The Tenth Annual

Undergraduate Research Symposium

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

Saturday April 8, 2017

Niagara University

NIAGARA UNIVERSITY

Education That Makes a Difference

Welcome Message

Curiosity. Look around the room today and I bet that we all hold this in common – we commit our time and efforts to chemistry and science due to curiosity. Not just passive interest, but interest in how things work, how we can improve things - make them a better way, understand them, apply them. I hope that you approach today's symposium with a fresh and curious mind – and that you find the presentations interesting and valuable simply for the sake of curiosity.

Each of the undergraduate students should be commended for engaging in research and for pursuing the opportunity to do something, to make something, and to contribute to the scientific endeavor. Events like this are a chance to celebrate this endeavor – whether the work is complete or is still underway, I hope you enjoy explaining your work to the like-minded folks who are here today.

Our keynote speaker, Dr. Christine Mahoney, has certainly followed her curiosity. After graduating from UB with a PhD in Analytical Chemistry, she started her career with pioneering work on the 3D analysis of polymers using Secondary Ion Mass Spectrometry (SIMS) at the National Institute for Standards and Technology (NIST). Since then, she has worked at other national labs, and is currently working in industry at Corning, Inc. Her research has touched on explosive analysis, biofilms and environmental samples, and other materials. Her talk today, *Surface Analysis Across Disciplines*, will touch on some of this work.

Niagara University is proud to host this event, and we hope you have a good time. Please take a moment to notice our sponsors and recognize their generosity in making this event possible!

On behalf of the organizing committee, welcome!

Dr. Robyn Goacher
Chair of 2017 Organizing Committee

2017 Symposium Organizing Committee

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

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

Dr. Dominic L. Ventura
Department of Math and Natural Sciences, D'Youville College

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

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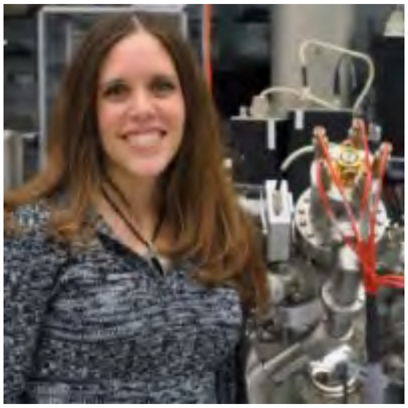

Surface Analysis Across Disciplines

Dr. Christine M. Mahoney

Dr. Mahoney is an analytical chemist, polymer chemistry expert and surface analyst, who has gained notoriety in the application of Secondary Ion Mass Spectrometry (SIMS) to the analysis of polymers and other organic materials. Dr. Mahoney has over 15 years of experience in materials characterization and method development. Following her formal education, she completed a National Research Council Post-Doctoral Fellow at NIST in Gaithersburg, MD, then joined NIST as a Senior Research Scientist where she maintained the TOF-SIMS research facility and developed “cluster SIMS” methodology characterization of polymeric biomaterials.

After NIST, Christine was a Senior Research Scientist at Pacific Northwest National Laboratory in Richland, WA where she served as a leader in the field of microscopy and microanalysis methods for both TOF and Nano SIMS, and worked towards developing this and other analytical approaches for forensics of explosives. She served a short stint at the Naval Research Laboratory furthering her research in the area of explosive forensics before joining Corning, Inc.

Christine holds a Bachelor’s degree in Chemistry from State University of NY at Potsdam and a PhD in Analytical Chemistry from State University of NY at Buffalo. Christine has more than 40 publications including a seminal work in Mass Spectrometry Reviews that has been cited over 200 times. She has authored several books and book chapters including being the editor and co-author of a book in the Wiley Series on Mass Spectrometry entitled “Cluster Secondary Ion Mass Spectrometry, Principles and Applications”.

Schedule of Events

April 8, 2017

University Dining Commons Addition
Niagara University, Lewiston NY

8:00 am - 8:50 am	**Registration**
8:50 am - 9:00 am	**Opening Remarks**
9:00 am-10:00 am	**Keynote Presentation:**

Dr. Christine M. Mahoney, Corning, Inc.

Surface Analysis Across Disciplines

10:00 am - 12:00 pm	**Student Oral Presentations**
12:00 pm - 1:00 pm	**Lunch**
1:00 pm - 2:30 pm	**Student Poster Session**
2:30 pm	**Symposium Awards and Closing remarks**

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ACS of Western New York

Oral Presentations

9:00 AM - 12:00 PM (University Dining Commons Addition)

Keynote Address

9:00 am **Christine M. Mahoney** Corning, Inc.

Surface Analysis Across Disciplines

Student Presentations

1. 10:00am **Zoe Vaughn** University at Buffalo

   The Application of (2-Hydroxyethyl Methacrylate) HEMA Hydrogel for Wound Healing

2. 10:20am **Andrew Fleischer** Rochester Institute of Technology

   Vacuum UV Photo-Oxidation of Poly(ethylene terephthalate)

3. 10:40am **Scott Laengert** McMaster University

   Sequential Functionalization of a Natural Cross-linker Leads to Designer Silicone Networks

4. 11:00am **Danny Belmona** Niagara University

   An Alternative Synthetic Pathway for a Cytotoxic Compound for Lymphocytic Leukemia

5. 11:20am **Thomas Bui** University at Buffalo

   Using Vibrational Sum-Generation Frequency to Study the Effects of Alkaline Salts and Sodium Dodecyl Sulfate on the Ordering of Single Wall Carbon Nanotubes

6. 11:40am **Kris Hoyt** Buffalo State College

   Freezing-induced Gold Nanoparticle Aggregation and its Effect on SERS

Student Abstracts

Talk 1

The Application of (2-Hydroxyethyl Methacrylate) HEMA Hydrogel for Wound Healing

Zoe Vaughn*, Christopher Heimburger, Austin Quinn and Joseph Gardella**

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

Chronic wound care has been gaining momentum due to drug delivery with the use of growth factors. Proteins such as Keratinocyte Growth Factor, KGF, leads to wound healing in the epithelial cells, and has also proven to promote wound closure. Hydrogels, water swollen structures composed mainly of hydrophilic polymers, serve as a vehicle that delivers the desired substance into the exact location needed for wound healing. Hydrogels aqueous nature allows the material to accommodate various therapeutic factors. 2-Hydroxythyl Methacrylate, HEMA, hydrogel is optimal because of its ability to achieve different characteristics without significant change to the polymer. Through swelling of HEMA and perfluoropolyether, PFPE, a cross linker, it was proven that HEMA holds up to 60% water by weight. Through the study it shows that HEMA is an excellent hydrogel to use when up taking protein such as KGF, proven through the results of the controlled release study. Knowledge that KGF is up taken was further proved by fluorescence and TOF SIMS. Uptake and release studies conducted on Green Fluorescence Protein, GFP, a reporter gene, also proved that HEMA can uptake protein. Through the various experiments indicate that HEMA hydrogel may be a highly effective route in wound healing.

Talk 2

Vacuum UV Photo-Oxidation of Poly(ethylene terephthalate)

Andrew Fleischer[a], *Andrew Morgan*[a], *Matthew Cocca*[a], *Katerine Vega*[a], *Surendra K. Gupta*[b], *Michael Mehan*[c] *and Gerald A. Takacs*[a]*

[a] School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY
[b] Department of Mechanical Engineering, Rochester Institute of Technology, Rochester, NY
[c] Xerox Corporation, Webster, NY

Poly(ethylene terephthalate)(PET) is a common thermoplastic polymer used in various industries where PET is often exposed to radiation as well as an oxygen environment. Because this type of exposure can change the chemistry unfavorably, it has become common to modify the surface by oxygen-containing plasma affecting the hydrophilicity at the surface. The PET studied was treated with Vacuum UV (VUV) ($\lambda = 104.8$ and 106.7 nm) photo-oxidation using a microwave (MW) plasma of Ar as the radiation source which was then compared to a similar treatment where oxygen atoms produced from a remote MW plasma of a gaseous mixture of Ar-O_2 in the absence of radiation. X-ray photo-electron spectroscopy (XPS) detected a lower saturation level for the atomic % of O with VUV photo-oxidation (32 at%) than with O atom treatment (34 at% O). The C 1s curve fitting results for both treatment methods show a decrease in aromatic sp^2 carbons and an increase in the amount of carbon-oxygen bonding due to the formation of the carbonyl (C=O) and carbonate-like (O-(C=O)-O) moieties for VUV photo-oxidation; and C-O-C, C=O, and O-C=O moieties for O atom treatment, respectively. Advancing water contact angle measurements showed more of an increase in hydrophilicity with the O atom treated samples than VUV photo-oxidation. Atomic Force Microscopy (AFM) images displayed smoother surfaces after VUV photo-oxidation while O atom treatment resulted in insignificant changes in surface roughness. Rinsing the treated surfaces with ethanol solvent partially decreased the at% O indicating the formation of a weak boundary during treatment.

Talk 3

Sequential Functionalization of a Natural Cross-linker Leads to Designer Silicone Networks

***Scott E. Laengert**, Alyssa F. Schneider, Eric Lovinger, Yang Chen, and Michael A. Brook**

Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON

Silicone polymers, or polysiloxanes, are used in a wide variety of practical applications including medical implants, industrial sealants, and electronic insulators. Silicones can be produced in various forms, such as oils, gels, elastomers, hard plastics, and foams, but achieving precision control of network structures is challenging, since functional groups introduced in industrial processing are often randomly distributed along the silicone backbone.

We have developed a system for the construction of precise silicone networks using the natural product eugenol, an extract of cloves and other plants, by taking advantage of its triple functionality in a selective and sequential manner (Figure 1). The boron-catalyzed Piers-Rubinsztajn reaction, using H-terminated silicones to create Si-O-C bonds, reacts fastest with the phenol group and slower with the methoxy group.[1] By adding a single equivalent amount of H-terminated silicone, the reaction at the phenol group takes place selectively, and subsequent addition of a second portion leads to reaction of the methoxy group. Adding a platinum catalyst and a third equivalent of Si-H leads to a hydrosilylation reaction of the silicone with the allyl group and the creation of an Si-C bond.[2] Remarkably, these two catalysts do not interfere with each other, and these three reactions can therefore be performed in any order, in the same reaction vessel, and without the need for workup of any kind. The result is that a variety of H-terminated polysiloxanes can be easily used to form chain extended polymers, elastomers, or foams in which the morphology of the material and its constituent parts can be manipulated at wi

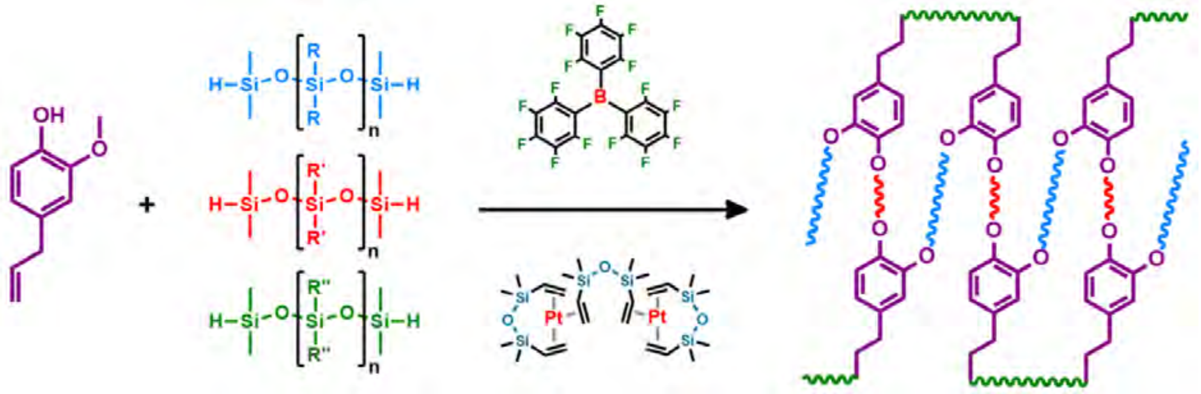


Figure 1. Eugenol can react selectively with a variety of different H-terminated polysiloxanes to produce ordered silicone networks with tunable properties.

References:

(1) Grande, J.; Gonzaga, F.; Brook, M.A. “Rapid assembly of explicit, functional silicones.” *Dalton Trans.*, **2010**, *39*, 9369

(2) Grande, J.; Urlich, T.; Dickie, T.; Brook, M.A. “Silicone dendrons and dendrimers from orthogonal SiH coupling reactions.” *Polym. Chem.*, **2014**, *5*, 6728

Talk 4

An Alternative Synthetic Pathway for a Cytotoxic Compound for Lymphocytic Leukemia

***Danny Belmona**, Zachary Mariani, Stephanie Scharmach and Luis Sanchez**

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

(−)-Communesin F is a naturally occurring compound isolated from marine and terrestrial Penicillium fungi. This compound sparked interest in the scientific community due to its significant cytotoxicity against lymphocytic leukemia cells in humans. (−)-Communesin F also has minimal effects on other cells making it highly selective against leukemia, however, extracting even trace amounts from natural sources is extremely costly, difficult, and time-consuming. Research on this compound has revealed that it can be biosynthesized from another natural product, (–)-aurantioclavine. Our goal is to efficiently synthesize (–)-aurantioclavine at a minimal cost, to be able to produce the final material in appropriate quantities. We are currently comparing two potential starting materials, tryptamine and 3-indolepropionic acid, which give us an inexpensive platform to start the synthesis. Our key synthetic steps include a Schmidt reaction and a Meyers chiral formamidine-based alkylation, to install two important structural features found in aurantioclavine: a seven-membered ring and a benzylic chirality center. Our progress in these efforts will be presented.

Talk 5

Using Vibrational Sum-Generation Frequency to Study the Effects of Alkaline Salts and Sodium Dodecyl Sulfate on the Ordering of Single Wall Carbon Nanotubes

Thomas T. Bui*, Sanghamitra Sengupta, Soha Talal Algoul and Luis Velarde**

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

We examine the effects of concentrations of sodium dodecyl sulfate (SDS) encapsulated with different diameters, (7,6) and (6,5), of single wall carbon nanotubes (SWCNT) with and without external alkaline chloride salts on thin glass film surfaces by using sum-frequency generation (SFG) spectroscopy. Studying SWCNT surfaces has been an interest due to their importance and applications to modern day material science. Understanding the nature of the interactions may help researchers develop a better technique to separate metallic and semi-conducting SWCNTs. We have found distinctive surfactant ordering between the (7,6) and (6,5) SWCNT as well as great reproducibility in our experimental data. The surfactant ordering lowers as we decrease the surfactant concentration on both SWCNT surfaces. Though there are weak van der waal forces working between just SDS-SWCNT molecules, the interactions shift to strong electrostatic interactions when alkaline salts are added to the system. 14mM and 10mM of SDS followed the trend that (6,5) was more ordered when compared to (7,6) SWCNTs, but when studying with 7mM, (7,6) showed to be more ordered than (6,5). When using our SFG spectra technique with the presence of ions, we found the ordering trend to be $K^+ > Na^+ > Ca^{2+}$ in (7,6), but the ordering shifted for (6,5) with the trend $Na^+ > K^+ > Ca^{2+}$, both at 14mM SDS concentration.

Talk 6

Freezing-Induced Gold Nanoparticle Aggregation and its Effect on SERS

Kris Hoyt *and Jinseok Heo**

Department of Chemistry, SUNY Buffalo State, Buffalo, NY

Here, we present that gold nanoparticle (AuNP) aggregates induced by quick freezing can be potentially useful as Surface Enhance Raman Scattering (SERS) substrates in the near-IR region. A near-IR SERS is an attractive method to obtain the Raman signals of an analyte in biological matrices that often show strong fluorescence background. The AuNP aggregates were prepared by freezing a solution of AuNPs with an average diameter of 70 nm in liquid nitrogen quickly and thawing it at room temperature slowly. After a cycle of the freezing and thawing process was completed, a plasmon band intensity of AuNPs at 542 nm, which originates from free AuNPs, significantly decreased but a plasmon band intensity in the near-IR region increased. These contrasting changes in the plasmon band strongly support the aggregation of AuNPs. The SERS spectra of Rhodamine 6G (R6G) were obtained with a 738 nm near IR laser in the presence of AuNPs before and after the freezing-induced aggregation. The SERS signals of R6G were ~2 x stronger with the AuNP aggregates. This signal enhancement is ascribed to the match of a plasmon wavelength of AuNP aggregates with a laser excitation wavelength of 738 nm. The freezing-induced AuNP aggregates were stable in a solution for at least a month, suggesting that this simple freezing method could be useful in producing near-IR SERS substrates.

Student Poster Presentations

Time: 1:00-2:30 PM (University Dining Commons Addition)

Poster 1 . **Dania Abdelhussein, Natalie Esadah**, Jerry Cartagena, Leander Bromley and Luis Velarde*

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

Using Sum Frequency Generation Spectroscopy to Examine Carbamate Pesticides on Silica Surfaces

Poster 2 . **James J. Rutowski**, **Anthony J. Berardi**, **Samantha T. Caico** and Jeremy L. Steinbacher*

Department of Chemistry and Biochemistry, Canisius College, Buffalo NY

Toward Novel Nanomaterials for ^{19}F Magnetic Resonance Imaging (MRI) Contrast Agents

Poster 3 . **James T. Marton, Ciara Pitman** and Robyn E. Goacher*

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

Analysis of Acid Digestion of Sugars from the Breakdown of Wood Using Multiple Analytical Methods

Poster 4 . **Korey Bedard**, **Scott Miskey**, Tomas Hudlicky* et al.

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

Chemoenzymatic Approach to Total Synthesis by the Hudlicky Research Group

Poster 5 . **Justin N. Bui** and Hou U. Ung*

Department of Chemistry, St. Bonaventure University, St. Bonaventure, NY

Probing the *i*-Motif Using Guanidinylated Cytosine

Poster 6 . **Kelli M. Burkholder** and Robyn E. Goacher*

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

Distributed Pharmaceutical Analysis Laboratory (DPAL) - Metformin Analyzed via HPLC

Poster 7 . **Alejandro Falca** and David F. Watson*

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

Excited-State Charge Transfer Between Covalently Tethered CdSe/CdTe Quantum Dots and Mesoporous TiO_2

Poster 8 . **Rebecca Ford,** Emily York and Luis Sanchez*

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

Preparation of L- and D-Vinylglycine-Based Building Blocks for the Synthesis of Medically Relevant Complex Molecules.

Poster 9 . **Filippo Gentile**, Isabelle Kozik and Timothy M. Gregg*
Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY

Substituent Effects in Aldol Reaction Rates

Poster 10 . **Etta J. Hanlon**, Jay Tinklepaugh, Britannia M. Smith, Yan Nie, Kelsey Moody, Kris Grohn, Fadi Bou-Abdallah and Robert P. Doyle*
Department of Chemistry, Syracuse University, Syracuse, NY

Saposin B Binds the Lipofuscin Bisretinoid A2E and Prevents its Enzymatic and Photo Oxidation

Poster 11 . **Kevin R. Huss** and M. Scott Goodman*
Department of Chemistry, SUNY Buffalo State, Buffalo, NY

What's In Your Friday Night? Locally Distilled Vodka Analysis

Poster 12 . **T. Huynh**, **J. Cubello**, J. F. McArthur, M. Q. Irving, J. Hughes, J. Schentag, L. M. Mielnicki and M. P. McCourt*
Department of Chemistry, Biochemistry and Physics, Niagara University, NY

Encapsulation and Delivery of Trastuzumab into Human Breast Cancer Cells Using Cholestosomes™

Poster 13 . **Jacob Kunz**, Sara Alam El Din, Allison Milano and Kelley Donaghy*
Department of Chemistry, SUNY College of Environmental Science and Forestry, Syracuse, NY

From Sludge to Silver: Creating Value-Added Materials from Teaching Laboratory Waste

Poster 14 . **Elliott Martin**, Steele Burgeson, and Luis Sanchez *
Department of Biochemistry, Chemistry, and Physics, Niagara University, NY

Development of a Biaryl Oxidative Coupling-Based Route to the Anti-Tumor Natural Products TMC-95

Poster 15 . **Ryan M. Becht** and Jeremy L. Steinbacher*
Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY

Developing Experiments for a Materials Chemistry Laboratory Course

Poster 16 . **Sean D. Mason**, Xaiolong Yang and Feng Li*
Department of Chemistry, Brock University, St. Catharines, ON

A Bipedal DNA Walking Device for Biosensing Applications

Poster 17 . **Dhvani Patel**, Yasser Heakal and Dominic L. Ventura*
Department of Chemistry, D'Youville College, Buffalo, NY

Design and Synthesis of Chloroquine Analogs

Poster 18 . **LeAnn Richert** and Luis Sanchez*
Department of Biochemistry, Chemistry, and Physics, Niagara University, NY

A Shapiro Elimination/Epoxidation-Based Strategy for the Synthesis of Cage Molecule Building Blocks

Poster 19 . **Arianna R. Rothfuss**, Tammy M. Milillo, Joshua S. Wallace and Joseph A. Gardella, Jr.*
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Tonawanda Coke Contamination Study

Poster 20 . **Kevin Lucas**, Christopher Swagler and Robyn Goacher*
Department of Biochemistry, Chemistry, and Physics, Niagara University, NY

Variability Among Options to Heat 96-well Plates

Poster 21 . **Benjamin Russ**, **Connor Tumiel**, Phillip Sheridan*, Matthew Bucchino, and Lucy Ziurys
Department of Chemistry and Biochemistry, Canisius College, Buffalo NY

The Pure Rotational Spectrum of KO: A Possible Circumstellar Molecule

Poster 22 . **Maoj Awad,** Saurabh Chauhan and David Watson*
Department of Chemistry, University at Buffalo, SUNY, Buffalo, NY

Effects of the Length of Bifunctional Molecular Linkers on the Lifetime of the Transferred Electron from Quantum Dots to Metal Oxides

Poster 23. **Emily Steiner,** Mary Hejna and Luis Sanchez*
Department of Biochemistry, Chemistry, and Physics, Niagara University, NY

Studies Toward the Synthesis of *ent*-Artemisinin, a Potential Anti-Malarial Compound

Poster 24 . **W. Benton Swanson**, John R. Verdi and Mariusz Kozik*
Department of Chemistry and Biochemistry, Canisius College, Buffalo, NY

Further Investigation of Transition-Metal Substituted Polyoxotungstates in Non-Polar Solvents using 2D DOSY ^{31}P NMR and Density Functional Theory

Student Abstracts

Poster 1

Using Sum Frequency Generation Spectroscopy to Examine Carbamate Pesticides on Silica Surfaces

Dania Abdelhussein, Natalie Esadah*, Jerry Cartagena, Leander Bromley and Luis Velarde**

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

According to the Environmental Protection Agency (EPA), over 1 billion pounds of pesticides are used in the United States yearly. Pesticides may spread by entering bodies of water and soil, and may also be absorbed by plants and animals due to the lack of pest control. One of the most widely used pesticides is Carbamate; which is used in homes, gardens, and agricultural environments. Carbamates harmful effects include inactivation of the acetylcholinesterase enzyme as well as interfering with the reproduction system and the fetal development**.** To know the mobility of a pesticide, the interactions between the pesticides and soil particles are important to understand. One of the most common minerals in the soil is silica, which is why in this study, carbamate was tested on silica surface to predict the interactions, which include the absorption and molecular level interactions between the pesticide carbamate and soil. The interactions of the molecules were observed by using sum frequency generation spectroscopy (SFG). SFG is a non-linear laser spectroscopy tool which provides vibrational spectra of molecules in surfaces and interfaces. By using SFG, we collected spectroscopic measurements of Propoxur and Carbaryl at the air/silica interface in order to identify the vibrational spectra of the interfaces at multiple infrared (IR) regions. After obtaining these results, we now have a better understanding of the pesticide mobility on the mineral surface and we will be able to avoid or minimize contamination of ground waters and water bodies.

Poster 2

Toward Novel Nanomaterials for ^{19}F Magnetic Resonance Imaging (MRI) Contrast Agents

***James J. Rutowski**, **Anthony J. Berardi**, **Samantha T. Caico** and Jeremy L. Steinbacher**

Department of Chemistry and Biochemistry, Canisius College, Buffalo NY

Targeted drug-delivery using multifunctional nanomaterials has become a major research focus as a means to overcome the limitations of low therapeutic efficacy and toxicity after systemic administration of chemotherapeutic drugs for treating cancer. The most advanced materials also incorporate an imaging contrast agent to enable simultaneous therapy and imaging of diseased tissues. There is currently no drug-delivery agent incorporating a fluorine magnetic resonance imaging (MRI) contrast agent that provides all of the characteristics of a multifunctional drug-delivery agent – choice of therapeutic payload, molecular targeting, biocompatibility, and imaging agent. Unless such a material is developed to fulfill this unmet need, fluorine MRI will remain underutilized as a cutting-edge means of detecting and treating human diseases such as cancer.

Here, we present work toward synthesizing new nanomaterials for use as multifunctional ^{19}F MRI contrast agents. We have synthesized a variety of fluorine-containing organic electrophiles for conjugation to nanomaterials that posses complementary nucleophiles. Many of the electrophiles contain hydrophilic groups to maximize solvation in aqueous environments relevant to biomedical imaging. To date, most of our work has centered on conjugating these fluorinated electrophiles to porous silica nanoparticles, a well-characterized platform for multifunctional drug-delivery agents. Our studies to-date show that functionalization of silica nanoparticles with fluorine is possible, but our system requires optimization. Moreover, we have begun work toward synthesizing fluorinated amphiphiles based on β-cyclodextrin, an inexpensive, safe, and natural nanomaterial.

Poster 3

Analysis of Acid Digestion of Sugars from the Breakdown of Wood Using Multiple Analytical Methods

James T. Marton, Ciara Pitman *and Robyn E. Goacher**

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

Second generation biofuels, whose feedstock includes wood chips and cornhusks, can be a new source of energy. Degradation of wood into sugars is an important step in the process. Previous work in our lab attempted to produce sugars from birch and spruce using cellulase and other enzymes. A 3,5-dinitrosalicylic acid (DNS) assay was performed to detect initial sugar production, but this analytical technique is not specific and measures only reducing ends. Analysis of glucose and xylose, the two sugars of interest, can be done using Liquid Chromatography-Electrospray Ionization-Mass Spectrometry (LC-ESI-MS). However, the concentrations of glucose and xylose monomers in the enzyme-digested wood supernatants were much lower with the LC-MS in comparison to the DNS assay. This indicated that the signal from the DNS assay may have arisen from soluble oligomers of the sugars. The aim of the acid digestion step is to break down these oligomers into monomeric glucose and xylose for LC-MS detection.

Acid digestion began by treating cellulose and xylan standards, which were analyzed using DNS and LC-MS. Furthermore, sugar standards of glucose and xylose were tested to ensure that the digestion method used did not degrade the original sugars. Then, the modified acid digestion procedure was applied to supernatants from the enzymatic digestion of both extracted and unextracted birch and spruce to see if it is possible to detect xylose and glucose sugars in the LC-MS. This work dovetails with efforts to determine whether the small molecule mediator ABTS, which is needed for laccase enzyme activity, causes matrix effects. Furthermore, the proteins themselves were studied for potential matrix effects, and sugars were present in the proteins used, which were assumed to have been added as stabilizers. Future work will involve continuing the acid digestion of the supernatants and determining which enzyme combinations will most effectively produce sugars, which can ultimately be used as fuel.

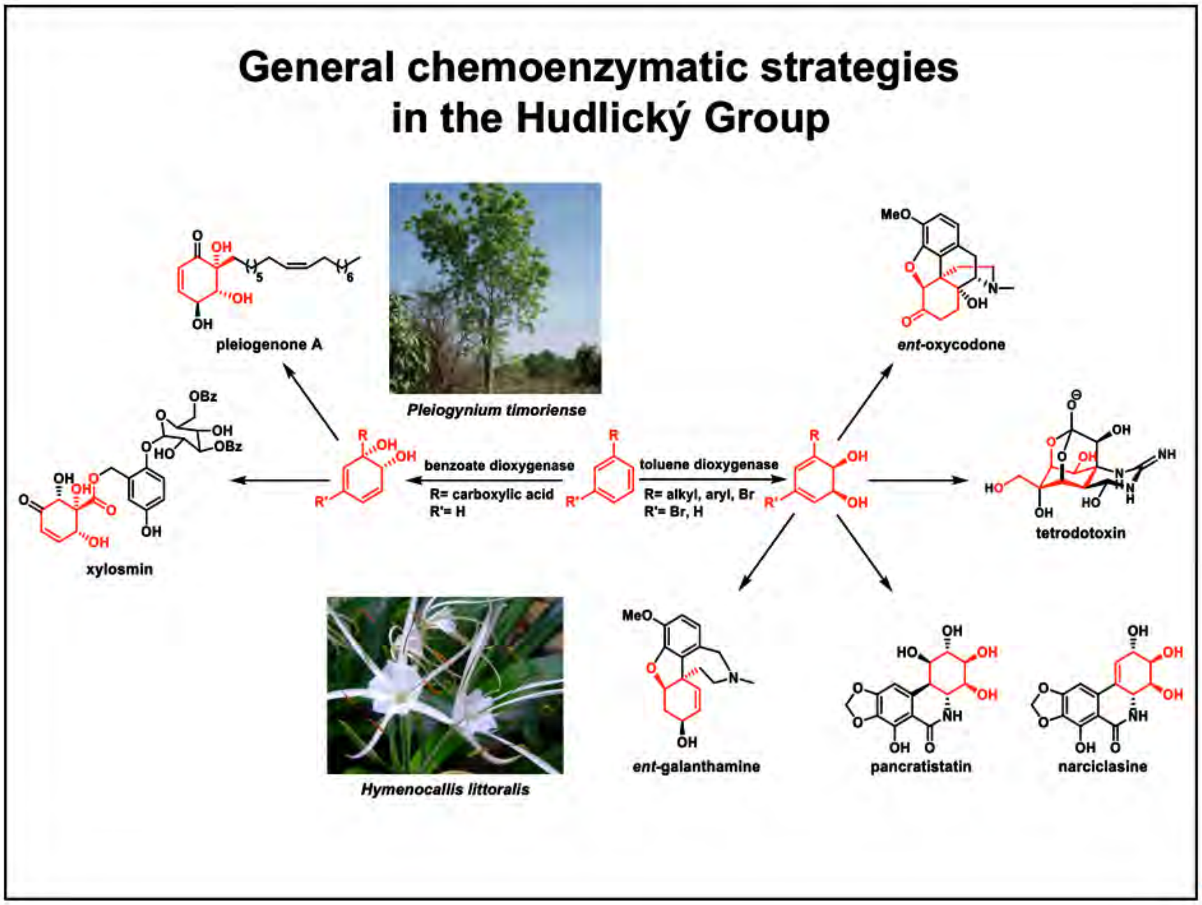
Poster 4

Chemoenzymatic Approach to Total Synthesis by the Hudlicky Research Group

***Korey Bedard**, **Scott Miskey**, Dale Lyons, Cameron Overbeeke, Daler Baidilov, Vincenzo Ticli, Mariia Makarova, Ringaile Lapinskaite, Tyler Bissett, Chelsea Rintelmann, Vimal Varghese, Jordan Froese, Brennan Murphy, John Trant, Lukas Rycek, Mukund Ghavre, Mary-Ann A. Endoma-Arias, Helen De La Paz, Razvan Simionescu, Josephine W. Reed and Tomas Hudlicky**

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

A description of chemoenzymatic methods for synthesis used by the Hudlicky group for approaches to complex natural products will be presented. The use of biotransformations has allowed for the enantioselective conversion of small aromatic substrates to highly oxygenated chiral pool intermediates, which have facilitated the preparation of numerous natural products in an enantiocontrolled manner. The *cis*-diols resulting from these transformations have been employed within our group in the synthesis of Amaryllidaceae alkaloids and morphinan-type alkaloids, among other natural products.



Poster 5

Probing the *i*-Motif Using Guanidinylated Cytosine

Justin N. Bui *and Hou U. Ung**

Department of Chemistry, St. Bonaventure University, St. Bonaventure, NY

Binding of DNA nucleobases makes use of hydrogen bonding, regardless of whether neutral nucleobases associate to form the Watson-Crick double-helix or to form alternative structures such as the G-quadruplex and the *i*-motif. DNA conformations such as the G-quadruplex and the *i*-motif form when guanine-rich regions and the complementary cytosine-rich strands separate and undergo single-strand self-association. Promoter regions of several oncogenes are believed to adopt *i*-motif conformations when underwound. If this hypothesis is correct, stabilizing the *i*-motif with small organic molecules *via* hydrogen bonding or other forms of intramolecular interactions may suppress the transcription of harmful mRNA, thus halting the spread of cancerous cells. Several guanidinylated cytosine derivatives have been synthesized. These cytosine derivatives are functionalized at the *N4*-position of cytosine with cyclic guanidine groups. These derivatives show favorable binding and stabilization of the *i*-motif. Several of the cytosine derivatives increased the UV melting points of *i*-motif forming DNA sequences by as much as 11°C.

Poster 6

Distributed Pharmaceutical Analysis Laboratory (DPAL) - Metformin Analyzed via HPLC

Kelli M. Burkholder *and Robyn E. Goacher**

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

Metformin is a widely used drug given to individuals suffering from Type-II diabetes. Metformin is currently being given to individuals in African countries. The DPAL project is working to find a method to analyze if the pills are correctly dosed and what is in the pills, as metformin has related compounds that may be present in the samples. Metformin was analyzed via an HPLC method to determine retention time and concentration when compared to a United States Pharmacopeia (USP)-metformin calibration curve. Upon analysis it was found that metformin has an average retention time of 1.96 min. Metformin related compounds B and C have retention times of 1.32 min and 4.20 min respectively. USP-metformin was determined to have a limit of detection of 0.2ppm and a lower limit of quantification of 0.7ppm. Expired metformin pills were also analyzed on the HPLC, no degradation products were detected but the concentration of the pill solution was used to calculate that the pill dosages were 5.9% to 7.5% lower than labeled. A spike recovery was performed on the expired metformin pill samples and matrix effects were not observed. Under dosed, correctly dosed, and overdosed USP-metformin solutions were prepared based on the concentration of the expired metformin pill sample that was analyzed. When these samples were run against a calibration curve, a 2-3% error was obtained that was systematically low. In the future it is hoped that a full USP-method will be put into place for those receiving metformin to be able to determine the dosage of the pill and if any degradation products are present.

Poster 7

Excited-State Charge Transfer Between Covalently Tethered CdSe/CdTe Quantum Dots and Mesoporous TiO_2

***Alejandro Falca** and David F. Watson**

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

Semiconductor quantum dots (QDs) are valuable light harvesters due to their size-dependent optoelectronic properties and large oscillator strengths. One major challenge is to maintain the separation of photogenerated charges. CdSe/CdTe heterostructures were assembled on TiO_2 films in order to spatially separate electrons and holes upon photoexcitation due to their Type II interface. *N,N'*-dicyclohexylcarbodiimide (DCC) mediated coupling chemistry was used to form the covalent linkage between quantum dots because it is selective, yielding heterostructures exclusively, and it allows for the control of the rate and extent of the coupling reactions. We expect that our configuration of QDs would minimize electron-hole recombination, improving the odds that photogenerated electrons and holes can be used to do work. Aqueous thioglycolic acid (TGA) capped CdSe QDs were synthesized by combining Cd and Se precursors under reflux. These TGA-capped CdSe QDs were then adsorbed to the surface of the TiO_2 film through soaking and activated via *N*-hydroxysuccinimide (NHS) coupling. Tetradecylphosphonic acid (TDPA) capped CdTe QDs were synthesized by combining and refluxing Cd and Te precursors under argon. The TDPA-capped CdTe QDs were chloride treated and coupled to 4-aminothiophenol (4-ATP) via ligand exchange. The CdSe/CdTe heterostructures were then synthesized via the *N,N'*-dicyclohexylcarbodiimide-mediated formation of amide bonds between capping ligands. QD synthesis and the products of ligand exchange and coupling reactions were characterized through ultraviolet-visible (UV-Vis) spectroscopy, ^1H nuclear magnetic resonance (^1H NMR) spectroscopy and attenuated total reflectance-Fourier Transform infrared (ATR-FTIR) spectroscopy.

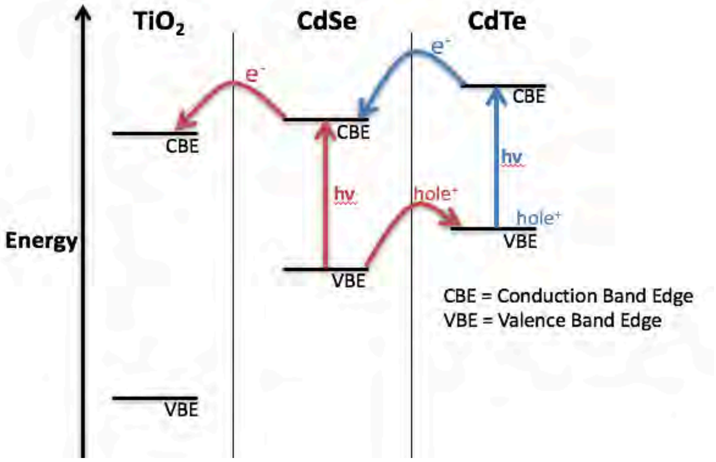


Figure 1. Estimated Energy Level Diagram of System

Poster 8

Preparation of L- and D-Vinylglycine-Based Building Blocks for the Synthesis of Medically Relevant Complex Molecules.

***Rebecca Ford**, Emily York and Luis Sanchez**

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

The unusual amino acid vinylglycine and a number of related compounds have been studied throughout the years for their involvement in certain biological processes and special reactivity. Given the presence of an alkene moiety, the structure of vinylglycine could be manipulated through a variety of chemical reactions, leading to larger and more valuable amino acid-like structures. Exploiting late-stage transformations on vinylglycine-containing peptide-like molecules could be of great use in the medicinal field.

While the preparation of vinylglycine has been extensively investigated in the past, its production is still problematical due to its sensitivity to racemization and isomerization, which renders key steps irreproducible during its synthesis. This project aims at developing an inexpensive approach to synthesize L- and D-vinylglycine derivatives as single enantiomers, using D- and L-serine respectively as starting materials. Additionally, we expect to find a means to protect this structure from racemization and isomerization via an appropriate derivatization. Our progress in these endeavors will be presented.

Poster 9

Substituent Effects in Aldol Reaction Rates

***Filippo Gentile**, Isabelle Kozik and Timothy M. Gregg**

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

The Aldol reaction is a staple of the undergraduate organic chemistry laboratory repertoire because it is operationally simple, the starting materials–ketones and aldehydes–are cheap and diverse, and it illustrates important concepts such as enolate chemistry and carbonyl electrophilicity. As electrophiles, benzaldehydes react rapidly, giving clean condensation products that are readily purified by recrystallization. The students at Canisius College perform an Aldol reaction experiment, in which they predict the effects of benzaldehyde substituents on the reaction rate, then make qualitative rate observations of which reactions actually proceed faster, and which slower. But, are observations of color change or precipitate formation reflecting the actual reaction rate?

To address this, question, Aldol reaction rates were measured by observing the disappearance of aldehyde by UV absorption at each aldehyde's λ_{max}, during progression of the reaction. With excess acetone, we were able to derive k_{obs} for the pseudo-first order reaction that involves rate-limiting attack of an enolate on the aldehyde carbonyl. These rates, using different aldehydes, correlate with Hammett sigma coefficients with slope of around 3, consistent with other studies of carbonyl additions.

We compared these reaction rates with the findings from the class experiment conducted at Canisius College in the spring of 2016. Students timed the first appearance of color change, but found this had no apparent correlation with substituent effects. On the other hand, the time to the first appearance of precipitate did appear to follow the expected rate trend. A rough translation of the class results into rate data allows a comparable Hammett plot that also exhibits slope > 1. This is good evidence that the observation of precipitation under the class conditions closely follows the rate-determining step of the reaction.

Poster 10

Saposin B Binds the Lipofuscin Bisretinoid A2E and Prevents its Enzymatic and Photo Oxidation

Etta J. Hanlon[1], *Jay Tinklepaugh*[1], *Britannia M. Smith*[2], *Yan Nie*[1], *Kelsey Moody*[3], *Kris Grohn*[3], *Fadi Bou-Abdallah*[2] *and Robert P. Doyle*[1,4]*

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[3] ICHOR Therapeutics, Lafayette, NY
[4] Department of Medicine, SUNY Upstate Medical University, Syracuse, NY

Vitamin A based bisretinoid accumulation in the retinal pigment epithelium is a major focus in the study of age-related macular degeneration (MD). The bisretinoid A2E is a pronounced bisretinoid in lipofuscin granules and accumulates in the lysosomes of retinal pigment epithelial cells. A2E has thus been extensively studied as a potential therapeutic target in the treatment of MD. However, whether or not endogenous lysosomal proteins can bind A2E and interfere with its enzymatic or photo induced oxidation has not been explored, providing an obstacle to any potential therapeutic agent. Herein, we demonstrate, using fluorescence and electronic absorption spectroscopy and mass spectrometry, that Saposin B, a critical protein in the degradation of sulfatides and 'flushing' of lipids, can bind A2E, preventing its H_2O_2-dependent enzymatic oxidation by horse radish peroxidase and photo oxidation by blue-light (450-460 nm).

Poster 11

What's in Your Friday Night? Locally Distilled Vodka Analysis

Kevin R. Huss *and M. Scott Goodman**

Department of Chemistry, SUNY Buffalo State, Buffalo, NY

Distilled vodka is typically 40% ethanol and 60% water (80 proof). However, during the distillation process the maximum percentage of ethanol is about 95.5% to 4.5% water and impurities (rectified spirit). This material is then diluted to achieve the desired percentages mentioned above. While the distilled ethanol is 95% pure, what could the impurities other than water in the initial distillation be? In order to address this question, samples of different "cuts" (heads, hearts and tails) were collected from local distilleries and analyzed using gas chromatography and mass spectrometry. Calibration curves were constructed for a few identified compounds to determine their percent. It was found that diethylacetal was sometimes identified in the hearts samples. Diethylacetal could be an indicator for aging in spirit alcohols, through the reaction of acetaldehyde, another impurity sometimes present in distilled spirits. In addition ethyl acetate was present in the head cuts, while various fusel oils were present in the tails cuts.

Poster 12

Encapsulation and Delivery of Trastuzumab into Human Breast Cancer Cells Using Cholestosomes™

T. Huynh[1], ***J. Cubello***[1], *J. F. McArthur*[2], *M. Q. Irving*[3], *J. Hughes*[1], *J. Schentag*[2,3,4], *L. M. Mielnicki*[1,3] *and M. P. McCourt*[1,3]*

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[2] Dept. of Pharmacy and Pharmaceutical Sciences, University at Buffalo, SUNY, Buffalo, NY
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According to the American Cancer Society, 1 in 8 (12%) of women in the United States develop invasive breast cancer. Among those individuals, approximately 25 to 30% of breast cancer cells exhibited elevated HER2 levels.[1] HER2 positive breast cancers identified by a pathologist typically exhibit amplification of the HER2 gene resulting in an overexpression of HER2 receptors.[2] The HER2 receptor (Human Epidermal Growth Factor Receptor 2) is a member of the epidermal growth factor family important for the intracellular signaling and regulation of cell growth. Trastuzumab (Herceptin®) is an IgG1 monoclonal antibody that has been proven to be effective in HER2 positive patients. Trastuzumab binding to HER2 interferes both directly and indirectly with downstream intracellular signaling pathways.[3,4] Unfortunately, less than about 35% of patients benefit from treatment with trastuzumab while the remainder exhibit initial or acquired resistance to treatment.[4,5] Importantly, brain metastasis frequently occurs in trastuzumab treated patients.[6] This population of resistant patients inspires efforts towards a more effective delivery system for trastuzumab, including those that can cross the blood-brain barrier. This laboratory has developed a neutral lipid based vesicle (the Cholestosome^{TM}), that uses naturally occurring lipids for the delivery of a wide variety of therapeutics, including small molecules, antibiotics, peptides, and proteins. Previous work has shown Cholestosome^{TM} -mediated delivery of FITC-labelled peptides into various mouse tissues (including brain) after oral administration. The Cholestosome^{TM} can therefore potentially be used to orally deliver compounds for which intravenous administration is the only effective dosing route. The present studies describe the initial efforts at Cholestosome^{TM} encapsulation of trastuzumab.

Poster 13

From Sludge to Silver: Creating Value-Added Materials from Teaching Laboratory Waste

***Jacob Kunz**, Sara Alam El Din, Allison Milano and Kelley Donaghy**

Department of Chemistry, SUNY College of Environmental Science and Forestry,
Syracuse, NY

Waste materials from chemistry teaching labs contain precious metal ions such as silver, copper and gold. Silver chloride and silver nitrate are found in the waste material from the Analytical Chemistry 1 Laboratory (FCH 380) *Experiment 8A, B. Precipitation & Titration of Chloride Ion* at SUNY ESF. Aqueous silver ions and suspended silver chloride are reduced to silver metal nanoparticles using sodium borohydride, isolation of the silver ions from the solution via vacuum filtration produces metal nanoparticles that can be used in the production of precious metal clays (PMC). PMC's, made from castoff metals from the electronics industry are marketed to jewelry artists as an alternative to using molten metal to form intricate shapes. PMC's were made by combining various amounts of wheat flour binder, oil, water and a dispersing agent poly-vinylalcohol with silver nanoparticles from laboratory waste, brass particles recovered from metal machining, as well as silver purchased from Sigma-Aldrich. Once PMC's were prepared, they were fired in a kiln. Brass clays were fired twice: once at low-temperature to burn off the organic binder and the second firing, in graphite. This second firing, called sintering, allows the metal atoms to close holes and create a homogenous metallic structure. Silver is fired once as it does not oxidize at high temperatures and does not require graphite immersion binder and sintering can be done in one firing. A scanning electron microscope (SEM) was used to compare particle size of the metal nanoparticles and the fired metal surfaces.

Poster 14

Development of a Biaryl Oxidative Coupling-Based Route to the Anti-Tumor Natural Products TMC-95

***Elliott Martin**, Steele Burgeson and Luis Sanchez* *

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

First isolated from the fermentation broth of *Apiospora montagnei* Sacc. TC 1093, the natural products TMC-95 A–D are of great interest because of their biological activity against the 20S proteasome. This distinctive activity makes them promising candidates as agents for the treatment of cancer. However, constructing such complex molecular structures requires many synthetic steps, which hinders their potential medical use. These active compounds feature a peptide-based structure composed of tyrosine, asparagine, a highly oxidized tryptophan, (*Z*)-1-propenylamine, and 3-methyl-2-oxopentanoic units. A particularly unusual bond is found in these natural products: a biaryl connection between the tryptophan and tyrosine residues and, as a result of this strange C–C linkage, axial chirality is observed around this bond. Our primary interest in this project is to develop chemical conditions to form this important biaryl linkage via oxidative coupling of suitable tripeptide-based building blocks. Such an oxidative coupling can make the synthetic production of TMC-95 significantly easier, by starting with the inexpensive and widely available natural amino acid units. With an easier synthetic route, TMC-95-based compounds could become viable anti-tumor drug candidates.

Poster 15

Developing Experiments for a Materials Chemistry Laboratory Course

Ryan M. Becht *and Jeremy L. Steinbacher**

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

Here we present experiments conducted in preparation for a new elective laboratory course, Materials Chemistry. In this work, we conducted experiments from the literature with the goal of adapting them to a lab setting for students. Polymerization experiments included the ring-opening polymerization of polycaprolactone and the atom-transfer radical polymerization of acrylate and styrene monomers. Additionally, we synthesized semiconductor quantum dots. Lastly, the mechanical properties of several metal wires were measured using a structure analyzer and the effects of various heat treatments on the wires were explored. These results were incorporated into the lab course, which ran for the first time in the fall of 2016.

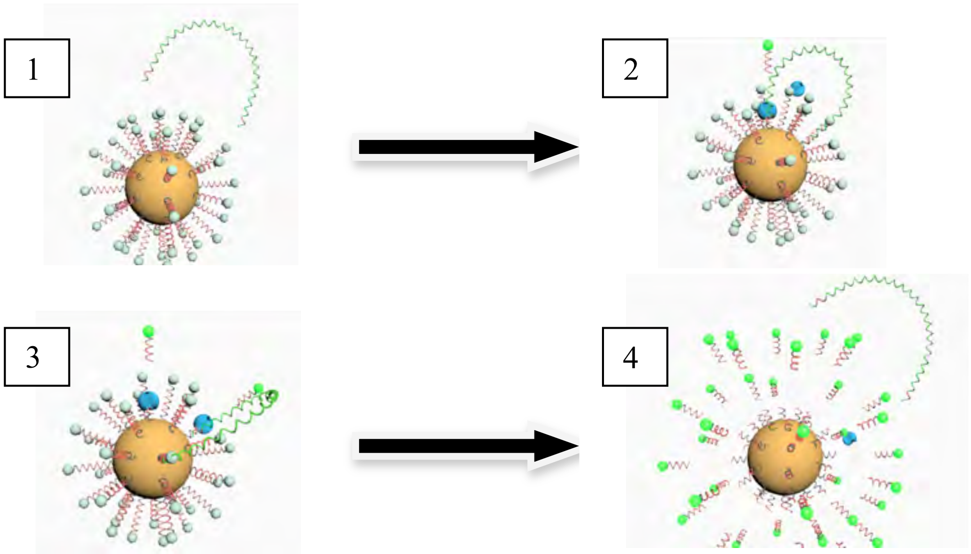
Poster 16

A Bipedal DNA Walking Device for Biosensing Applications

***Sean D. Mason**, Xaiolong Yang and Feng Li**

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

This project outlines the development of a bipedal DNA walking device. There are two DNA motifs in the walking device. The first is a single-stranded DNA walker which contains two identical nicking cleavage sites. The second is a fluorescently-labeled signal reporter (SR) containing a complimentary nicking cleavage site. The signal reporter is functionalized to a gold nanoparticle. In the presence of a nicking endonuclease enzyme, the DNA walker moves along a 3-D AuNP track by hybridizing and subsequently cleaving SRs. Since the fluorescence is initially quenched by the AuNP, operation of the DNA walker amplifies fluorescence signal. The question asked was if this walking device traversed a 3-D DNA track in a concerted walking fashion, or if it would traverse the track randomly. The mechanism was monitored by using two signal reporters, each with the same sequence, but a different fluorophore. Each signal reporter was functionalized to a separate gold nanoparticle. The bipedal DNA walking device was incubated to one type of gold nanoparticle for 30 minutes and the other type of gold nanoparticles were added to the solution afterwards. Nicking endonuclease was then added to initiate the DNA walking, and fluorescence was monitored using two channels, each corresponding to the signal generation from the two SRs on the different gold nanoparticles. We found that the signal generated from the DNA track which the bipedal was hybridized to saturated before the signal of the DNA track of the added gold nanoparticle. This suggested that the bipedal DNA walking device does traverse a three dimensional DNA track in a step-by-step walking fashion. This DNA walking device has potential to be used in biosensing applications by altering the sequence of the DNA walker.



Poster 17

Design and Synthesis of Chloroquine Analogs

Dhvani Patel[†]*, Yasser Heakal*[‡] *and Dominic L. Ventura**[†]

[†]Department of Chemistry, D'Youville College, Buffalo, NY
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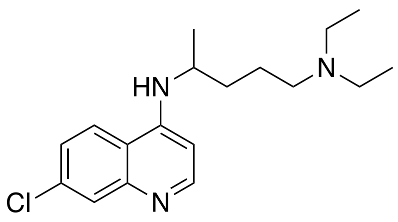
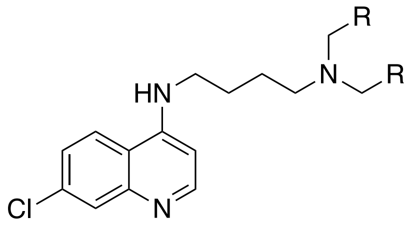
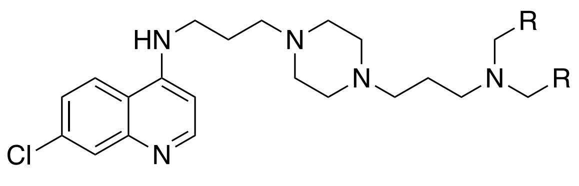
Chloroquine (CQ) is a chemotherapeutic agent and was also the foremost treatment of malaria for many years. First, a series of CQ analogs were designed/studied and the desired analog was then synthesized by reacting 4,7-dicholoroquinoline and 1,4-bis(3-aminopropyl) piperazine in 1-pentanol. The mixture was heated and held at reflux overnight. Then, various aldehydes with sodium triacetoxyborohydride were used to add a variety of alkyl or aromatic rings to the terminal amine. Next, it was washed, dried and purified by flash column chromatography to yield the desired, CQ analog.

Over the summer, we will be testing the synthesized CQ analog for inhibition of autophagy in triple-negative breast cancer cells. This part of the project will focus on taking advantage of polyamine transporters in targeting and delivering CQ, intracellularly.



Chloroquine





R = CH_3 , $CH(CH_3)_2$, Ph, (*p*-Cl)Ph, (*p*-NO_2)Ph, (*p*-F)Ph, (*p*-OCH_3)Ph

Poster 18

A Shapiro Elimination/Epoxidation-Based Strategy for the Synthesis of Cage Molecule Building Blocks

LeAnn Richert *and Luis Sanchez**

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

Platonic hydrocarbons and highly symmetric cage molecules have attracted the attention of chemists for decades. The first total synthesis of dodecahedrane, the simplest hydrocarbon with full icosahedral symmetry, more than thirty years ago was a remarkable and notorious achievement in organic chemistry. Still to date, however, the preparation of such compounds involves lengthy processes. Exploiting the elements of symmetry of the target cage molecules, as a tactic to minimize the necessary synthetic steps, is especially desirable.

We noticed that building blocks containing fused five-membered rings have been the central theme of a number of studies related to cage molecules. The idea of synthesizing symmetric compounds using polycyclizations, cycloadditions, and domino reactions continues to appear, even in very recent reports, but the preparation of the required substrates for such transformations has been generally unsuccessful. The present project offers both an alternative strategy and a method for the synthesis of C_2-symmetric cage molecule building blocks, which is based on a Shapiro reaction, an *m*CPBA-promoted epoxidation, and a β-elimination executed in sequence. Our approach and progress will be presented.

Poster 19

Tonawanda Coke Contamination Study

***Arianna R. Rothfuss**, Tammy M. Milillo, Joshua S. Wallace and Joseph A. Gardella, Jr.**

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

The Tonawanda Coke Corporation was found guilty of violating the Clean Air Act, Clean Water Act, and the Emergency Planning and Community Right-to-Know Act. The coke oven gases were allowed to leak benzene, formaldehyde, and other harmful chemicals into the air. Contamination was also leaked into the surrounding neighborhoods. One condition of the lawsuit was that the company must fund a multi-year study on the contamination and emissions from the Tonawanda Coke Corporation. To determine how the contamination spread, geographic information systems (or GIS) will be used. GIS is able to map out data concerning the spread of the contamination, along with the contamination levels. The data for the GIS maps will come from soil samples taken from residences in the areas near the Tonawanda Coke Corporation. The levels of various contaminations (from volatile organic compounds to metals) will be determined and mapped out.

Poster 20

Variability Among Options to Heat 96-well Plates

***Kevin Lucas**, Christopher Swagler and Robyn Goacher**

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

The 3,5-dinitrosalicylic acid (DNS) assay is commonly used for the measurement of sugars in solution, via reaction with the reducing ends of the sugars. In our lab, it is used to measure sugars produced by degrading lignocellulose with xylanase and cellulase enzymes. This colorimetric assay results in a color change from bright yellow to burnt orange as the reaction proceeds to completion. The DNS assay, like many others, requires heating to proceed. Originally, this reaction was done in test tubes in a boiling water bath, with large volumes of toxic chemicals used each time. With our research, we use 96-well plates heated at lower temperatures. Through this approach, we can generate large numbers of reactions using small volumes, limiting the hazardous waste used. We began the research by heating the 96-well flat-bottom plates on a dry bath with a heating block. However, when generating calibration curves, we were only able to obtain data with limited linearity. This poster will present data generated to troubleshoot the cause of this. The reproducibility of the plate-reader spectrometer was tested with dye solutions and found to be <2% RSD. However, when solutions of constant sugar concentration were reacted on the 96-well plate on the dry bath, we observed deviation across the 96-wells of >35% RSD. To fix the issues related to the high percent RSD and non-linearity, we evaluated the direct heating of 96-well plates using several methods. The Mx-Stratagene Thermocycler provided us with the most reproducible method for heating the enzyme reactions, limiting the deviations to ~5% across the 96-well thermocycler plate and providing for highly linear calibration curves. It is recommended that any lab group performing an assay or reaction requiring heating of a 96-well plate carefully consider the impact that variability in heating can have on the results.

Poster 21

The Pure Rotational Spectrum of KO: A Possible Circumstellar Molecule

***Benjamin Russ*[1], *Connor Tumiel*[1], *Phillip Sheridan**[1], *Matthew Bucchino*[2], *and Lucy Ziurys*[2]

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[2] Department of Chemistry and Biochemistry, The University of Arizona, Tucson, AZ

The potassium monoxide (KO) molecule is of interest for two primary reasons. First, the ground electronic state of KO is controversial. Two possibilities exist, $^2\Pi$ or $^2\Sigma$, however these two states are very close in energy. Second, KO is postulated to be present in the circumstellar envelope of the oxygen-rich star VY Canis Majoris. In order to investigate both issues, we have used millimeter-wave spectroscopy to measure pure rotational transitions of the KO molecule in the gas phase. KO was synthesized by the reaction of potassium vapor with nitrous oxide in a vacuum chamber. We have recorded continuous rotational spectra of KO in the 250 – 300 GHz region. From these spectra we have so far identified 11 rotational transitions belonging to the $^2\Pi$ electronic state. The frequencies of these transitions are currently being used to conduct a radioastronomical search for KO in VY Canis Majoris. The rotational spectra continue to be analyzed for additional transitions arising from KO.

Poster 22

Effects of the Length of Bifunctional Molecular Linkers on the Lifetime of the Transferred Electron from Quantum Dots to Metal Oxides

Maoj Awad, *Saurabh Chauhan and David Watson**

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

Quantum dots (QDs) are semiconductor with a bandgap that can be controlled across a wide range of energy levels by controlling their size. As the QDs get smaller the, the difference between the conduction and valence band increases, requiring more energy to excite the electrons. QDs are intriguing light-harvesters and excited-state charge donors. This advantage makes them favorable for solar cell production. One way to employ this property of QDs is to tether them to electron or hole accepting semiconductor substrate using bifiunctional molecular linkers. The properties of these ligands affect the process of electron transfer. Our group has reported these effects in dispersions of QD-molecular linker-semiconductor constructs. This poster will present an extension of this effort to study the effect of the length of these linkers on the process of electron transfer within nanocrystalline thin films. Excited-state electron transfer process was characterized using time correlated single photon counting (TCSPC). The difference in the lifetimes of the transferred electron between the four different lengths linkers suggest that the electron transfer yields depend significantly on the properties of the molecular linkers.

Poster 23

Studies Toward the Synthesis of *ent*-Artemisinin, a Potential Anti-Malarial Compound

***Emily Steiner**, Mary Hejna and Luis Sanchez**

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

Artemisinin is a natural product isolated from the plant *Artemisia annua* that is currently the fastest-acting treatment available against *Plasmodium falciparum*—the protozoan parasite that causes the deadliest form of malaria. The low bioavailability of this compound and its short half-life, however, make the cost of artemisinin therapies very high. Anti-malarial *combination* therapies involving artemisinin are employed to avoid the development of resistance to the drug by the parasite, as recommended by the World Health Organization.

Artemisinin's structure contains a unique peroxide bridge that is believed to be responsible for the drug's mechanism of action. We gather that the exceptional biological activity of this compound may originate in the fine-tuned chemical reactivity of its peroxide bridge, rather than the topology of the structure itself. Consequently, we hypothesize that its enantiomer (*ent*-artemisinin)—a yet unreported compound—could exhibit comparable anti-malarial properties. Seeking an affordable synthetic route, our current goal is to develop a reaction sequence to produce *ent*-artemisinin from zingiberene, a compound found in ginger oil. Thus far we have successfully isolated a ginger oil fraction in which zingiberene is the primary component (as per NMR analysis) and further purified it via a series of reactions. We have recently begun studies into the synthesis of the *ent*-artemesinin precursor molecule, *ent*-amorphadiene, from zingiberene, and have been analyzing this process via LCMS. If this proposed synthetic route is successful, we believe that the low cost and high availability of ginger oil would allow for the large-scale production of *ent*-artemisinin.

Poster 24

Further Investigation of Transition-Metal Substituted Polyoxotungstates in Non-Polar Solvents using 2D DOSY ^{31}P NMR and Density Functional Theory

***W. Benton Swanson**, John R. Verdi and Mariusz Kozik**

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

Transition-metal substituted polyoxotungstates (TMSPOTs), when transferred into nonpolar solvents, have been reported by several groups as potential catalysts for carbon dioxide reduction. Therefore, their structures in nonpolar solvents are of great interest. Recently we reported 2D DOSY ^{31}P NMR and DFT data that proved the existence of dimers in dry toluene solutions of tetraheptylammonium salts of cobalt substituted Keggin anion, $[PW_{11}CoO_{39}]^{5-}$, and trimers in THA solutions of Weakley's anions, $[PW_9O_{34}Co_4O_{34}W_9P]^{10-}$. However, the differences in intensity of the NMR signals between monomers and dimers or monomers and trimers were very large, making data interpretation questionable.

This poster reports the 2D DOSY NMR data for THA salts of nickel substituted Keggin anion in dry toluene. The intensities for both monomer and dimer are comparable this time. Therefore, we are totally confident that indeed there are dimers and monomers present. In addition, the ratio of radii obtained from DOSY and from DFT calculations are in better agreement for Ni-substituted than for Co-substituted Keggin anion. Also, as with previously reported TMSHPTs, the DFT calculations show that in dry toluene, for THA salts of Ni-substituted Keggin anions, the dimers are more stable than monomers. Interestingly, the DFT calculations confirm that the signal intensity ratio of dimer to monomer should indeed be closer to one for Ni-substituted anions than for Co-substituted anions.

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