pair. The Boron-Sulfur FLP will then be using to activate small molecules such as nitric oxide and carbon monoxide. This presentation will feature our ongoing research to synthesize simple Boron-Sulfur Frustrated Lewis Pair through simple acid-base reaction as well as hydroboration reaction.

Poster 9.

Adsorption and Surface Coverage of Mercaptohexadecanoic Acid on SnO_2 Thin Films

Elizabeth R. Hinterberger *and Gregory R. Soja**

Department of Chemistry, D'Youville College, Buffalo, NY

The chemisorption and surface coverage of mercaptohexadecanoic acid (MHDA) adsorbed on nanocrystalline SnO_2 thin films is presented. MHDA can act as a molecular linker in the attachment of quantum dots to the SnO_2 film, which would have applications in sensing and photovoltaic devices. SnO_2 thin films were prepared via a low cost doctor blade method, in which colloidal SnO_2 is spread across a glass substrate using a Pasteur pipette. Films were immersed in a 2 mM solution of MHDA in THF for at least 2 hours. FTIR spectroscopy was used to confirm chemisorption as well as surface coverage using a modified Beer-Lambert equation. The surface coverage of MHDA on the SnO_2 film was calculated to be $1.1 \pm 0.1 \times 10^{-7}$ mol/cm^2, which closely agrees with previously reported surface coverages of MHDA on nanocrystalline TiO_2 thin films. Future studies will explore the catalytic nature of these SnO_2 films.

Poster 10.

Self-Assembled Cofacial Prisms and Their Applications Towards O_2 Catalytic Reduction

***Daoyang Zhang**, Matthew R. Crawley and Timothy R. Cook**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Herein we report the study of the oxygen reduction reaction (ORR) catalyzed by coordination-driven self-assembled cofacial cobalt porphyrin prisms. Two equivalents of CoTPyP (cobalt(II) tetra(meso-4-pyridyl)porphyrinate) and four equivalents of functionalized molecular clips comprise each prism. Ruthenium molecular clips were synthesized by treatment of functionalized oxamido-bridging ligands with a μ_2-chloro-bridged ruthenium dimer molecule, resulting in yields greater than 50%. Cofacial prisms were obtained in self-assembly yields in excess of 90%. One of these prisms, $[Ru_8(\eta^6\text{–}i\text{Pr-}C_6H_4Me)_8(oxa)_4(CoTPyP)_2][OTf]_8$ (oxa = oxamido , OTf = triflate), has been shown in a previous report to affect the ORR with high selectivity towards H_2O over H_2O_2. We hypothesize that the molecular clip used in these prisms can have a steric influence, determine metal–metal separation, and also have an electronic effect, which all contribute to the selectivity and kinetics of catalysis. Our current studies seek to deepen our understanding of ORR at dinuclear active sites. The ORR catalytic activity was investigated using cyclic voltammetry for both homogenous and heterogeneous conditions.

Poster 11.

Metformin and Metformin-Related Compounds: Stability and Quantification

***Maham Alamgir**, Brent Boleslav and Robyn E. Goacher**

Department of Biochemistry, Chemistry and Physics, Niagara University, NY

The Distributed Pharmaceutical Analysis Laboratory (DPAL) is a project focused on the analysis of drugs in Africa, to identify mis-labeled or mis-dosed pills. Metformin is a pharmaceutical that is widely taken by individuals with Type-II diabetes. At Niagara University, we have worked to validate an HPLC method to determine whether metformin pills are indeed metformin, if they are dosed correctly, and whether there may be degraded products in the metformin. After this method passed system suitability checks and was approved by the DPAL project, the authors and analytical lab students at Niagara University analyzed 62 metformin tablets from Kenya against a calibration curve. Of these, 60 were found to be within 10% error of the labeled dosages. The remaining two pills were determined to be other pharmaceuticals in their corresponding packaging, which had been mixed into the metformin samples at some point between purchase and analysis. We are currently studying the stability of standard metformin solutions when stored at room temperature, and in the refrigerator (4°C) and freezer (-80°C). We are also working on separating additional metformin related compounds (MRCs) from metformin via HPLC, and on quantifying these MRCs. Quantifying includes establishing linearity, precision and finding LOD/LLOQ for both metformin and its related compounds. This will then be used to quantify the concentration of any degraded products or leftover reactants in the metformin chromatograms. It is hoped that the stability evaluation and MRC study will streamline and expand the utility of our HPLC analysis of metformin pills in the future.

Poster 12.

Identification of Products of Metallophthalocyanine (MPc) Catalyzed 2,3-Sigmatropic Rearrangements

***Timeka Snead**, David T.R. Stewart and Dominic L. Ventura**

Department of Chemistry, D'Youville College, Buffalo, NY

The objective of this laboratory experiment is to identify and quantify the products of metallophthalocyanine (MPc) catalyzed 2,3-sigmatropic rearrangements. During the reaction, a diazo compound reacts with an allyl methyl sulfide. When the products were tested on the NMR, nuclear magnetic resonance spectroscopy, the results showed two main products in each sample, which agreed with the given equation. One product of the reaction includes a straight chain and the other includes a cyclopropyl ring. Different metal catalysts including copper, cobalt, nickel, iron, silver, zinc and manganese were used to catalyze each set of substrates. Gas Chromatography-Mass Spectrometry (GC-MS) was used to separate and quantify each compound in the product mixture. The data produced included a chromatogram of each sample, which consisted of peaks at certain retention times, and the mass spectrum for each peak, which consisted of several peaks at different mass ions.

Poster 13.

Explaining Common Fragmentation Patterns in HEMA via Quantum Molecular Dynamics Calculations

Anxhela Nezha, *Shohini San-Britain and Joseph A. Gardella Jr**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Polymeric HEMA (hydroxyethylmethacrylate) was analyzed via ToF-SIMS (time of flight – static secondary ion mass spectrometry) to observe common fragmentation patterns. Previous literature reveals that C_2HO^+, $C_2H_5O^+$, etc. are the more common fragmentation structures observed for HEMA during any SIMS analysis. Utilizing the software Avogadro, each common structure of HEMA was depicted in order to conduct quantum molecular dynamic calculations via the additional software, GAMESS. The aforementioned calculations were used to ascertain bond dissociation energies of each analyzed fragment. Based on the obtained data, the hope is to determine why certain fragments of HEMA are more common than others during ToF-SIMS analysis.

Poster 14.

Molecular Solvation in Phosphonium Ionic Liquids

Rachel I. Riga *and Mark P. Heitz**

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The goal of this research is to determine the solvation dynamics in four environmentally-friendly, "green", phosphonium ionic liquids (PILs) + cosolvent binary mixtures. Rose Bengal is a prototypical fluorescent molecule known for its spectral sensitivity and is used to probe the IL mixtures. Neat ILs and methanol (MeOH) solvents were used to form an array of IL mixtures in which rose Bengal was dissolved. Solvation of rose Bengal was determined using steady-state and time-resolved fluorescence spectroscopy. The rose Bengal steady state data shows a systematic blue shift as PIL is added to solution. The solute emission intensity is quenched most effectively at a mole fraction of xPIL ~0.1 suggesting that the solvent-solute interactions are most unique in this range of mole fraction. Similarly, the lifetime data shows a minimum value at xPIL ~0.1 mol fraction PIL, also implying quenching of the probe at this solution composition. Rose Bengal is better solvated, more relaxed, at MeOH-rich mole fractions. The time-resolved center of gravity and associated solvation correlation function, C(t), shows that solvation of rose Bengal occurs at a faster rate in solutions of lower mole fraction PIL.

Poster 15.

Effect of Chalcogenoxanthene Dye Chain Length on Electron Injection and Recombination on Zirconium Dioxide and Titanium Dioxide

Justin A. Maxwell[1]*, Zachery Schmidt*[2]*, David F. Watson*[2]** and Kacie R. Liwosz*[1,2]****

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[2]Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Solar energy is the most abundant natural and renewable energy source. By using dye-sensitized solar cells this energy can be converted into useable electricity. Dye structures are easily tunable to have desired photo-physical properties. Increasing light harvesting and higher electron collection capabilities are very desirable characteristics for the dyes that are used in solar cells. We use chalcogenorxanthene dyes for their ability to sensitize nanocrystalline TiO_2. We are investigating how increasing the number of thiophene rings changes electron recombination, forward electron transfer, and backwards electron transfer. The dyes that are under investigation contain one, two, or three thiophene rings. Using transient absorption spectroscopy, we can characterize electron injection of the excited state of the dye. It is hypothesized that the charge recombination will be slower with dyes that have more thiophene rings, and the back-electron transfer will decrease with multiple thiophene rings as well. Previously it has been found that the lifetime of 1-Se-2 was longer than the lifetime of 1-Se-1.

Poster 16.

FeTOB and Its Uses as a CEST MRI Contrast Dye

***Nicholas Nordblum-Sinclair**, Akanksha Patel and Janet R. Morrow**

Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

The purpose of our research is to develop a safer alternative contrast dye for use in CEST MRI. Our affiliation with Roswell Park of Buffalo allows us to test these dyes in a safe setting using basic laboratory techniques like injecting the dye into laboratory rats and then test the effects under an MRI machine. The findings from these experiments have given us ample reason to believe our dye is working correctly and that we are moving in the correct direction.

Poster 17.

Synthesis and Analysis of Novel Compounds for Spectroscopy Lab

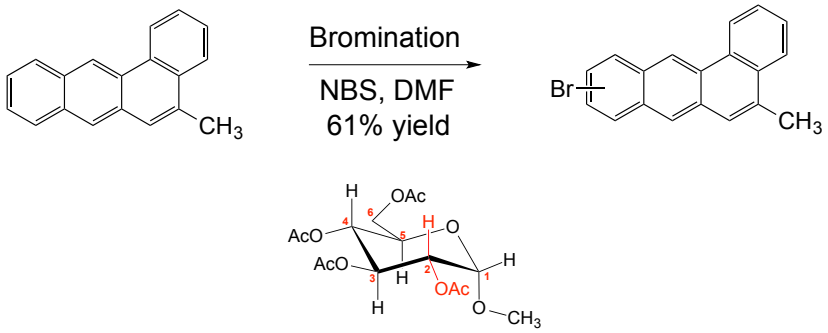
Jennifer Sescil *and Timothy M. Gregg**

Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY

Students studying Organic Spectroscopy have to consider a molecule's structure and how that is reflected in spectra, and conversely, they look at spectra (from NMR, IR and Mass Spec instruments) and consider what structure caused them. However, online databases of spectra now allow many common organic chemicals to be identified merely by searching using spectral data. To foster rigorous spectral interpretation skills, we are constantly seeking challenging structures, that, nonetheless, give clear NMR, IR and Mass Spectra, so they will be pedagogically useful for spectroscopy students. Generally, preparing likely candidate compounds requires 1 or more synthesis steps, as well as purification and extensive spectral characterization to ensure their use will be of value.

In the first project, we synthesized 5-methylbenz[a]anthracene. Electrophilic Aromatic Substitution of this compound with bromine gives a single major monobromination product, even though there are 11 different potential sites of substitution on the molecule. We sought to unambiguously assign ^{1}H and ^{13}C NMR resonances of this product in order to identify the site of bromination. Although the site of bromination is likely the 7-position, extensive analysis of 2D NMR data showed that coincidental overlaps in the spectra make it an unlikely teaching compound.

In the second project, we synthesized and studied the NMR spectra of a variety of sugar derivatives. Both per-acetylated pyranose structures and methyl glycosides were examined in terms of signal overlap in their $^{!}H$ NMR spectra. Two compounds were identified that are well-suited for use as unknowns in spectroscopy lab. Their COSY spectra allow unambiguous assignment of H resonances. With complete assignments, coupling constant analysis enables the student to determine the stereochemistry at each sugar backbone position, including the anomeric position, and to identify the sugar.



Poster 18.

Syntheses of Piperazine Derivatives Through Reductive Amination

***Victoire-Grace Karambizi**, Mahmuda Rahman, Elifnur Yeldez, Greg O'Brien, Julianna Du-Hart and Sujit Suwal**

Department of Chemistry, SUNY Buffalo State College, Buffalo, NY

Piperazine derivatives are widely used as the privileged-scaffold in modern drug discovery. Piperazines are known to improve lipophilicity of the small molecules, therefore, they are selected as the primary line of chemical motif within the complex molecular framework that are used for drug screening. Kinase inhibitors, CNS drugs, and Anthelmintic are few drugs, where piperazines are present as an essential chemical moiety. In addition, they are also used to syntheses of heterocyclic polymers. A synthetic approach that offer a variety of piperazine analogs is still in high demand. Importantly, piperazine derivatives that contain amino acid side-chain would offer additional diversity that has high reward potential in the diversity-oriented synthesis and combinatorial chemistry. To this point, we envisioned to synthesize piperazine derivatives, starting from reductive amination of amino acid esters with protected-glycine aldehyde, which would offer secondary amines. We hypothesize a deprotection of t-boc group followed by an intramolecular cyclization and subsequent amide reduction would offer the optically pure mono-substituted piperazine derivatives. Using this approach, we are synthesizing nearly a half-dozen of piperazine derivatives that comprises different amino acid side chain.

Poster 19.

Production of Organo-Mercury Compounds in the Atmosphere

Taiylor Q. Cristman *and Theodore S. Dibble**

Department of Chemistry, SUNY ESF, Syracuse, NY

We present studies of a previously neglected pathway in the oxidation of mercury in the atmosphere. Mercury emitted to the atmosphere and travels around the globe before being transferred to ecosystems. These emissions are mostly as atomic mercury, Hg(0), but mercury transfer to ecosystems mostly occurs in the form of Hg(II) compounds. Most Hg(0) oxidation in the atmosphere is believed to be initiated by trace amounts of atomic bromine:

$$Br + Hg \rightarrow BrHg\bullet \qquad (1)$$

followed by reaction of the BrHg radical with a variety of atmospheric radicals, •Y:

$$BrHg\bullet + \bullet Y \rightarrow BrHgY \qquad (2)$$

(Y= NO_2, HOO, BrO, etc.). Given that BrHg• can react with HOO• to make stable BrHgOOH, it seemed likely that BrHg could react with organic peroxy radicals (ROO•) in the atmosphere to make BrHgOOR. We turn to quantum chemistry, using CH_3OO as a model for the class of ROO• compounds, to study the possible reaction products:

$$BrHg\bullet + CH_3OO\bullet \rightarrow BrHgOOCH_3 \text{(3a)}$$

$$BrHg\bullet + CH_3OO\bullet \rightarrow BrHgH + CH_2OO \qquad (3b)$$

$$BrHg\bullet + CH_3OO\bullet \rightarrow Hg + BrOOCH_3 \qquad (3c)$$

$$BrHg\bullet + CH_3OO\bullet \rightarrow BrHgO\bullet + \bullet OCH_3 \qquad (3d)$$

$$BrHg\bullet + CH_3OO\bullet \rightarrow BrHgCH_3 + O_2 \qquad (3e)$$

All these reactions correspond to oxidation of Hg(I) to Hg(II), except Reaction (3c), which corresponds to reduction. Reactions (3d) and (3e) are roughly thermoneutral, but reactions (3a) and (3b) are exothermic by about 30 kcal/mole. Kinetically, the only reaction which appears not to have a barrier is reaction (3a). So the most favorable path appears to be reaction (3a).

The product of reaction (3a) is an organomercury compound. The toxicity of mercury raises largely from organomercury compounds, which are potent neurotoxins. Formation of organomercury compounds was previously thought to only occur in ecosystems via biological processes. The formation of organomercury compounds from the gas-phase oxidation of mercury raises concern, as this would tend to increase the toxicity of mercury above that predicted by fate and transport models.

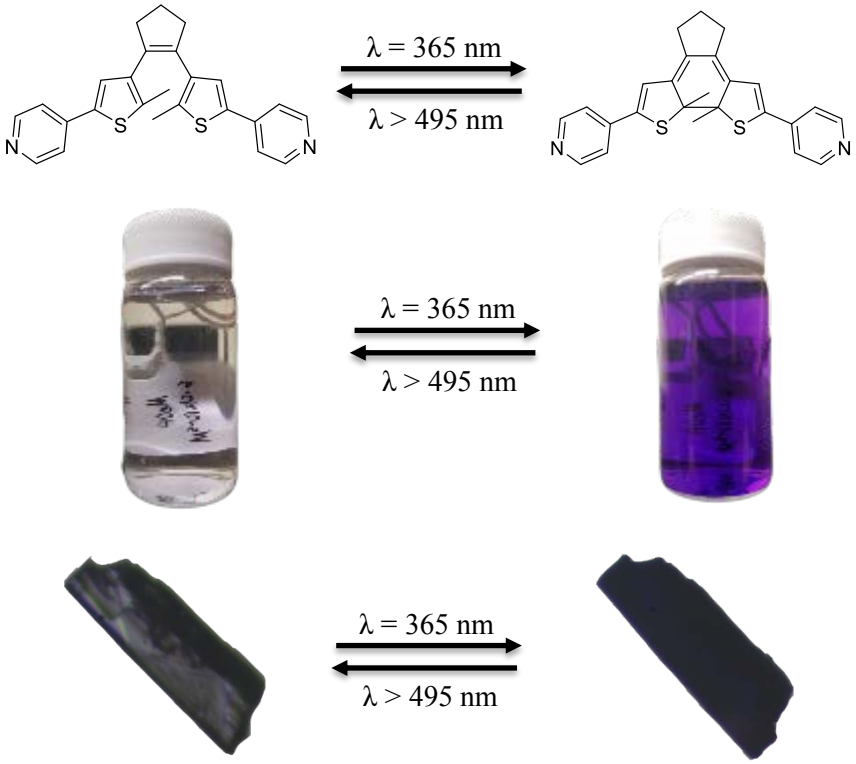
Poster 20.

Engineering (?) Photoactive Crystalline Solids

Ronald T. Jerozal*, Travis B. Mitchell and Jason B. Benedict**

Department of Chemistry, University at Buffalo, SUNY, Buffalo NY

Crystal engineering is the task of designing and predicting the properties and structure of a crystal based on the molecular structure of its components and the potential intermolecular interactions that can occur. This idea can be used to transform ordinary crystals into dynamic or reactive systems, and one way to make these dynamic systems is to incorporate photoresponsive molecules such as diarylethenes. Diarylethenes are appealing due to their isomers often being thermally stable, fatigue resistance, and able to rapidly undergo photocyclization. This has led them to have many applications as photoresponsive materials such as molecular switches, fluorescent sensors, and memory storage. It is paramount that these compounds be reactive in the solid state to have applications in materials; however, this is a challenge for diarylethenes, which can only photoisomerize when they adopt one of two conformations. Crystal engineering was used to attempt to synthesize crystals containing diarylethenes in the required conformation, so that the photochemical properties of these compounds can be studied in the solid state. This was done by designing supramolecular assemblies, such as co-crystals and metal-organic frameworks, held together by non-covalent interactions in structural moieties known as supramolecular synthons. After characterizing multiple supramolecular assemblies using single crystal X-ray diffraction, it became apparent that designing crystal structures based on potential synthon interactions is insufficient to predict photoreactivity of these diarylethene systems.



Poster 21.

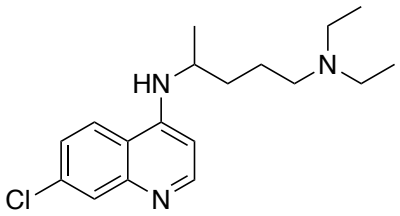
Synthesis and Evaluation of Chloroquine Analogs in Breast Cancer Cells

Catherine C. Lincourt[1]*, Dhvani Patel*[1,2]*, Peter Cao*[2]*, Yasser Heakal*[2]** and Dominic L. Ventura*[1]***

[1]Department of Chemistry, D'Youville College, Buffalo, NY
[2]Department of Pharmaceutical Sciences, D'Youville College, Buffalo, NY

Chloroquine (CQ) is a chemotherapeutic agent and has also been the foremost treatment of malaria for many years. Chloroquine has recently been investigated in the pharmacological inhibition of autophagy, although in high concentrations. Potentially, chloroquine derivatives may inhibit autophagy of breast cancer cells in much lower concentrations. In this study, we aimed to design and synthesize a group of CQ analogs through various methods. Utilizing various amines, we were able to produce a small library of compounds for this study.

Once synthesized, the CQ analogs were tested for inhibition of autophagy in triple-negative breast cancer cells. This part of the project focused on taking advantage of polyamine transporters in targeting and delivering CQ, intracellularly.



Chloroquine (CQ)

Poster 22.

Distributed Pharmaceutical Analysis Laboratory (DPAL): Developing an HPLC Method for Ampicillin and Cloxacillin Quantitation in Ampiclox Pills

***Jenna Schlosser**, Julia Freemire, Kaitlin Schreader and Robyn E. Goacher**

Department of Biochemistry, Chemistry and Physics, Niagara University, NY

The greater purpose of the Distributed Pharmaceutical Analysis Laboratory (DPAL) is to analyze medicines from Africa to identify drugs that are mislabeled, mis-dosed or degraded. The mixed antibiotic "Ampiclox" contains ampicillin and cloxacillin and is commonly prescribed in Africa. This medicine has not previously been analyzed by members of the DPAL project. Currently, Niagara University is developing an HPLC method for the analysis of Ampiclox. Literature methods using a nonpolar C-18 column and gradient elution with a phosphate buffer and acetonitrile are being adapted to fit the system suitability requirements established by the University of Notre Dame's DPAL project. Work so far includes testing of varying phosphate buffer pHs and concentrations, with evaluation of tailing factors, linearity, precision, and limits of detection and quantitation. Further, the adapted method is being tested for its ability to resolve degradation products from the ampicillin and cloxacillin, and for accuracy in regular and degraded matrices. Once these steps are complete and the method passes system suitability requirements, the method will be shared with other universities and analysis of medicines from African markets will begin.

Poster 23.

Towards the Synthesis of a Library of Foldamers Using Amino Acid Surrogates

***Mahmuda Rahman**, **Elifnur Yildiz**, Greg O'Brien, Victoire-Grace Karambizi and Sujit Suwal**

Department of Chemistry, SUNY Buffalo State College, Buffalo, NY

Suzuki-Miyaura cross-coupling is widely used for creating biaryl molecules. However, the cross-coupled products that contain heterocyclic moieties with different substituent predisposed around benzene architecture is limited. Heterocyclic moieties are indispensable fragments among FDA-approved drugs, such as Gleevec, Dasatinib, Erlotinib, etc. We, therefore, aimed to create Suzuki cross-coupled heterocyclic molecules that also contain N-protected amine and carboxylic acid, so that the resultant molecules can further be utilized in the synthesis of oligomers. We anticipate a presence of heterocyclic moieties would amplify a chance of finding hit molecules while screening against targeted biomolecules.

To increase the molecular diversity, we used arenes that contain protected amine disposed ortho, meta- or para to the boronic moiety. With these molecules, we will be manipulating the number of torsional degrees of freedom per pitch and potential energy surfaces within the oligomers while synthesizing a library of foldamers. Also, it allows us to tune the location and number of noncovalent interactions while avoiding energetically unfavorable conformations. Currently, we successfully synthesized half a dozen Suzuki cross-coupled molecules and also testing compatibility in solid phase synthesis of peptidomimetics.

Poster 24.

Interference of Ionic Liquids on the Bradford Assay: A Spectroscopic Study

Tyler Johnston *and Mark P. Heitz**

Department of Chemistry and Biochemistry, The College at Brockport, SUNY, Brockport, NY

With the growing popularity of ionic liquids (ILs) in industry these substances are entering the environment. As these liquid salts become more widely used, it is essential that the effects and possible interference of these liquids on common laboratory techniques are characterized. The Bradford assay is a UV-vis absorption method used for protein quantification that relies on the specific interactions that occur between a protein and Coomassie Brilliant Blue G-250 (CBBG). Specifically, the assay depends on CBBG's color change when in the presence of protein. The bound form of the dye absorbs at 595 nm. Using known protein concentrations, a standard curve can be constructed. These data points are the baseline against which we can determine unknown protein solution concentration. The Bradford Assay is susceptible to interference from a large variety of chemicals, including surfactants and typical chemical denaturants. The similarity of IL/ surfactants structure suggests that ILs can perturb the determination of protein concentration via the Bradford assay. Therefore, the focus of our study is the spectroscopic measurement of the effects of imidazolium chloride ILs ($[Im_{x,1}]^+$ Cl^-) on the Bradford assay. Our results show that in neat IL solution, there is a systematic increase in the absorbance at 595 nm indicating that CBBG responds to presence of ionic liquid. The similar response of CBBG to both protein and $[Im_{10,1}]^+$ Cl^- creates a problem in that the presence of IL can result in a measured protein concentration that appears to be higher than what is actually present in solution.

Poster 25.

Selection of an Extraction Method for Nonpolar Organic Compounds from Silicone Wristbands

***Caitlin M. Massimi**, Connor Gould and David T.R. Stewart**

Department of Chemistry, D'Youville College, Buffalo, NY

Silicone wristbands have been studied to absorb numerous chemicals from the atmosphere. The idea behind using silicone wristbands is to determine the exposure a person experiences to harmful chemicals, on a daily basis. This project has taken that idea and is developing a method to extract such compounds, out of wristbands, and then measure them through gas chromatography coupled with mass spectrometry. So far, a method has been developed to measure the concentrations of chemicals using the GCMS. The objective of this current project is to determine the best method for the extraction of chemicals out of silicone wristbands. Multiple peer-reviewed articles were thoroughly read in order to analyze different extraction methods. A method was then determined from the articles. The extraction method involves a pre-rinse of the wristbands, a post-rinse, after the absorption of chemicals, a solvent extraction, and a concentration step. In the future, the extraction method will be tested and used. The plan is to test the extraction with known concentrations of samples in order to determine the effectiveness of the method. After it is refined, then the combined use of the extraction and GCMS method will be used to determine unknown concentrations of chemicals, from the atmosphere, as absorbed into silicone wristbands.

Poster 26.

Synthesis and Characterization of a Biomimetic Copper Complex of CuZnSOD

Jonathan M. DeMaria *and Allan Jay P. Cardenas**

Department of Chemistry and Biochemistry, SUNY Fredonia, Fredonia, NY

The synthesis of nitric oxide from arginine facilitated by nitric oxide synthase is well established. However, the involvement of Copper-Zinc Superoxide Dismutase (CuZnSOD) in the conversion of HNO to NO in the process is still an ongoing debate. In order to gain insights on how the CuZnSOD interacts with HNO to produce NO, the activation site of this enzyme is being modeled using a copper complex of the pyridine diimine (PDI) and diamide (PDA) ligands. This presentation will include the synthesis and characterization of the copper complexes.

Poster 27.

Work Towards the Use of Silicone Wristbands as Personal Passive Sampling Devices for Environmental Contaminants

Connor Gould, *CeDrice B. Howard and David T.R. Stewart**

Department of Chemistry, D'Youville College, Buffalo, NY

Silicon wrist bands (SWB) can be used to detect personal exposure to harmful chemicals present in the environment. They are efficient at collecting a wide range of nonpolar organic compounds [1]. Silicon wristbands are an easy and affordable method of collecting data without interrupting the daily activities of the wearers. A completed method would consist of three general steps: 1) a human subject would wear the SWB for a defined period, 2) the chemicals absorbed by the SWB would be extracted into a liquid solvent, 3) the solvent would be analyzed by gas chromatography mass spectrometry (GCMS) for quantitative analysis. The detected chemicals and the relative amounts and concentrations found may correlate to various socio-demographic differences.

The chemicals selected for this initial process include toluene, oxybenzone, chlorobenzene, and *N,N*-diethyl-meta-toluamide (DEET). GCMS can separate and qualitatively determine the presence of the target compounds from an extraction. External calibration curves that will allow the concentrations of the target compounds to be determined are currently under development. The current chromatographic method can accommodate future compounds without extensive modification. Future work will include the development of a method for extracting the target compounds from silicon wristbands consistent yields.

The portion of the project presented currently is work towards objective number 3.

[1] Kile, M. L.; Scott, R. P.; O'Connell, S. G.; Lipscomb, S.; MacDonald, M.; McClelland, M.; Anderson, K. A. Using silicone wristbands to evaluate preschool children's exposure to flame retardants. *Environmental Research* **2016**, *147*, 365-372.

Poster 28.

Synthesis and Characterization of Modified Anticancer Chalcone Analogues

Kaycie R. Malyk *and Mark Janik**

Department of Chemistry and Biochemistry, SUNY Fredonia, Fredonia, NY

Chalcones are biologically active molecules that are known for their numerous medicinal properties. Within the recent past, these compounds have been explored as potential drug candidates in cancer research due to their anticancer properties. Molecules with a chalcone-like structure have the ability to bind to the protein tubulin, which then inhibits the polymerization of tubulin into microtubules. It is this inhibition that can impart to these compounds their anticancer ability. There are three primary binding sites on tubulin that different chemotherapeutic agents utilize, the colchicine, the vinca alkaloid, and the paclitaxel site. For these analogs, the colchicine site will be of focus regarding the proposed anti-cancer mechanism of chalcones. This poster will discuss the background, synthesis, and characterization of modified chalcone analogues with the potential to act as tubulin binding agents.

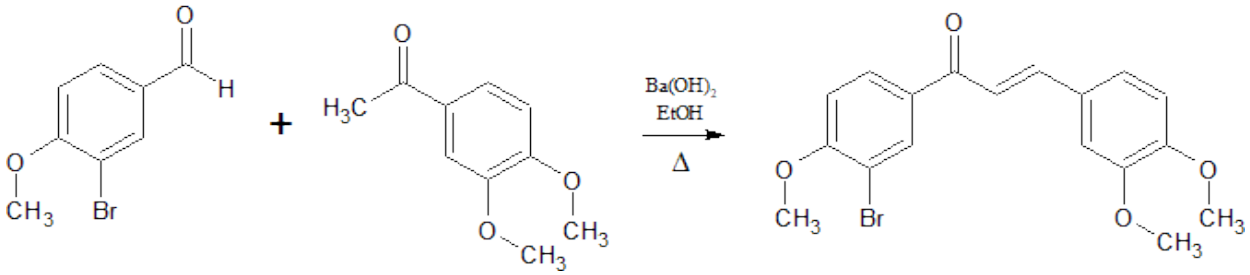


Figure 1. Reaction of 3-bromo-4-methoxybenzaldehyde, 3,4-dimethoxyacetophenone, and barium hydroxide to produce a chalcone analogue

NOTES: