2024 ROCACS Student Research Symposium

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The 68th Annual

Collegiate Research Symposium

Sponsored by the Rochester Section

of the American Chemical Society

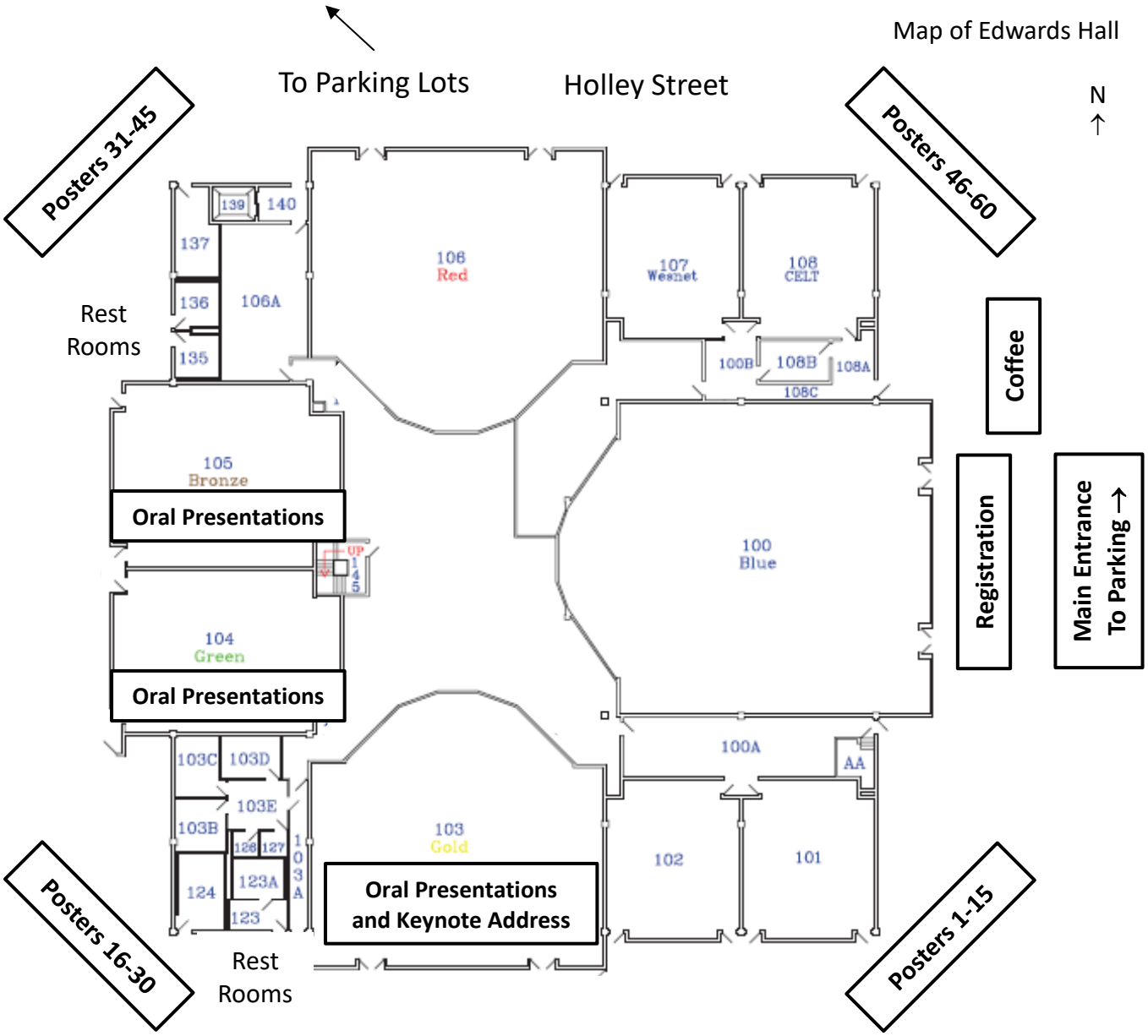
Saturday April 20, 2024

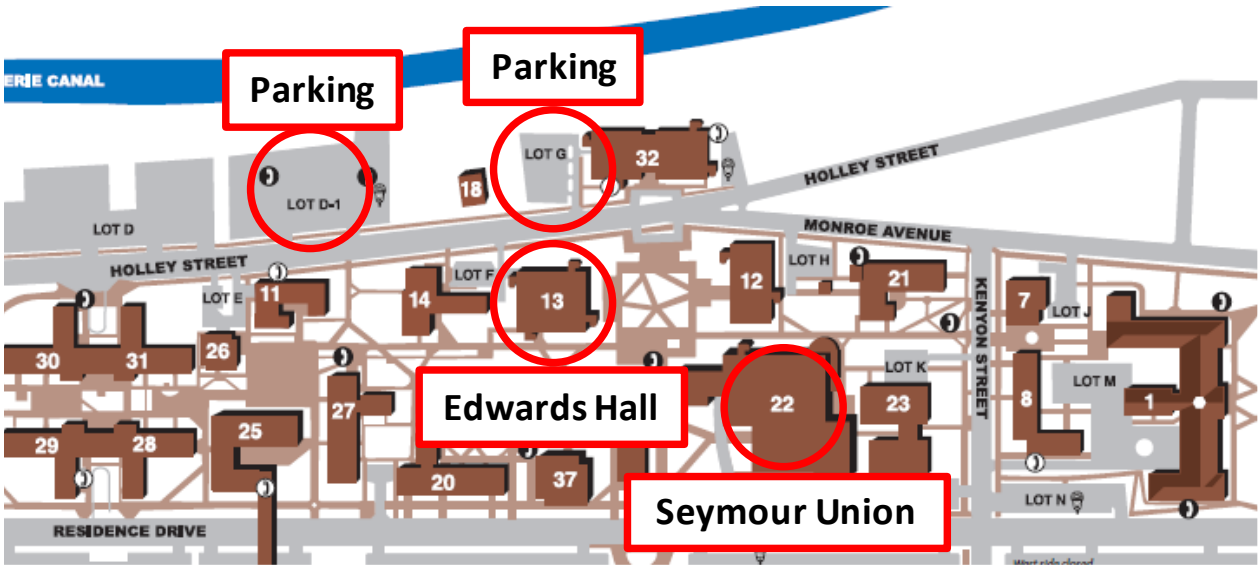
SUNY Brockport

Department of Chemistry and Biochemistry

SUNY BROCKPORT

Map of Edwards Hall





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Welcome Message

All of the students presenting here are to be commended for their hard work and dedication, 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 time to celebrate accomplishments – whether the work is complete or still underway. It is our hope that you enjoy sharing your work with like-minded folks who are in attendance today.

Our day's events will begin with a keynote address delivered by Dr. Lea Vacca Michel from Rochester Institute of Technology. Dr. Michel will present a talk titled "**Triggering toxicity: How antibiotics enhance the release of extracellular vesicles from Escherichia coli**". Dr. Michel is now Professor of Biochemistry at RIT. Lea received her B.A. degree in Physics and Math from Colgate University, her Ph.D. in Biophysics from the University of Rochester, and performed her postdoctoral research at Cornell University. After a brief stint in industry, Dr. Michel started her faculty position in 2009 at the Rochester Institute of Technology, where she is now a Professor in the School of Chemistry and Materials Science. In 2022, Dr. Michel was named the College's first Director of Diversity, Equity, and Inclusion. Currently, her research is focused on the role of proteins in disease. Dr. Michel strives to increase the participation of women and students with historically marginalized identities (including those who are d/Deaf and hard-of-hearing) in science and math.

Brockport University is pleased to host this event. Thanks to all who have participated in this year's event and especially all those who have volunteered their time and energy to make this happen. We hope you have a great day of conversation, collaboration, and discovery!

On behalf of the organizing committee, welcome!

Mark Heitz and Michael Coleman, Co-Chairs

2024 Rochester ACS Student Research Symposium

Symposium Schedule of Events

Saturday, April 20, 2024

Edwards Hall

SUNY Brockport, Brockport NY

8:00 am	Registration begins
8:00 am - 8:45 am	Oral and Poster Presentation Setup
8:50 am - 8:55 am	Opening Remarks, Edwards Hall, Room 103
9:00 am - 10:00 am	Keynote Presentation

Dr. Lea Vacca Michel, Rochester Institute of Technology

Triggering toxicity: How antibiotics enhance the release of extracellular vesicles from Escherichia coli

10:10 am - 11:30 am	Student Oral Presentations
11:30 am - 12:30 pm	Lunch and conversations, Edwards Hall
12:30 pm – 1:15 pm	Student Poster Session I – Odd Numbered Posters
1:15 pm - 2:00 pm	Student Poster Session II – Even Numbered Posters
2:00 pm	Symposium Awards, Closing Remarks

2024 ACS Student Research Symposium Acknowledgements

The Rochester Local Section of the American Chemical Society

SUNY Brockport Students, Faculty, and Staff
- Faculty of the Department of Chemistry and Biochemistry
  - Drs. Robert LeSuer, Carly Reed, Joshua Blose, and Markus Hoffmann
  - Provost Martin Abraham
- Ms. Kimberly Vonburen, Administrative Assistant - Poster supplies, name tags

- Brockport Student Volunteers
  - Silas Martin, Jaylyn Hill, Troy Smith, and Kachiri Guzman

- Other Volunteers
  - Nathaniel A. Coleman, Melissa Chandler (Agilent Technologies)

Keynote Speaker

Triggering toxicity: How antibiotics enhance the release of extracellular vesicles from Escherichia coli

Dr. Lea Vacca Michel

Lea Vacca Michel received her B.A. degree in Physics and Math from Colgate University, her Ph.D. in Biophysics from the University of Rochester, and performed her postdoctoral research at Cornell University. After a brief stint in industry, Dr. Michel started her faculty position in 2009 at the Rochester Institute of Technology, where she is now a Professor in the School of Chemistry and Materials Science. In 2022, Dr. Michel was named the College's first Director of Diversity, Equity, and Inclusion. Currently, her research is focused on the role of proteins in disease. Dr. Michel strives to increase the participation of women and students with historically marginalized identities (including those who are d/Deaf and hard-of-hearing) in science and math.

Abstract: Bacterial extracellular vesicles (BEVs) are nano-sized spherical particles released from bacteria and containing cellular biomolecules from their parent bacterium. While BEVs are constitutively released from Gram-negative bacteria (such as Escherichia coli), environmental factors such as temperature changes, stress, and antibiotics can enhance their release. We proposed that some antibiotics, such as beta lactams that target the peptidoglycan layer of the bacterial cell, enhance BEV release more than other types of antibiotics. We used ultracentrifugation, immunoblotting, and nanoparticle tracking analysis to isolate, detect, and quantify BEVs released from Escherichia coli in the presence of different antibiotics. Several beta-lactam antibiotics caused significantly more EV release, while quinolone and aminoglycosides caused relatively less vesiculation. These results underline the importance of antibiotic choice when treating sepsis patients.

Part of the research reported in this presentation was supported by NIAID of the National Institutes of Health under award number R21AI163782 (to LVM and TG).

Undergraduate Award for Outstanding Achievement in Chemistry

History

In 1989, the Rochester Section, Inc. of the American Chemical Society began recognizing undergraduates for their outstanding academic achievement by sponsoring an award for each college or university within the six-county area of the Rochester Section.

Criteria

The following criteria have been established for the award:

- Each department at a college or university within the geographic area of the Rochester Section that offers an undergraduate degree in chemistry or chemical engineering may nominate **one** graduating undergraduate student per year.
- The nominated student must be a full-time student who is expected to complete an undergraduate degree in chemistry or chemical engineering during the calendar year of nomination.
- The nominated student must have an outstanding academic record of achievement in chemistry and/or chemical engineering as rigorously measured by GPA (minimum 3.5/4.0), participation in research or other scholarly work, service to the department, and additional awards earned.
- Each nominating department may establish additional guidelines and criteria for use in selecting its recipient.

Congratulations to the 2024 Award Winners

Trevor Gienau	SUNY Brockport Department of Chemistry and Biochemistry
Isiah McMurray	Nazareth University Department of Chemistry and Biochemistry
Martina Videva	Rochester Institute of Technology School of Chemistry and Materials Science
Hope Silva	University of Rochester Department of Chemistry
Rebecca Choi	University of Rochester Department of Chemical Engineering

Oral Presentations

Session A, Edwards Hall 103

10:10 AM (OP1)
LITERATURE STUDY OF VITAMIN A AND A CHEMICAL UNDERSTANDING OF THE BIOLOGICAL SYSTEM TO DELVE DEEPER INTO THE RELATIONSHIP BETWEEN OTHER VITAMINS AND MINERALS
Logan Abaldo
Rochester Institute of Technology, Rochester, NY

10:25 AM (OP2)
PREPARATIONS OF POLYMETHINE AND RHODANINE DYES
Liam Almekinder*, Dr. Jeremy Cody*
School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY

10:40 AM (OP3)
PROSTATE-SPECIFIC MEMBRANE ANTIGEN
Andrew O'Brien
School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY

10:55 AM (OP4)
AMPHIPHILIC DENDRONS AS SUPRAMOLECULAR HOLDASE CHAPERONES
Elizabeth R. Piedmont*,[1] Erin E. Christensen,[1] Todd D. Krauss,[1,2] Benjamin E. Partridge[1]*
[1]Department of Chemistry, University of Rochester, Rochester; [2]Institute of Optics, University of Rochester, Rochester, NY

11:10 AM (OP5)
HARNESSING NOVEL CONJUGATION INHIBITORS TO HELP COMBAT ANTIBIOTIC RESISTANCE
Mary Emily Visingard[1], *Lizabeth McKenzie Watts[2], André O Hudson[1,2], Renata Rezende Miranda[1]**
School of Chemistry and Materials Science[1], Gosnell School of Life Sciences[2], Rochester Institute of Technology, Rochester, NY

Session B, Edwards Hall 105

10:10 AM (OP6)
INVESTIGATING THE PAL-TOLB INTERACTION
***Tahaara Gazali**, Adeaze Collins, Dr. Lea Michel*
School of Chemistry and Materials Science[1], Gosnell School of Life Sciences[2], Rochester Institute of Technology, Rochester, NY. 14623

10:25 AM (OP7)
ATTEMPT OF STUDYING AMYLOID OLIGOMERS IN THE ALZHEIMER'S DISEASE RAT BY UTILIZING GOLD COLLOID AGGREGATES
***J. Mukkatt**,* K. Yokoyama*
Department of Chemistry , SUNY Geneseo, Geneseo, NY

10:40 AM (OP8)
VISUALIZING CYTOSKELETAL PROTEIN RECONSTRUCTION OF VULVAR CANCER WITH SURFACE-ENHANCED RAMAN SPECTROSCOPY AND GOLD NANOPARTICLES
***Patrick Loss**, Nicole Mathewson, Kia Haering, Jani Lewis, Kazushige Yokoyama**
Department of Chemistry , SUNY Geneseo, Geneseo, NY

10:55 AM (OP9)
CHARACTERIZATION OF WEAKLY BOUND COMPLEXES BETWEEN WATER AND N-METHYL-2-PYRROLIDONE
***Isiah M. McMurray** and Josh J. Newby**
Chemistry Department, Nazareth University, Rochester, NY

11:10 AM (OP10)
INVESTIGATING CAVITY QUANTUM ELECTRODYNAMICS-ENABLED ENDO/EXO- SELECTIVITIES IN A DIELS-ALDER REACTION
***Jialong Wang**,[1] Braden M. Weight,[2] and Pengfei Huo*,[1,3]*
[1] Department of Chemistry, University of Rochester, Rochester, NY
[2] Department of Physics and Astronomy, University of Rochester, Rochester, NY
[3] The Institute of Optics, Hajim School of Engineering, University of Rochester, Rochester, NY

Oral Presentation Abstracts

OP1

Literature Study of Vitamin A and a Chemical Understanding of the Biological System to Delve Deeper into the Relationship between Other Vitamins and Minerals

Logan Abaldo

Department of Chemistry, Rochester Institute of Technology, Rochester, NY 14623

Vitamins are organic molecules which are required for the body to carry out a variety of functions, with vitamin A being primarily responsible for vision. Popular media distorts nutritional facts about vitamins, leaving people misinformed on how to maintain healthy levels. In this talk, primary literature is studied to delve deeper into the relationships between vitamin A and other vitamins and minerals by applying an organic chemical perspective to the mechanisms throughout the metabolism pathway. Often, literature meta-analysis can highlight existing knowledge in a different light that can uncover new connections and hypotheses.

OP2

Preparations of Polymethine and Rhodanine Dyes

Liam Almekinder, *Dr. Jeremy Cody*

School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY 14623

Complex organic dyes continue to be important synthetic targets with a wide range of potential applications. Our work on the synthesis of polymethine and rhodanine based dyes with applications ranging from pharmaceutical targets to fluorescence agents and organo-photovoltaic cells will be discussed. These dyes contain a wide variety of functionalities, and multiple synthetic approaches are possible.

OP3

Prostate-Specific Membrane Antigen

Andrew O'Brien

School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester NY 14623

Prostate-specific membrane antigen (PSMA) is a biomarker that is overexpressed in prostate cancer cells and can be targeted by PSMA inhibitors for imaging or therapy. Our group synthesizes prostate-cancer-targeted molecular imaging probes containing the PSMA inhibitor

N-[N-[(S)-1,3-dicarboxypropyl]carbamoyl]-(S)-L-lysine (DCL, Glu-urea-Lys), connected via a disuccinimidyl suberate (DSS) linker, to imaging modules such as MRI contrast agents or near-infrared dyes. However, difficulty in synthesizing DCL has hampered further work toward these targeted imaging probes. This presentation outlines the improved synthesis of DCL, guided by the principles of being scalable, safe, straightforward, and saving money. Optimizations include protecting carboxylic acids as tert-butyl esters rather than 4-methoxybenzyl (PMB) esters, using carbonyldiimidazole (CDI) in place of triphosgene to form the asymmetric urea core, and purifying all intermediates and final products using automated flash chromatography. These improvements enabled the gram-scale synthesis of DCL, facilitating further progress towards targeted molecular imaging probes.

OP4

Amphiphilic Dendrons as Supramolecular Holdase Chaperones

Elizabeth R. Piedmont,[1] *Erin E. Christensen,*[1] *Todd D. Krauss,*[1,2] *Benjamin E. Partridge*[1]

[1]Department of Chemistry, University of Rochester, Rochester; [2]Institute of Optics, University of Rochester, Rochester, NY.

Proteins are important biomolecules that are involved in most biological processes ranging from cell movement to transportation of cargo and catalysis. Proper folding into tertiary and quaternary structures typically dictates protein function. Post translation from the ribosome, proteins are susceptible to misfolding and aggregation due to exposed hydrophobic residues and the crowded environment found in cells.[1,2] Protein aggregates are implicated in a variety of diseases such as cataracts, Parkinson's disease, and Alzheimer's disease. Therefore, chaperones have been utilized to aid protein folding. Artificial systems have been explored to mimic natural chaperones and have successfully refolded proteins and prevented aggregation, but are limited by low substrate scope, high concentration, and difficulties achieving substrate specificity through their polydisperse nature.[3] In this presentation, I'll discuss a new type of artificial chaperone based on amphiphilic dendrons containing naphthyl and benzyl ethers and tetraethylene glycol tails. The tetraethylene glycol chains increase water solubility of these molecules, which can be tuned further with the structure of the hydrophobic core and generation number. In aqueous solution, these dendrons assemble into sphere–like aggregates, as shown via UV-vis and atomic force microscopy (AFM). Fluorescent studies with the solvatochromic dye Rhodamine 6G suggest that these molecules induce a hydrophobic environment. Finally, these dendrons display chaperone activity similar to a holdase by reducing the extent of fibrillization of an amyloid beta fragment, verified using circular dichroism, AFM, and Congo red binding assays. This work shows that amphiphilic dendrons display chaperone activity and showcases their potential as molecular chaperone mimics.[4]

References

1. Y. E. Kim, M.S Hipp, A. Bracher, M. Hayer-Hartl, F. Ulrich Hartl, *Annu. Rev. Biochem.* **2013**, *82*, 323–355.
2. F. Ma, C. Li, Y. Liu, L. Shi, *Adv. Mater.* **2020**, *32*, 1805945.
3. O. Hanpanich, A. Maruyama, *Biomaterials* **2020**, *254*, 120150.
4. E. R. Piedmont, E. E. Christensen, T. D. Krauss, B. E. Partridge, *RSC Chem. Biol.* **2023**,

4, 754-759.

OP5

Harnessing Novel Conjugation Inhibitors to Help Combat Antibiotic Resistance

Mary Emily Visingard*[1]*, *Lizabeth McKenzie Watts2, André O Hudson1,2, Renata Rezende Miranda1**

School of Chemistry and Materials Science[1], Gosnell School of Life Sciences[2], Rochester Institute of Technology, Rochester, NY.14623

Bacterial conjugation is a horizontal gene transfer mechanism associated with the dissemination of antibiotic resistance genes among human pathogens. This process occurs via conjugative plasmids that are transferred through a type IV secretion system (T4SS), a multi-protein complex. As conjugative plasmids are ubiquitous in the bacterial kingdom, inhibition of T4SS is a potential drug-design target to prevent the dissemination of antibiotic-resistance genes. Several small molecules, called “conjugation inhibitors” (COINs), have been reported to inhibit conjugation in Escherichia coli, including tanzawaic acid (TZAs) derivatives, but their protein targets and mechanisms of action are currently unknown. Our research aims to produce new TZA analogs with efficacy surpassing previously identified COINs and identify the targets and biochemical mechanisms by which they inhibit conjugation. Our design approach consisted of 1) simplifying the overall TZA scaffold to facilitate the synthesis while maintaining the chemical features that are important for COIN activity, and 2) adding a terminal alkyne to "click" to a reporter molecule in our future characterization studies. The molecules were synthesized using a two-step synthetic route involving a Horner-Emmons olefination reaction followed by ester hydrolysis. A fluorescence-based conjugation assay confirmed that our COIN probes inhibited conjugation in E. coli cells without affecting bacterial growth, which is important to avoid selection pressure that would favor resistant genetic variants. Future work will involve using our novel COIN probes for the specific and quantitative analyses of their protein target(s) and mechanisms of action in E. coli cells expressing the conjugation machinery.

OP6

Investigating the Pal-TolB Interaction

Tahaara Gazali*, Adeaze Collins, Dr. Lea Michel*

School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY 14623

Bacterial infections caused by Gram-negative bacteria, such as Escherichia coli (E. coli), are a significant challenge to the medical community, especially considering the emergency of new antibiotic resistant bacteria. This study investigates the Pal-TolB protein complex as a new target for antibiotic development against E. coli infections. The Pal-TolB complex plays important roles in maintaining the integrity of E. coli's cell envelope and in the constriction

step of cell division. Our study aims to better understand the Pal-TolB interaction by disrupting Pal-TolB binding using site-directed mutagenesis. We prepared single point mutations in Pal that we hypothesize are in the Pal-TolB binding interface and then tested for changes to Pal-TolB binding using enzyme linked immunosorbent assays (ELISAs). Our preliminary findings suggest that we were able to identify several key residues that dictate the Pal-TolB interaction, which we aim to target with novel antibiotics in the future.

OP7

Attempt of Studying Amyloid Oligomers in the Alzheimer's Disease Rat by Utilizing Gold Colloid Aggregates

***J. Mukkatt**,* K. Yokoyama*

Department of Chemistry , SUNY Geneseo, Geneseo, NY

Utilizing Raman imaging, in-situ detection of gold-colloid aggregates in the brains of the Alzheimer's disease rat was conducted. Through Raman imaging, we can find that the aggregates exhibited a distinctive physical identity compared to the gold colloid aggregates that were observed and formed from the Ab1-42-fibrill coated gold colloid. While analysis is still underway, our data has shown that a b-sheet conformation is a significant piece in the formation of the gold colloid aggregates.

OP8

Visualizing Cytoskeletal Protein Reconstruction of Vulvar Cancer With Surface-enhanced Raman Spectroscopy and Gold Nanoparticles

***Patrick Loss**, Nicole Mathewson, Kia Haering, Jani Lewis, Kazushige Yokoyama**

Biology & Chemistry Department, SUNY Geneseo, Geneseo, NY

When treated with the corticosteroid known as clobetasol, the epithelial vulvar cancer cell line A431 undergoes a predictable cellular reconstruction. Changes in cytoskeletal protein biomarkers in treated cells are indicative of an epithelial-mesenchymal transition. This transformation could be a useful model to demonstrate the interactions of involved proteins from a chemical perspective. Its internal validity is supported by successful replications of the experiment. The use of surface-enhanced Raman spectroscopy (SERS) paired with colloidal gold nanoparticles is a promising approach to quantify these interactions. We attempted to use a 3-dimensional SERS imaging technique to characterize the change in cytoskeletal proteins of a single cell. The mechanisms of this expected cellular reconstruction can be visualized through tracking the protein interactions and surface composition during this transition. While spectral assignments reveal the order of gains and losses of protein, the collected signals and their comparison from signals in literature sheds light on the binding, folding, and repelling forces between these cytoskeletal proteins.

OP9

Characterization of Weakly Bound Complexes Between Water and N-methyl-2-pyrrolidone

Isiah M. McMurray *and Josh J. Newby**

Chemistry Department, Nazareth University, Rochester, NY, 14618

Weakly-bound complexes are molecules that are bound to other molecules by only intermolecular forces. Studying these interactions helps the scientific community better understand how larger systems (e.g. proteins and enzymes) are structured and how they function. Previous research in this area focused on homocyclic ring molecules' interactions with water. Recently, there has been more research involving heterocyclic molecules. The current study looks into the interactions between N-methyl-2-pyrrolidone (NMP) and water. NMP is a common chemical used in paint thinners and removal products. It is chemically interesting as it contains multiple electronegative atoms, π-electrons, and a bulky substituent group that can all impact the binding of a water molecule. Previous studies focused on the NMP : water interactions in bulk systems. One study did posit a favored orientation, but did not confirm it. In the current study, computational analysis and matrix isolation FTIR were used to characterize the interactions of NMP and water on the molecular scale. Our computational findings suggest that there are four orientations in which the weakly bound NMP : water complex can form. The most energetically favorable structure was observed to form a hydrogen bond from the water molecule to the ketone of NMP. Spectroscopic analysis also supports this interaction as the most favored state.

OP10

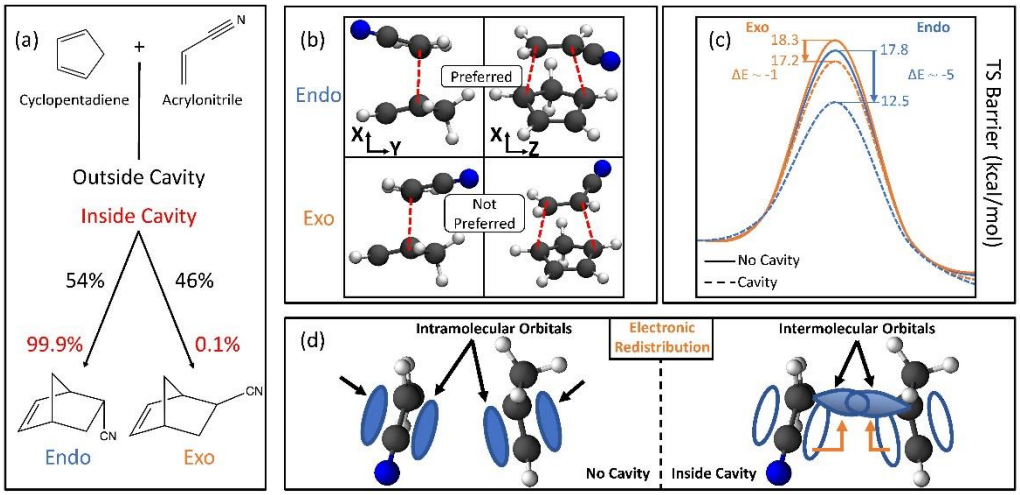
Investigating Cavity Quantum Electrodynamics-Enabled Endo/Exo- Selectivities in a Diels-Alder Reaction

Jialong Wang,[1] *Braden M. Weight,*[2] *and Pengfei Huo**,[1,3]

[1] Department of Chemistry, University of Rochester, Rochester, NY
[2] Department of Physics and Astronomy, University of Rochester, Rochester, NY
[3] The Institute of Optics, Hajim School of Engineering, University of Rochester, Rochester, NY

Coupling molecules to a quantized radiation field inside an optical cavity has shown great promise in modifying chemical reactivity. It was recently proposed that strong light-matter interactions are able to differentiate endo/exo products of a Diels-Alder reaction at the transition state. Using the recently developed parameterized quantum electrodynamic ab initio polariton chemistry approach along with time-dependent density functional theory, we theoretically confirm that the ground state selectivity of a Diels-Alder reaction can be fundamentally changed by strongly coupling to the cavity, generating preferential endo or exo

isomers which are formed with equal probability for the same reaction outside the cavity. This provides an important and necessary benchmark with the high-level self-consistent QED coupled cluster approach. In addition, by computing the ground state difference density, we show that the cavity induces a redistribution of electron density from intramolecular π-bonding orbitals to intermolecular bonding orbitals, thus providing chemically relavent description of the cavity-induced changes to the ground state chemistry and thus changes to the molecular orbital theory inside the cavity. We extend this exploration to an arbitrary cavity polarization vector which leads to critical polarization angles that maximize the endo/exo selectivity of the reaction. Finally, we decompose the energy contributions from the Hamiltonian and provide discussion relating to the dominant dipole self-energy effects on the ground state.



Poster Presentations

12:30-2:00 PM **Edwards Hall**
Odd Numbered Posters: 12:30-1:15 PM
Even Numbered Posters: 1:15-2:00 PM

Poster 1
SOLVATION IN NOVEL IONIC LIQUIDS: COSOLVENT SOLUTIONS WITH WATER
Mandy Huynh*[1]*, Gary A. Baker*[2]*, and Mark P. Heitz*[1,]**
[1]Department of Chemistry and Biochemistry, SUNY Brockport, Brockport, NY
[2]Department of Chemistry, University of Missouri, Columbia, MO

Poster 2
TOWARDS THE SYNTHESIS OF NOVEL FLUOROMETRIC PROBES INSPIRED BY ORGANOCATALYTIC RING-OPENING OF A LACTONE
PJ Nikolai*, Hunter Heineman, Christina Goudreau Collison*
School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, New York

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Ryan M. Hacker*, Daniela M. Grimard, Katie A. Morgan, Michael I. Webb**
Department of Chemistry, SUNY Geneseo, 1 College Circle, Geneseo, New York

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Gabriela Gonzalez
School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, New York

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Silas Martin*[1]*, *Trevor Gienau*[1]*, William. W. Brennessel*[2]*, Joshua Blose*[1]*, and Carly Reed*[1]***
[1]Department of Chemistry and Biochemistry, SUNY Brockport, Brockport, NY.
[2]Department of Chemistry, University of Rochester, Rochester, NY

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SIMULATION STUDIES TO PREDICT PROTEIN-PEPTIDE BINDING AFFINITIES VIA MELD-ACCELERATED MOLECULAR DYNAMICS
Maria Ciko *and Emiliano Brini*
School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, New York

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ROLE OF CYTOCHROMES C BIOMOLECULAR WIRES IN A BIOHYBRID SYSTEM FOR PHOTOCHEMICAL HYDROGEN EVOLUTION
Soraya Ngarnim*, Ryan Kosko, Farwa Awan, Manasi Gangan, Anne Meyer, Todd Krauss, Kara L. Bren*
Department of Chemistry, University of Rochester, Rochester, NY

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Navraj Singh[1]*, Gabriela Gonzalez[1], Panteha Torabian[2], Tom Gaborski[2], and Lea V. Michel[1]**
[1]School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY
[2]Department of Biomedical Engineering, Rochester Institute of Technology, Rochester, NY

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BIODIESEL
Annabel Rupp
Department of Chemistry, SUNY Geneseo, 1 College Circle, Geneseo, NY

Poster 10
INVESTIGATING THE PAL-TOLB INTERACTION
Tahaara Gazali*, Adeaze Collins, Dr. Lea Michel*
School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY

Poster 11
DETECTING BACTERIAL EXTRACELLULAR VESICLES IN HUMAN PLASMA FOR SEPSIS DIAGNOSIS
Martina Videva[1]*, Nico Burgado[1], Nikita Robinson[1], Anthony Pietropaoli[3], Tom Gaborski[2], and Lea V. Michel[1,*]*
[1]School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY
[2]Department of Biomedical Engineering, Rochester Institute of Technology, Rochester, NY
[3]Pulmonary and Critical Care Medicine, University of Rochester Medicine, Rochester, NY

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MOLECULAR SOLVATION IN PEG200 SOLUTIONS
Kennedy A. Mueller*, Markus M. Hoffmann*, and Mark P. Heitz**
Department of Chemistry and Biochemistry, SUNY Brockport, Brockport, NY

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Peggy Chen, ***Mya L. Soto,*** *Nana Aikins, Kenneth Gerien, Joshua Thomas, Sarah Denial, Christopher Daley, Emmanuella Delva, Elizabeth Richter, Brent Cotman, David N. Frick**, Julie A. Thomas*, and Suzanne F. O'Handley*
Department of Chemistry and Materials Science, Rochester Institute of Technology
*Gosnell School of Life Sciences, Rochester Institute of Technology
**Department of Chemistry and Biochemistry, University of Wisconsin-Milwaukee

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DEVELOPING PHOTORESPONSIVE ARTIFICIAL CHAPERONES
Hannah Claus*, Elizabeth R. Piedmont and Benjamin E. Partridge**
University of Rochester, Rochester, NY

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Serena Tuytschaevers[1]*, André O. Hudson[1], Emiliano Brini[2], Renata Rezende Miranda[2*]*
[1]Thomas H. Gosnell School of Life Sciences, Rochester Institute of Technology, Rochester, NY
[2]School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY

Poster 16
BIODIESEL
Colden Grossman
Department of Chemistry, SUNY Geneseo, 1 College Circle, Geneseo, NY

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TIMING MATTERS: HOW THE ORDER OF CONTENT DELIVERY AFFECTS STUDENT EXAM PERFORMANCE IN ORGANIC CHEMISTRY
Kevin Shrestha*, **Katie Miller****, Isabelle Ormond, Eric Reyes, Christina Goudreau Collison*
School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY

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Parbhat Kumar*, Aiden J. Ward, Alejandro Lazaro, and Benjamin E. Partridge*
Department of Chemistry, University of Rochester, Rochester, NY

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Malachi Clay[1]*, Trevor Gienau[1], Silas Martin[1], Joshua Blose[1], William. W. Brennessel[2] and Carly Reed[1]**
[1]Department of Chemistry and Biochemistry, SUNY Brockport, Brockport, NY.
[2]Department of Chemistry, University of Rochester, Rochester, NY

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Lee E. Schoneman[1], *Adam N. Robinson[1], Rachel H. Horowitz[2], Carly R. Reed[2], and Michael L. Gleghorn[1]**
[1]School of Chemistry and Materials Science, College of Science, Rochester Institute of Technology, Rochester, NY
[2]Department of Chemistry and Biochemistry, SUNY Brockport, Brockport, NY

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Priscilla Peters, *Amanda Canfield, and Shauna M. Paradine**
Department of Chemistry, University of Rochester, Rochester, NY

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Alex Wilkinson
Department of Chemistry, SUNY Geneseo, 1 College Circle, Geneseo, NY

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Eva Reilly, *Andrew Seyler, Peipei Zhu, and Suzanne F. O'Handley**
School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester NY

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UPCYCLING BOTTLES INTO 3-D PRINTING FILAMENT
Aurora Pardun
Department of Chemistry and Biochemistry, SUNY Brockport, Brockport NY

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School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY

Poster Presentation Abstracts

Poster 1

Critical Bone Fracture Repairs: A Comparison of the Mechanical Properties of Calcium Phosphate Bioactive Cement and Pig Bones

Mandy Huynh[1]*, Gary A. Baker*[2]*, and Mark P. Heitz*[1,*]

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[2]Department of Chemistry, University of Missouri, Columbia, MO

Ionic liquids (ILs) have had a prominent place in liquids research over several decades because of their potential use alternatives to organic solvents in a wide variety of chemical applications in diverse areas such as chemical synthesis, electrolyte media for batteries, fuel cells, and solar cells. Given the large number of potential cation/anion combinations, this allows for specific tailoring of ILs to create task-specific "designer" solvents. While this affords interesting and novel media formulations, the associated solution physicochemical properties ultimately govern their utility. Commonly, these solvents can be rather viscous (> 10 cP, and up to ~70,000 cP), which implicates molecular transport properties. One viscosity mitigation strategy is to form solutions using molecular cosolvents. While much has been published on neat ILs, primarily focused on imidazolium, phosphonium, and ammonium derivatives, we have very recently developed a novel IL system using an ether-based zwitterionic liquid. In addition, our work gives attention to the study of water-modified IL. Water is usually implicated as an impurity, and we are interested in how the presence of water modifies solvation in these novel ILs. To address this general question, static and time-resolved 2D electronic spectroscopic techniques are used to examine molecular solvation through characterizing the solvation dynamics using the classic fluorescent solvation probe, coumarin 153.

Poster 2

Towards the Synthesis of Novel Fluorometric Probes Inspired by Organocatalytic Ring-Opening of a Lactone

PJ Nikolai*, Hunter Heineman, Christina Goudreau Collison*

School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, New York

Di-fluorometric probes are of interest due to their fluorescent properties in both hydrophilic and hydrophobic regions. Such fluorescent properties allow for greater monitoring of interactions between amphiphilic probes and cell membranes, which can contribute to advancing the understanding of cell membranes and drug delivery methods. Our research focuses on the synthesis of a library of di-fluorometric probes of differing carbon chain length that will be furthered studied by our collaborators to investigate their therapeutic potential. Our

goal is to optimize the substitution reaction to afford the dansyl head upon a carbon chain and to begin exploring a reaction path that involves a more stable intermediate compared to prior attempts to produce the di-fluorometric probe. My research goals will address the synthesis of di-fluorometric probes comprised of commercially available dansyl chloride, 7-amino-4-methylcoumarin, and a macro lactone.

Poster 3

Synthesis and Evaluation of Ruthenium-Arene Complexes to Modulate the Aggregation of the Amyloid-β Peptide

Ryan M. Hacker*, Daniela M. Grimard, Katie A. Morgan, Michael I. Webb**

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Alzheimer's Disease (AD) is a neurological disorder characterized by a buildup of the amyloid beta (Aβ) peptide as aggregate species in the brain. Recent advances using antibody based treatments which target Aβ have seen clinical success, achieving FDA approval. However, they come at a significant cost, ranging from $20,000-40,000 a year. Ruthenium-based therapeutics are promising alternatives, as they have shown an ability to modulate the aggregation of Aβ in solution and prevent its cytotoxicity. Despite their initial success, significant questions regarding the affinity of the complexes for Aβ relative to endogenous proteins remain unknown. Therefore, we have synthesized a series of ruthenium-based complexes and assessed their respective ability to modulate Aβ aggregation while also evaluating their association with the serum protein albumin (HSA). The impact on Aβ aggregation for the complexes was assessed using thioflavin T fluorescence, dynamic light scattering, and transmission electron microscopy. Alternatively, the affinity of the complexes for Aβ and HSA was determined using isothermal titration calorimetry and fluorescence binding assays. The results of these experiments will be discussed, where structure-activity relationships will be established.

Poster 4

Antibiotic Impact on the Release of Extracellular Vesicles from E. coli

Gabriela Gonzalez

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[‡] Department of Chemistry, University of Rochester, Rochester, NY

Four alkyl substituted acetoacetic acids were prepared and their rate of decarboxylation was studied in aqueous solutions in the temperature range 30-50 °C. Activation energies were calculated based on the first order rate law and compared to the DFT calculated activation energies in the gas phase. We have confirmed that the concerted mechanism of beta keto acids decarboxylation in solutions is not supported.

Alkyl substituted acetoacetic acids have been characterized by single crystal x-ray data analysis for the first time. It was found that acids are packed in crystals by making hydrogen bonding in pairs between carboxylic groups. We were trying to explain experimental activation energies in solution by the distance of the C-C bond that will break in the decarboxylation reaction.

Poster 5

The synthesis of [Ir(2-phenyl-1H-imidazo[4,5-f] [1,10]phenanthroline)(L)2](PF6) complexes for G-quadruplex biosensors

Silas Martin[1], *Trevor Gienau[1], William. W. Brennessel[2], Joshua Blose[1], and Carly Reed[1]**

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[2]Department of Chemistry, University of Rochester, Rochester, NY

G-quadruplex (GQ) nucleic acid structures have gained attention in the field of biosensing in recent years due to their cost-effectiveness, easy modification, stability, and ability to act as either the target recognition component or the signal transducer within a biosensor. Cyclometallated iridium (III) complexes have emerged as luminescent signaling agents that can be integrated into GQ biosensing assays. The present advantages over organic and other transition metal lumophores include strong, long-lived phosphorescence; high photostability; and selectivity over other forms of DNA. Structural changes to the iridium complex, as well as, GQ sequence and topology impact the binding affinity and luminescence enhancement of signaling agents. In this work we explore the synthesis, characterization, and luminescence enhancement of a series of iridium (III) complexes containing the 2-phenyl-1H-imidazo[4,5-f][1,10]phenanthroline ligand. Fluorescence titrations were conducted to determine if luminescence enhancement occurred. It was found that three of the four complexes exhibit luminescence enhancement in the presence of GQ DNA. X-ray crystallography was used to characterize the iridium(III) structures. Luminescence differences as they relate to structural differences will be discussed.

Poster 6

Simulation Studies to Predict Protein-Peptide Binding Affinities via MELD-accelerated Molecular Dynamics

Maria Ciko *and Emiliano Brini*

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Peptide drug discovery and structure-based drug design investigate the biological function and behavior of proteins in human cancers. In this study, I explore complex formation via protein-ligand binding affinities, a valuable resource in disrupting the interactions that enable cancer growth. Proteins have many degrees of freedom of internal and relative motion that are

simplified by Molecular Dynamics (MD), though at a high computational cost. MELD, or Modeling Employing Limited Data, is a probabilistic approach that uses Bayesian integration of external information to accelerate the process. In addition to locating the most frequent, lowest free energy conformations, it also facilitates flexibility in protein-peptide interactions for biomimetic applications. I use RMSD values to indicate the accuracy of nine bound structures comprising an MDM-protein and a peptide with a distinctive mutation. MD analysis through OpenMM confirmed that stable conformations can be reached for each docked system and that low RMSD values showed a good binding affinity, such that the protein did not drastically change its conformation upon binding. In a study conducted by Morrone, MELD demonstrated correct outcomes in a competitive inhibition environment across the nine systems. My hypothesis is that I can effectively compute the relative binding affinities in a way that minimizes ligands' steric hindrance and mitigates the effect of slowed diffusion on simulation convergence time. Given the consistency of the method implemented, I anticipate these computations to be congruent with experimental results.

Poster 7

Role of Cytochromes c Biomolecular Wires in a Biohybrid System for Photochemical Hydrogen Evolution

***Soraya Ngarnim**, Ryan Kosko, Farwa Awan, Manasi Gangan, Anne Meyer, Todd Krauss, Kara L. Bren*

Department of Chemistry, University of Rochester, Rochester, NY

Understanding the mechanical properties of bone is critical to the design of materials that are to be used in repair of bone fractures. The mechanical properties of the materials in turn determine the behavior of the body under a load or force. This study compares the mechanical properties of Calcium Phosphate Cement (CPC) to pig bone with the aim of determining its suitability and applicability for use on load bearing bone fracture sites. CPC has been reported to be a bioactive and biodegradable material with potential resorbability, molding capabilities, and easy manipulation. It is composed of hydroxyapatite (HA), a major component of human bone, and a base constituent of the cement. Due to the potential resorbability and also the ability to initiate bone growth, our continuing efforts are geared toward addressing challenges of adequate mechanical strength of the cement to ensure compatibility to human bone. The cement was synthesized and characterized using published methods, mechanical strength tested and the data obtained is presented and discussed herewith.

Poster 8

Investigating the Effects of Antibiotics on the Production of Extracellular Vesicles in E. coli

***Navraj Singh**[1], Gabriela Gonzalez[1], Panteha Torabian[2], Tom Gaborski[2], and Lea V. Michel[1]**

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NY
[2]Department of Biomedical Engineering, Rochester Institute of Technology, Rochester, NY

Extracellular vesicles (EVs) are nano-sized, membrane-bound spheres constitutively released by most cell types, including Gram-negative bacteria. EVs contain many similar molecules to their cell "parent," some of which are toxic and have been shown to contribute to the inflammatory response in host tissue. Studies have shown that EV production is enhanced by the presence of environmental stressors, such as antibiotic exposure. We hypothesized that some antibiotics, depending on their mechanism of action, might enhance EV release from Gram-negative Escherichia coli (E. coli) more than other antibiotic types. After incubation of E. coli with nine antibiotics at their clinically relevant concentrations, we isolated the EVs using ultracentrifugation and characterized them using immunoblotting, nanoparticle tracking analysis, and transmission electron microscopy. The results of our study suggest that some antibiotics, specifically beta-lactams, do indeed enhance EV release more than others, such as aminoglycoside antibiotics. Since EVs, as well as the molecules inside EVs, can trigger inflammation, these results may have important implications for doctors who prescribe antibiotics to sepsis patients.

Poster 9

Biodiesel

Annabel Rupp

Department of Chemistry, SUNY Geneseo, 1 College Circle, Geneseo, NY

Fossil fuels are the largest contributors to global climate change, accounting for nearly 75% of total greenhouse gas emissions. A green energy solution can be found in autotrophs, which both sequester carbon in their growth and can be made into biodiesel. Chlorella vulgaris has been studied for lipid extraction and production, both of which were made more efficient through means of culturing the algae in different media and by evaluating the biodiesel produced via IR spectroscopies. Synechococcus, a genus of cyanobacteria that grows prolifically in Conesus Lake, may be an even better source of fuel than C. vulgaris because it grows at a rate nearly twice as fast and is known to be a strong carbon sequester. (This species has not yet been specified, but is believed to be of the vulcanococcus species.) Growth of Synechococcus was observed in a variety of media and it was determined that BG-11 profosters the most prolific growth. Synechococcus phospholipids will be extracted from dead cells and converted into biodiesel using a transesterification process. Finally, we will compare our results from Synechococcus with previous studies on C. vulgaris to determine which organism is the better source of biodiesel.

Poster 10

Investigating the Pal-TolB Interaction

***Tahaara Gazali**, Adeaze Collins, Dr. Lea Michel*

School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY

Bacterial infections caused by Gram-negative bacteria, such as Escherichia coli (E. coli), are a significant challenge to the medical community, especially considering the emergency of new antibiotic resistant bacteria. This study investigates the Pal-TolB protein complex as a new target for antibiotic development against E. coli infections. The Pal-TolB complex plays important roles in maintaining the integrity of E. coli's cell envelope and in the constriction step of cell division. Our study aims to better understand the Pal-TolB interaction by disrupting Pal-TolB binding using site-directed mutagenesis. We prepared single point mutations in Pal that we hypothesize are in the Pal-TolB binding interface and then tested for changes to Pal-TolB binding using enzyme linked immunosorbent assays (ELISAs). Our preliminary findings suggest that we were able to identify several key residues that dictate the Pal-TolB interaction, which we aim to target with novel antibiotics in the future.

Poster 11

Detecting Bacterial Extracellular Vesicles in Human Plasma for Sepsis Diagnosis

***Martina Videva[1]**, Nico Burgado[1], Nikita Robinson[1], Anthony Pietropaoli[3], Tom Gaborski[2], and Lea V. Michel[1,*]*

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Sepsis is a clinical syndrome that occurs when the host proinflammatory immune responses become elevated in response to an infection. If untreated, sepsis can result in severe sepsis, causing organ failure or hypotension, known as septic shock. Outer membrane biomolecules LPS, OmpA, and Pal have been implicated in the pathophysiology of Escherichia coli (E. coli) sepsis, specifically, the over-inflammatory response observed in sepsis patients. Notably, all of these biomolecules are released as a complex inside outer membrane vesicles (OMVs) from E. coli and other Gram-negative bacteria. We hypothesize that these proteins and OMVs themselves may serve as excellent biomarkers for the diagnosis of sepsis. The purpose of this study was to optimize the detection of OMVs from complex human biofluids, like plasma. Specifically, a set of 20 patient plasma samples were obtained from the Intensive Care Unit (ICU) at Strong Memorial Hospital, and purified using centrifugation, syringe-filtration, and ultracentrifugation, to isolate OMVs and other extracellular vesicles (EVs). These samples were then analyzed using immunoblotting to specific E. coli antigens. Here, we describe the

results of our preliminary study, which demonstrates that we are able to isolate OMVs and other EVs from human plasma, and characterize them using immunoblots to E. coli antigens, such as LPS, OmpA, and Pal.

Poster 12

Molecular Solvation in PEG200 Solutions

***Kennedy A. Mueller**, Markus M. Hoffmann*, and Mark P. Heitz**

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In recent years, peptide synthesis has become more prevalent due to the capabilities with solid-phase peptide synthesis (SPPS). Using a resin to build the peptide with Fmoc-protected amino acids allows for simple, high efficiency, high yield production of peptides. Before removing the peptide from the resin, modifications such as the addition of a fluorophore can be done. However, a protocol outlining which dye derivative, activating agent, activation time, and reaction time are needed for attachment has not been elucidated. In fact, the results reported in the literature dictate chemical amounts much higher than those typically needed for SPPS and the use of more activating agents than needed. To test the applicability of using different fluorescein derivatives, attachment to alanine-methyl ester was first tested. Then, optimization of all parameters was begun using a 6-mer peptide. Liquid chromatography-mass spectrometry and spectroscopy was used to analyze the success of the synthesis.

Poster 13

A CTPase Nudix Hydrolase from Mycobacterium tuberculosis as a Potential Novel Antibiotic Target

*Peggy Chen, **Mya L. Soto,** Nana Aikins, Kenneth Gerien, Joshua Thomas, Sarah Denial, Christopher Daley, Emmanuella Delva, Elizabeth Richter, Brent Cotman, David N. Frick**, Julie A. Thomas*, and Suzanne F. O'Handley*

Department of Chemistry and Materials Science, Rochester Institute of Technology
*Gosnell School of Life Sciences, Rochester Institute of Technology
**Department of Chemistry and Biochemistry, University of Wisconsin-Milwaukee

Organosilicon complexes of the form $RSi(QNO)_2Cl$ (QNO = 8-oxyquinoline N-oxide; R = ^{t}Bu, *p*-tolyl, Bn) were synthesized and characterized by ^{1}H, ^{13}C, and ^{29}Si NMR spectroscopy. Organosilicon complexes of the same form (R = Me, Ph) were synthesized and characterized by ^{1}H, ^{13}C, and ^{29}Si NMR spectroscopy, and elemental analysis. Multiple X-ray crystal structure solvates of $MeSi(QNO)_2Cl$ and of $MeSi(QNO)_2(OSO_2CF_3)$ revealed separated ion pairs with trigonal bipyramidal complex cations in each. In all cases, a single isomer is formed with both N-oxide groups in axial positions. The similarity of the NMR spectra of $MeSi(QNO)_2(OSO_2CF_3)$ and $MeSi(QNO)_2Cl$ suggest that they also exist as separate ion pairs in $CDCl_3$ solution.

Poster 14

Developing Photoresponsive Artificial Chaperones

***Hannah Claus**, Elizabeth R. Piedmont and Benjamin E. Partridge**

Department of Chemistry, University of Rochester, NY

A series of organosilicon complexes containing the OPTO (1-oxo-2-pyridinethione) ligand were synthesized and characterized by ^{1}H, ^{13}C, and ^{29}Si NMR spectroscopy as well as X-ray crystallography. The crystal structures of a series of silacycloalkanes of the form $(CH_2)_xSi(OPTO)_2$ (x = 3, 4, 5) were compared along with $Me_2Si(OPTO)_2$ to examine the influence of ring size on chelate strength as well as the effect of the silacycle relative to the open-chain structures. The carbon resonances of the ligand in various complexes were identified using ^{1}H-^{13}C HMQC NMR experiments. The relative order of several of the carbon resonances was found to depend on temperature and the substituents bonded to silicon. Variable-temperature NMR studies revealed dynamic chelation equilibria involving dissociation of the Si←S=C bond.

Poster 15

Computational Assessment of Novel Bacterial Conjugation Inhibitors

***Serena Tuytschaevers[1]**, André O. Hudson[1], Emiliano Brini[2], Renata Rezende Miranda[2*]*

[1]Thomas H. Gosnell School of Life Sciences, Rochester Institute of Technology, Rochester, NY
[2]School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY

Antimicrobial resistance (AMR) is a global threat, causing an estimated 700,000 annual deaths. Conjugation is the primary means of spreading AMR genes among bacteria, underscoring the importance of conjugation inhibitors (COINs) in combating AMR. Known COINs include unsaturated fatty acids (uFAs), 2-alkynoic fatty acids (2-aFA), and tanzawaic acids (TZAs). However, many COINs lack identified targets or mechanisms of action. Identifying effective COINs is essential to prevent AMR gene dissemination. Previous analyses of 2-aFA COINs have pinpointed key features that may be essential to their activity such as a hydrophobic tail, unsaturations, and a polar head. Leveraging the efficacy of 2-hexadecynoic acid (2-HDA) and the low toxicity of TZA-A, we designed two sets of new TZA analogs with diverse hydrophobic tails and varying unsaturation levels for a structure-activity relationship assessment to identify optimal analogs for future studies. To accelerate discovery, we will employ molecular dynamics and Modeling Employing Limited Data (MELD), a Bayesian computational method, to analyze the compounds. This approach predicts binding affinities of novel TZA-derived COIN analogs with potential bacterial protein targets, facilitating compound selection for synthesis and biological characterization. Integrating structure-guided design, molecular dynamics, and advanced computational methods presents a comprehensive strategy to combat AMR.

Poster 16

Biodiesel

Colden Grossman

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Fossil fuels are the largest contributors to global climate change, accounting for nearly 75% of total greenhouse gas emissions. A green energy solution can be found in autotrophs, which both sequester carbon in their growth and can be made into biodiesel. Chlorella vulgaris has been studied for lipid extraction and production, both of which were made more efficient through means of culturing the algae in different media and by evaluating the biodiesel produced via IR spectroscopies. Synechococcus, a genus of cyanobacteria that grows prolifically in Conesus Lake, may be an even better source of fuel than C. vulgaris because it grows at a rate nearly twice as fast and is known to be a strong carbon sequester. (This species has not yet been specified, but is believed to be of the vulcanococcus species.) Growth of Synechococcus was observed in a variety of media and it was determined that BG-11 profosters the most prolific growth. Synechococcus phospholipids will be extracted from dead cells and converted into biodiesel using a transesterification process. Finally, we will compare our results from Synechococcus with previous studies on C. vulgaris to determine which organism is the better source of biodiesel.

Poster 17

Timing Matters: How the Order of Content Delivery Affects Student Exam Performance in Organic Chemistry

Kevin Shrestha*, Katie Miller*, *Isabelle Ormond, Eric Reyes, Christina Goudreau Collison*

School of Chemistry and Materials Science, Rochester Institute of Technology, Rochester, NY

The order prescribed by an adopted organic chemistry textbook may largely influence the timing of when certain concepts are taught during the semester. It was hypothesized that changing the order of content delivery would positively affect student exam performance. During our trial year, it was discovered that students scored higher on both the last exam of Organic I and the first exam of Organic II when a reorganization of the content was implemented compared to the control years. Interestingly, the reorganization did not adversely affect exam performance for traditionally timed content.

Poster 18

Designing Hydrogen-Bonding Motifs to Program Hierarchical Assembly

Parbhat Kumar*, Aiden J. Ward, Alejandro Lazaro, and Benjamin E. Partridge*

Department of Chemistry, University of Rochester, Rochester, NY

Hierarchical assembly is the basis of numerous biological structures that are crucial for life, such as folded proteins, cell membranes, double-stranded DNA, and muscle fibers. Nature employs hierarchy so extensively because it provides efficient access to complex architectures. These biological structures are inherently dynamic and achieve this dynamic nature by incorporating non-covalent interactions which are reversible and cooperative. In this study, we aim to program the hierarchical assembly of synthetic building blocks to design complex fibrous materials. Initial studies have focused on designing a series of bifacial nucleobases to interact with each other via non-covalent interactions, including hydrogen bonding, π–π stacking, and dispersion interactions. Synthetic routes have been developed and validated for five novel compounds, each capable of hydrogen bonding on two distinct faces. For two of these molecules, denoted G^A and H^C, their assembly has been explored via a combination of X-ray crystallography (in the solid state) and UV-vis spectroscopy (in solution). These studies demonstrate that bifacial nucleobases engage in hydrogen bonding and base-pair stacking, akin to natural DNA. In future work, we hypothesize that controlling the relative strength of the interactions between building blocks will permit the sequence of assembly to be programmed and thus hierarchical structures to be accessed. The resulting architectures will find potential applications as mimics of the extracellular matrix and as impact-resistant soft materials.

Poster 19

Structural Analysis of a Series of Iridium(III) Complexes for Biosensors

Malachi Clay*[1]*, Trevor Gienau*[1]*, Silas Martin*[1]*, Joshua Blose*[1]*, William. W. Brennessel*[2] *and Carly Reed*[1]**

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School of Chemistry & Materials Science, Rochester Institute of Technology, Rochester NY

Cyclometallated iridium(III) complexes have recently emerged as luminescent signaling agents that can be integrated into G-quadruplex (GQ) biosensing assays. GQ nucleic acid structures are being readily applied in biosensors due to their cost-effectiveness, stability, and ability to act as either the target recognition component or the signal transducer within a biosensor. Structural changes to the iridium complex as well as GQ sequence and topology impact the binding affinity and luminescence enhancement. In this work we explore the synthesis, structural analysis, and luminescence enhancement of a series of iridium(III) complexes containing the 2,9-dimethyl-1,10-phenanthroline ligand. X-ray crystallography was used to characterize the iridium(III) structures. Fluorescence titrations were conducted to determine the extent of the luminescence enhancement. It was found that the methyl substituents on the phenanthroline ligand impact bond lengths and angles around the iridium center when compared to the unsubstituted phenanthroline ligand. All four complexes in the series exhibited luminescence enhancement in the presence of GQ DNA. The impact of

structural variation among the iridium complexes on luminescence enhancement will be discussed.

Poster 20

Crystallized DNA G-Quadruplex Structure Bound to an Iridium Complex Ligand

***Lee E. Schoneman[1]**, Adam N. Robinson[1], Rachel H. Horowitz[2], Carly R. Reed[2], and Michael L. Gleghorn[1]**

[1]School of Chemistry and Materials Science, College of Science, Rochester Institute of Technology, Rochester, NY
[2]Department of Chemistry and Biochemistry, SUNY Brockport, Brockport, NY

Proto-oncogenes such as c-MYC contain many tumor survival pathways that, when overexpressed, can result in carcinogenesis. One method that is currently being explored to hinder gene overexpression is the formation of different DNA arrangements in the promoter region. The G-quadruplex structure consists of numerous subunits of 4 hydrogen-bound guanines, known as G-quartets, that stack upon each other as opposed to traditional Watson-Crick base pairing. These structures tend to form naturally in guanine-rich environments, which includes the promoter regions of many proto-oncogenes. Due to the size and complexity of the quadruplex, RNA polymerase cannot advance past the structure, halting transcription. To prevent the quadruplex from dissociating, it may be possible to stabilize a quadruplex *in vivo* using ligands that may be able to bind on top of or in the grooves of the quadruplex. Before creating drugs to stabilize G-quadruplexes in vivo, however, their presence must be confirmed first. Due to its increased luminescence when bound to G-quadruplexes as well as its selectivity against typical double-stranded and single-stranded DNA, a cyclometalated iridium (III) imidazole phenanthroline complex will be co-crystallized alongside an annealed oligonucleotide sequence known to form G-quadruplexes (5'-TGGGGT-3'). These crystals will then be analyzed using X-ray diffraction to determine how the iridium complex binds to the G-quadruplex. While structure determination is still in progress, understanding these interactions will provide insight into how to locate G-quadruplexes in vivo.

Poster 21

Copper-Catalyzed Free-Radical Cyclization of Olefins

***Priscilla Peters**, Amanda Canfield, and Shauna M. Paradine**

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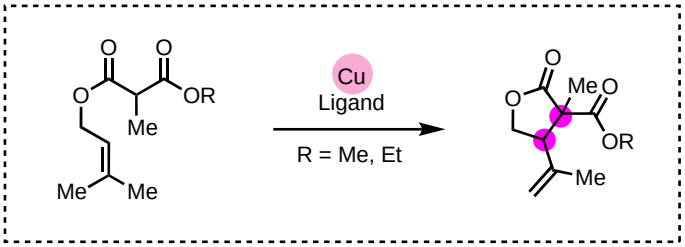
We are reporting a copper-catalyzed, oxidative radical cyclization of olefins to generate lactones and carbocycles. This method addresses challenges associated with manganese (III) mediated approaches to rapidly generate complex scaffolds. Limitations of previous approaches include use of stoichiometric amounts of metal, poor chemoselectivity, and requirement of copper as a co-reagent. Our method is a ligand-enabled, catalytically-controlled

cyclization of unsaturated β-keto esters and malonate diesters followed by elimination with the final product containing an olefin, which serves as a functional handle for future derivatization. Following optimization of our reaction conditions, we report good yields of five member lactones in the presence of an electron withdrawing bipyridine ligand and air as an oxidant. Substrate diversification is ongoing.



Poster 22

Biodiesel

Alex Wilkinson

Department of Chemistry, SUNY Geneseo, 1 College Circle, Geneseo, NY

Fossil fuels are the largest contributors to global climate change, accounting for nearly 75% of total greenhouse gas emissions. A green energy solution can be found in autotrophs, which both sequester carbon in their growth and can be made into biodiesel. Chlorella vulgaris has been studied for lipid extraction and production, both of which were made more efficient through means of culturing the algae in different media and by evaluating the biodiesel produced via H1NMR, C13NMR, and IR spectroscopies. Synechococcus, a genus of cyanobacteria that grows prolifically in Conesus Lake, may be an even better source of fuel than C. vulgaris because it grows at a rate nearly twice as fast and is known to be a strong carbon sequester. (This species has not yet been specified, but is believed to be of the vulcanococcus species.) Growth of Synechococcus will be observed in a variety of media to determine which yields the most lipids. Synechococcus phospholipids will be extracted from dead cells and converted into biodiesel using a transesterification process. Finally, we will compare our results from Synechococcus with previous studies on C. vulgaris to determine which organism is the better source of biodiesel.

Poster 23

Characterization of diadenosine polyphosphatases of the Nudix hydrolase superfamily in M. tuberculosis and M. leprae

***Eva Reilly**, Andrew Seyler, Peipei Zhu, and Suzanne F. O'Handley**

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M. tuberculosis and *M. leprae* contain diadenosine polyphosphatase mRNA decapping Nudix

hydrolases, and we are characterizing these enzymes as potential novel antibiotic targets. In *M. tuberculosis* there is the primary Nudix Ap_nAase and the secondary Nudix Ap_nAase, and there are orthologs of these two enzymes in *M. leprae*. The diadenosine polyphosphatases from *Legionella pneumophilia* and *Bartonella bacilliformis* are considered "invasion enzymes"; when the genes for these enzymes are knocked out, these bacteria are less able to invade their host cells. It is of interest to know whether these enzymes have the same or similar function in *M. tuberculosis* and *M. leprae*. If they are found to be involved in invasiveness and thus in virulence, then these enzymes could be novel antibiotic targets. We have cloned and overexpressed each protein and have subcloned each protein into a HisTag vector to optimize purification. The *M. leprae* enzymes express too insolubly to purify and characterize, and thus we are working on increasing the expression of soluble protein so that we can study these enzymes as well; currently, we know that they each have Ap_nAase activity. We have tried to increase enzyme solubility by changing the overexpression conditions including lower temperatures, less IPTG, the addition of GroESL, the use of Rosetta E. coli, and the addition of diglycine. This research has been supported by an NIH AREA grant, a CUR-Goldwater Scholars Faculty Mentor Award, an ASBMB undergraduate research award, and a RIT honors SURF.

Poster 24

Upcycling Bottles into 3-D Printing Filament

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The goal of this research was to turn plastic bottles into 3-D printing filament. Providing a way to create specialized equipment in a relatively accessible manner was one of the main objectives of this research. To make this transformation possible, we had to shred plastic bottles using a residential paper shredder. The shredded plastic was then fed into the filastruder. The filastruder is a device that heats the plastic up to about 250◦ C then slowly extrudes the plastic through a nozzle. Eventually, we will produce enough material to wind the filament onto a spool using the filawinder and print with it. The ability to use this material to create functional pieces will be discussed during the event. The filastruder and filawinder were commercially available kits that I have constructed independently. Doing so posed many challenges. Incomplete instructions and faulty parts made completion difficult. However, these challenges have been overcome with creativity and ingenuity. For example, I have designed and 3-D printed multiple versions of replacement couplers. I have also 3-D printed a vertical hopper that allows us to mount the filastruder vertically.

Poster 25

Exploring ALPHA-FOLD Predicted Structures of Nudix Proteins to Investigate Binding Site Dynamics through Implicit Solvent Molecular Dynamics Simulations

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Understanding the binding dynamics of molecules to proteins is pivotal for drug design, particularly in targeting specific sites crucial for therapeutic intervention. Experimental methods to identify these sites, while accurate, are often time-consuming and expensive. Molecular dynamics (MD) simulations emerge as a powerful, cost-effective alternative, offering insights into the structural, dynamical, and thermodynamic properties of molecular systems. Utilizing OpenMM, a high-performance computing library, this study focuses on utilizing the power of Alpha-Fold predicted structures of Nudix hydrolases—enzymes that catalyze the hydrolysis of nucleoside diphosphate derivatives across a broad substrate spectrum. Given the presence of intrinsically disordered regions (IDRs) in some Nudix proteins, which complicate traditional experimental analysis, MD simulations are particularly advantageous. They provide a detailed, atomistic view of these dynamic regions, enhancing our understanding of protein-protein interactions (PPIs) and their implications for drug discovery.

Our approach, which includes analyzing protein stability and conformational changes through Root Mean Square Deviation (RMSD) and examining binding site dynamics, leverages implicit solvent models and the AmberFF-14SB force field over extensive 500 ns trajectories. The findings underscore the potential of MD simulations in identifying and assessing the drug ability of the Alpha-Fold Predicted Structures of Nudix proteins, thereby informing the development of targeted therapeutics.

Poster 26

A New Synthesis for Alanine-Based Self-Assembling High-Relaxivity Contrast Agents

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High-relaxivity contrast agents have emerged as powerful tools for the imaging of cancer through MRI. The previously synthesized Fmoc-D-Trp-Ala(Gd-DO3A)-OH is one such contrast agent, and has displayed a promising r_1 relaxivity of 24.5 ± 1.2 $mM^{-1}s^{-1}$ at 1.0 T through self assembly. However, further evaluation of this contrast agent was limited by a difficult synthesis. A new synesis route for Fmoc-D-Trp-Ala(Gd-DO3A)-OH has been implemented that bypasses many of the problems found within the original synthesis. The success of this pathway enables research into the effect of a C-terminal carboxylate vs. carboxamide on the agent's relativity, as a C-terminal carboxamide version could likely be synthesized using the same pathway. It could also provide easier access to a foundational module for larger, more complex targeted contrast agents.

Poster 27

Inter- and Intramolecular Hydrogen Bonding in n-Octanol Related Ether Alcohols

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We have conducted a molecular dynamics (MD) study investigating the effect of ether position on the hydrogen bonding present in isomeric species of octanol-related ether alcohols. This work was motivated by the need to understand the fundamental interactions in polyethylene glycol (PEG) systems. PEG has garnished significant attention in recent decades due to its role in green chemistry, being a sustainable feedstock demonstrated to have minimal environmental toxicity. This study is part of an ongoing work dedicated to the understanding of PEG as a chemical solvent, thereby promoting further use in research and development. Data extracted from the simulations include physical properties such as density and viscosity that were compared with experimental measurements, as well as values more difficult to obtain experimentally, such as radial distribution functions and number of hydrogen bonds. As one preliminary result, intramolecular hydrogen bonding was found to be most prevalent when the ether moiety is centrally located to the molecular structure of the ether alcohol. We attribute this finding to two effects, namely ring constraints and entropic effects with increased configuration space with increased distance between ether and hydroxy moiety. Another remarkable finding suggests that intermolecular hydrogen bonding in the case of 1-hexoxymethan-1-ol leads to highly stable 6-membered ring formations as shown in Figure 1.

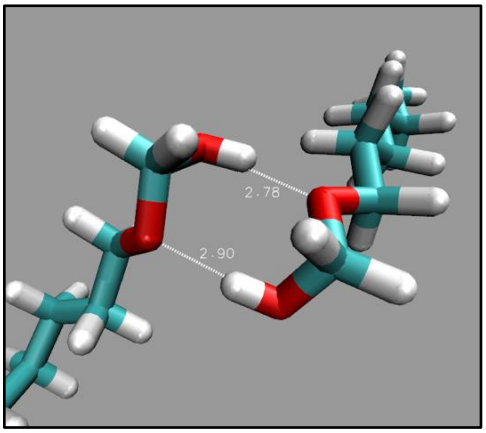

Figure 1. 6-membered ring formation through the intermolecular hydrogen bonding observed for 1-hexoxymethan-1-ol species in a MD simulation at 298K.

Poster 28

Clustering Protein Structures Using Energy Instead of Atomic Displacement

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Clustering is a process which groups similar protein structures using a chosen criterion, in this case, structure energy. This has traditionally been used with geometric considerations such as RMSD, which measures the average displacement between two structures. In chemistry, the energy difference and the system's thermal energy is a much better representation of a system's state than the moment to moment positions of a molecule's constituent atoms. That is not to say that there is not a strong correlation between low RMDS between and similar proteins, but this often becomes less clear cut with multicomponent systems. Throughout this presentation, we will further explore the benefits of clustering using energetic principles rather than geometric ones. The method that is used here to classify a protein's energy is an elastic network model called FlexE which can be used to quickly and accurately compute the energy of a protein structure. Using this method, an energy-based similarity matrix can be generated that can now be fed to any clustering algorithm to separate protein structures into clusters based on their thermal energies. We will compare the clustering performance of this method to the geometric approach through the analysis of several systems including a protein monomer, dimer, and protein peptide systems. The effectiveness of these two approaches will be discussed as well as their relative advantages and disadvantages.

Poster 29

Bioethanol from Rice husks as a Second-Generation Biofuel: Glucose Quantification Using Dinitrosalicylic Acid Analysis

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The preferred usage of fossil fuels over renewable energy sources has resulted in the extraneous release of greenhouse gasses into the atmosphere. Greenhouse gasses pollute the atmosphere and contribute significantly to the problem of global warming. As a result, alternative, renewable energy sources have become a central topic for discussion. Biomass is one of many alternatives. Biomass is a more environmentally friendly, renewable organic matter that can be used as fuel. Biofuels that use foods high in carbohydrates, including rice, bread, potatoes, and other crops, are often referred to as first-generation biofuels. However, the problem with first-generation biofuels is that they take away a food source and increase global food prices. Therefore, research has turned to second-generation biofuels, which acquire ethanol from biomass as an alternative to first-generation biofuels. Second-generation biofuels are made from lignocellulose which composes the inedible part of a plant's cell wall composed of cellulose and lignin. This project centralizes utilizing one of the most abundant and readily

available biomasses, rice husks. The main objective of this research project is to determine if rice husks are an efficient biofuel. This is determined by converting the rice husk into biofuel using the ionic liquid, known as 1-Butyl-3-methylimidazolium chloride, and quantifying the amount of glucose obtained from this process through the use of dinitrosalicylic acid analysis (DNS), glucose refractometry, and ultraviolet-visible spectroscopy. The greater the amount of glucose in the samples, the more ethanol that can be produced via fermentation to be used as fuel.

Poster 30

Crystallization of a Diadenosine Polyphosphatase of the Nudix Hydrolase Superfamily from M. tuberculosis

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M. tuberculosis contains 11 potential Nudix hydrolases, and we are characterizing these enzymes as potential novel antibiotic targets. The diadenosine polyphosphatases (ApnAases) / mRNA decapping enzymes are a family of enzymes within the Nudix hydrolase superfamily. In M. tuberculosis there is the primary Nudix ApnAase and the secondary Nudix ApnAase. The diadenosine polyphosphatases from Legionella pneumophilia and Bartonella bacilliformis have been found to be important in each pathogen's ability to invade its host cells. We are interested in whether these enzymes have a similar role in M. tuberculosis. If they are found to be involved in invasiveness and thus in virulence, then these enzymes could be novel antibiotic targets. Solving the X-ray crystal structure of this enzyme could be used for novel drug design against M. tuberculosis. We have cloned and overexpressed the primary Nudix ApnAase from M. tuberculosis and have subcloned it into a HisTag vector to optimize purification. This enzyme has been purified and characterized, and we are in the process of crystallization for structure determination. We have identified multiple crystallization conditions, and have sent crystal samples to the National Synchrotron Light Source II at Brookhaven National Laboratory for data collection. This research has been supported by an NIH AREA grant, a CUR-Goldwater Scholars Faculty Mentor Award, an ASBMB undergraduate research award, a RAS student research grant, and a RIT COS Emerson SURF.

Poster 31

Timing Matters: How the Order of Content Delivery Affects Student Exam Performance in Organic Chemistry

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The order prescribed by an adopted organic chemistry textbook may largely influence the timing of when certain concepts are taught during the semester. It was hypothesized that

changing the order of content delivery would positively affect student exam performance. During our trial year, it was discovered that students scored higher on both the last exam of Organic I and the first exam of Organic II when a reorganization of the content was implemented compared to the control years. Interestingly, the reorganization did not adversely affect exam performance for traditionally timed content.