



The Mid-Hudson American Chemical Society

25th Annual

UNDERGRADUATE RESEARCH SYMPOSIUM

Friday, April 25, 2025



25th Annual Mid-Hudson ACS
Undergraduate Research Symposium
April 25, 2025

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Program

3:30 – 4:00 PM: Check-In & Poster Set-Up (*Science Hall*)

4:00 – 4:40 PM: Poster session A

4:40 – 5:20 PM: Poster session B

5:30 – 6:00 PM: Awards & Announcements (*Coykendall Science Building Auditorium*)

6:00 PM: Lecture by Dr. Karena Chapman, Stony Brook University
(*Coykendall Science Building Auditorium*)

7:00 PM: Buffet Dinner (*Science Hall, reservations required*)

Guest Speaker

Dr. Karena Chapman
Stony Brook University

X-RAY VISION: BRINGING FUTURE MATERIALS INTO FOCUS

Our need for clean energy drives widespread materials research, from energy storage in lithium-ion batteries to efficient catalytic conversions of chemical fuels to the capture of CO₂ from the air around us. Breakthroughs can be driven by discoveries of new materials or advances in the tools that we use to understand how these materials form, function, and fail. Our research uses advanced characterization tools to probe the structure of energy materials in situ, as they function or react. This allows us to identify how their functional behaviors are governed by their structure and chemistry. These fundamental insights serve as a road map towards next-generation clean energy solutions.



KARENA CHAPMAN

Endowed Chair in Materials
Chemistry

Stony Brook University

Stony Brook, NY

Karena Chapman is at the forefront of a materials revolution as the Endowed Chair in Materials Chemistry at Stony Brook University. Prior to her tenure at Stony Brook, she embraced synchrotron science as a tool for chemistry at Argonne National Laboratory, where she led the development of the world's first dedicated X-ray Pair Distribution Function instrument at the Advanced Photon Source.

With roots in Australia, she earned both her undergraduate and graduate degrees from the University of Sydney. Her research lies at the intersection of structure, function, and reactivity in energy-relevant materials, often pushing the boundaries of what can be revealed through advanced synchrotron techniques. Her work spans diverse fields, from nuclear waste storage solutions to nanoporous frameworks for catalysis, CO₂ capture, and novel materials discovery.

Recognized as one of the American Chemical Society's Talented 12 in 2016 and recipient of the 2022 Hanawalt award and 2015 MRS Outstanding Young Investigator Award, Karena's contributions to the field are widely recognized. As an editor for ACS Energy Letters, and the Deputy Director of GENESIS, a Next Generation Synthesis Center funded by the Department of Energy, she continues to shape the future of materials chemistry.

Abstracts (Session A = Odd, Session B = Even)

(1) EXPLORING THE CATALYTIC POWER OF ACYLTRANSFERASE FROM *MYCOBACTERIUM SMEGMATIS*

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New biocatalytic enzymes are being discovered and celebrated for their ability to lower reaction rates and yield high enantiomeric excess. Traditional chemical catalysis in synthetic chemistry often employs metals, many of which are dwindling on our planet, whereas enzymes and biological organisms, which are regenerative and accessible, are worthy alternatives to metal catalysis. In this work, we focus on the acyltransferase enzyme from *Mycobacterium smegmatis* (MsAct). MsAct has been shown to favor condensation reactions over hydrolysis in aqueous conditions due to its hydrophobic pocket, making it a promising candidate for a wide range of industrial applications. The enzyme has been previously reported to perform trans-esterification, amidation, trans-amidation, and per hydrolysis reactions exceptionally well, and can withstand a wide range of pH (6-10) environments compared to that of other known biocatalysts. Previous studies have also reported MsAct's performance of the reverse reaction, specifically hydrolysis of the newly formed ester product, after prolonged reaction times, highlighting its dynamic catalytic capabilities. Herein this study explores the relationship between MsAct concentration to perform acetylation reactions, as well as exploring MsAct's enantioselectivity and its activity towards more polar substrates.

(2) QUANTIFYING SCS3-MEDIATED ER HOMEOSTASIS THROUGH REPORTER GENE ASSAYS

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The mammalian endoplasmic reticulum (ER) resident enzyme FIT2, and its yeast counterpart, SCS3, play a crucial role in ER lipid and proteo-homeostasis. Through mechanisms that remain under investigation, these fatty acetyl coenzyme A diphosphatases regulate key metabolic pathways responsible for proper lipid droplet formation and ER morphology. This study employs an SCS3-deleted (*scs3* Δ) yeast strain alongside engineered cells overexpressing key genes identified in a prior genetic screen. By overexpressing these candidate genes and exposing cells to stress-inducing growth conditions, the study aims to elucidate the functional role of SCS3—and, by extension, FIT2—in maintaining ER homeostasis.

This study was made possible by a newly optimized ER-stress assay utilizing a UPRE-*lacZ* reporter system to assess unfolded protein response activation. Two experimental approaches were employed: (1) five cell strains were analyzed under normal conditions, with dithiothreitol (DTT) or tunicamycin to induce proteotoxic ER stress, and (2) five cell strains were tested in standard media and inositol-depleted media to evaluate lipotoxic ER stress response. These assays quantify SCS3's role in ER stress mitigation and demonstrate how candidate gene overexpression in *scs3* Δ cells provides differing levels of rescue. Ultimately, this study validates prior qualitative observations with quantitative data.

(3) PURIFICATION OF *Salmonella* TYPHIMURIUM pCU1 TRAI CONSTRUCTS AND STRUCTURAL ANALYSES OF *Bacteroides ovatus* PDA

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Structural characterization of microbial proteins is an essential part of developing new drugs. We studied the protein TraI encoded on antibiotic resistant plasmid pCU1 from *Salmonella* Typhimurium and a polysaccharide deacetylase from gut microbe *Bacteroides ovatus*. Antibiotic resistance is a global public health issue, and a route that bacteria acquire resistance is conjugative plasmid transfer (CPT). In CPT, the relaxosome protein complex processes plasmids for transfer between bacterial cells. The pCU1 relaxosome contains TraI, a bifunctional enzyme with relaxase and helicase domains. To investigate binding interactions between TraI and other relaxosome proteins, we obtained relaxase and helicase-only TraI constructs. We expressed and purified the relaxase construct TraI_299 using intein affinity and size exclusion chromatography. However, our initial attempt to purify the helicase construct TraI_311-1078 yielded low amounts of target protein due to insufficient overexpression. After modifying our methods, we achieved successful overexpression of TraI_311-1078. The next phase in the TraI project is to purify additional TraI constructs and perform isothermal titration calorimetry with other relaxosome proteins. Gut microbe *B. ovatus* has capsular polysaccharide carbohydrates (CPS) on its cellular surface. CPS can serve as a protective barrier to antibiotics and may influence the human immune system. Despite its importance, CPS synthesis in *B. ovatus* is unknown. We structurally analyzed two crystal structures of CPS biosynthetic protein *B. ovatus* PDA (BoPDA). To gain insight into its mechanisms, crystal structures of BoPDA bound to Cu^{2+} and Zn^{2+} were solved, using programs Coot and Phenix we improved the models. The BoPDA Cu^{2+} and Zn^{2+} bound structures will be compared to Co^{2+} and Ni^{2+} bound structures. Our research is important for broader understanding of microbes and supports the development of new antimicrobials.

(4) SOLVENTLESS SYNTHESIS OF CHALCONES

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Chalcones (1,3-diaryl-2-propene-1-ones) in which two aromatic rings are linked by a three-carbon α,β -unsaturated carbonyl system have been shown to display a wealth of biological properties. Piperonal is an aromatic heterocyclic aldehyde consisting of a benzene ring fused to a pyran ring. Many compounds containing this 3,4-methylenedioxy group have shown very strong antibacterial activity. A small library of chalcones containing a piperonal moiety have been synthesized by Claisen-Schmidt condensation with acetophenone derivatives substituted at the para position with various electron-donating and electron-withdrawing substituents for a structure-activity relationship study. Although most aldol condensation reactions are run in organic solvents at elevated temperatures, solventless synthesis of chalcones have recently been shown to be efficient. Solvents are a significant component of industrial chemical waste. This reaction highlights green chemistry principles as the synthesis minimizes waste production (no reaction solvent) and proceeds with high atom economy. The synthesis and characterization will be discussed.

(5) SYNTHESIS OF 2-BUTYL-4-OXOAZETIDINE

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Antibiotics are continuing to be used now more than ever, and bacteria are rapidly evolving mechanisms of resistance. Historically, the most effective class of antibiotics are the β -lactams, a 4-membered cyclic amide. By acylating serine residues, they inactivate enzymes that catalyze the formation of peptidoglycan, weakening the cell wall and causing osmotic stress. Bacteria have evolved various classes of enzymes that hydrolyze the peptide bond and destroy the lactam ring. The aim of this research was to synthesize 2-butyl-4-oxoazetidine by reacting 1-hexene with chlorosulfonyl isocyanate, followed by reduction. The product was purified and analyzed using various spectroscopic methods. The results of this study will be presented along with implications for future studies.

(6) BUFFER AND ELECTROLYTE CONSIDERATIONS FOR LIGHT DEPENDENT CURRENT GENERATION BY REACTION CENTERS ON GRAPHENE OXIDE

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Photosynthetic reaction centers (RCCs) from *Cereibacter sphaeroides* generate light-dependent current when covalently attached to an electrode. In our previous work, we have collected evidence that utilizing lysine residues on the outside surface of RCCs resulted in a light dependent cathodic current when covalently attached to graphene oxide (GO) electrodes. Recently, we were able to attain a twenty-fold increase in such light-dependent current by changing the buffer during the crosslinking step. In this project, we plan to optimize electrolyte concentrations and consider other electrolytes. Initially, we are utilizing the Cottrell equation to predict the current. We propose to model light absorption in GO, charge carrier generation, and transport, while systematically varying electrolyte properties (e.g., pH, ion concentration) to predict the optimal conditions for maximizing photocurrent. Experimental validation will involve fabricating GO electrodes, testing them in selected electrolytes, and measuring photocurrent using cyclic voltammetry and chronoamperometry. Future efforts might include DFT, MD, and COMSOL to provide a detailed, actionable roadmap for optimizing electrolyte-GO interactions, directly enhancing the development of efficient light-driven energy conversion systems.

(7) THERMAL DEGRADATION MODELING OF POLYTETRAFLUOROETHYLENE APPLICATIONS

**Bret J. Copeland, Kai D. Palam, Charles M. Aronov, Amelia J. Kitlinski, Daniel E. McGinnis, Aryanna S. Cargle, Benjamin R. Johnson, Nijel Rogers, Justin Hunter, Justin R. Toole, Victor A. Jaffett, Pamela Sheehan,
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Synthetic fluoropolymers, particularly poly- and perfluorinated alkyl substances (PFAS), are widely used across various industries, including kitchenware, textiles, and flame-resistant materials. Their unique properties - such as high wettability, thermal and chemical stability, and low friction - originate from the strength of their carbon-fluorine (C–F) bonds. However, increasing concerns have emerged over the toxicity of fluoropolymers in living organisms, largely due to their strong protein-binding affinity and environmental persistence. Combustion-based methods have been proposed to reduce the concentration of these substances in open-air environments. Yet, identifying the key decomposition products generated during combustion remains a significant challenge. To investigate the thermodynamic and kinetic aspects of the degradation mechanism of polytetrafluoroethylene (PTFE), we employed an integrated approach combining ChemCAD chemical process simulation with density functional theory (DFT)-based microkinetic modeling. Through ChemCAD bulk process models, we determined the mass and energy balance of the degradation of products resulting from the polymer breakdown. Moreover, the microkinetic modeling results indicate that COF_2 and C_2F_4 are the predominant degradation products compared to C_3F_6 . Notably, the concentration of O_2 in the system plays a critical role in activating specific degradation pathways and determining the resulting product distribution. Therefore, careful control of oxygen levels within the combustion chamber is essential for manipulating PTFE degradation toward desired conditions.

(8) DETERMINATION OF TRAK'S OLIGOMERIZATION STATE WITHIN THE PCU1 RELAXOSOME USING ATOMIC FORCE MICROSCOPY

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Antibiotic resistance has become an increasing and prevalent health crisis, projected to kill millions of people per year. A major contributor to this spread of antibiotic resistance is conjugative plasmid transfer, an evolved bacterial mechanism that uses the relaxosome protein complex to facilitate the transfer of DNA containing antibiotic-resistant information between bacteria. This study focuses on the pCU1 relaxosome, which includes the proteins TraK, TraI, and an Integration Host Factor, from the bacteria *Salmonella* Typhimurium. We aim to determine TraK's oligomerization state through a method of volume analysis that uses atomic force microscopy (AFM) imaging to correlate measured protein volume with its molecular weight. To facilitate accurate molecular volume determination, we created a standard curve by comparing the molecular weights and measured volumes of a set of stable proteins imaged by the AFM. The proteins were analyzed by comparing three volume determination methods considering AFM tip convolution in the images to yield the most consistent protein volumes for the standard curve. This standard curve is a valuable tool for determining the oligomerization state of TraK and other proteins within the pCU1 relaxosome, including their stoichiometric ratios when bound to DNA.

(9) ORGANIC CHEMISTRY WEBSITE AND REACTION GENERATOR

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The goal of this project was to develop a web application to help students further learn and practice organic chemistry (reactions). This work is a continuation of a previous project, “Organic Chemistry Reaction Question Generator,” which we developed into a website for reinforcing reactions and principles. We created a random problem generator for reactions that include both functional group transformations and carbon chain reactions. This process was done computationally using the HTML and JavaScript languages. To support the learning experience, we built a spinning wheel to learn functional group identification, quizzes, and a guide to each reaction covered in Organic Chemistry I. Throughout the semester, we have gathered student feedback and incorporated their suggestions into our website design, which positively impacted their learning outcomes. In the future, we want to add more advanced reactions, build more games, and have a way to track progress to further enhance student engagement and success.

**(10) INVESTIGATING THE ANTIBIOTIC PROPERTIES OF
PHENOTHIAZINE, DIBENZAZEPINE, AND
BUTYROPHENONE DERIVATIVE ANTIPSYCHOTIC
COMPOUNDS**

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Antimicrobial resistance is a rapidly worsening global health crisis, contributing to millions of deaths per year. Synthesizing, isolating, and general development of novel antimicrobials has stalled within the 21st century due to the high cost of resources, and its investment by pharmaceutical companies has dropped. A new eye has recently turned towards screening and repurposing previously existing compounds for their potential antimicrobial properties.

Antipsychotics have antimicrobial roots, having originated from the antimalarial agent and later discovered monoamine oxidase inhibitor (MAOI), methylene blue. Throughout the 1950s, the phenothiazine core of the dye proved to be especially promiscuous, with neuroleptic derivatives becoming FDA approved within the decade. This study investigates the antibacterial activity of three structurally distinct antipsychotic drugs—thioridazine, clozapine, and haloperidol—against *Bacillus subtilis*, a gram-positive model organism. While prior research has focused on pathogenic gram-positive species such as antibiotic-resistant *Staphylococcus aureus*, these bacteria often contain efflux pumps that obscure potential mechanisms of action. By studying *B. subtilis*, a non-pathogenic species with well-characterized genetics, this project aims to establish a clearer foundation for understanding the antibacterial effects of antipsychotics and support future investigations into their mechanisms of action.

(11) ANTIMICROBIAL POTENTIAL OF SYNTHESIZED MONO/BIS LACTAMS

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Antibiotic resistance is becoming a critical threat to human health, making the synthesis of novel antibiotics invaluable. β -lactams are a class of 4-membered cyclic amides that display significant antimicrobial activity. They acylate essential serine residues in the cell walls of bacteria, leading to cell lysis and death. The objective of this research was to treat various alkenes with chlorosulfonyl isocyanate (CSI) to form N-sulfonyl chloride β -lactams and then reduce them to their corresponding β -lactam. Products were purified using recrystallization and/or column chromatography then analyzed using spectroscopic methods. Several β -lactams were synthesized, and disc diffusion bioassays were conducted on gram-positive (*M. phlei*, *Staph. aureus*, *Strep. faecalis*) and gram-negative (*E. coli*, *Ps. fluorescens*) bacteria to evaluate their antimicrobial potential.

**(12) OXIDATION OF A LIGNIN MODEL COMPOUND BY THE
LACCASE MEDIATOR SYSTEM:
A STUDY OF MEDIATOR EFFECTIVENESS**

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Mediators of the laccase-catalyzed oxidation of a lignin model compound were studied to aid development of a benign process for biomass valorization. An enzyme-based approach, such as one utilizing the laccase mediator system (LMS), would avoid the need for harsh chlorine-based delignification reagents. Limitations of the LMS are known, however, including toxicity and expense associated with the most common mediator, 1-hydroxybenzotriazole (HBT). To further investigate these limitations, five additional natural and synthetic laccase mediators were examined to analyze the effect of the mediator on laccase activity, as well as to assess the ability of the LMS to oxidize veratryl alcohol, a lignin model compound. The synthetic mediators, HBT and 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS), proved to be the most powerful, exhibiting almost quantitative oxidation of veratryl alcohol, as determined via HPLC; yet with HBT as mediator, laccase was rendered inactive. Natural mediators, including acetosyringone and syringaldehyde, were not as effective, consistent with their lower redox potential. Since our laboratory has previously reported that alginate encapsulation protects enzymes against oxidative damage, this work sets the stage for future studies employing immobilized laccase.

(13) INVESTIGATING THE ENZYMATIC AND BINDING CHARACTERISTICS OF MICROBIAL PROTEIN *B. OVATUS* POLYSACCHARIDE DEACETYLASE (*BoPDA*)

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Bacteroides, perhaps the most common species found in the human gut microbiome, confer advantages upon their host. One species, *Bacteroides ovatus* (*B. ovatus*) has been demonstrated to provide benefits such as suppression of intestinal inflammation, but can also be linked to autoimmune diseases such as systemic lupus erythematosus (SLE). External cellular carbohydrates such as capsular polysaccharides (CPS) can play a role in modulating these microbe-host interactions, however CPS loci in *Bacteroides* are understudied. One CPS locus in *B. ovatus* encodes a carbohydrate deacetylating enzyme, *BoPDA*. Previous characterizations of *BoPDA* found no enzymatic activity with large polysaccharides. In this study, we have performed biochemical assays to identify a suitable ligand for *BoPDA*. Deacetylase assays with the general esterases substrate 4-methylumbelliferyl acetate were completed. Binding affinity for polysaccharides xylan and chitin, and oligosaccharides triacetyl-chitotriose and 2,3,4-O-triacetyl-D-xylopyranose was studied through carbohydrate affinity polyacrylamide gel electrophoresis (CA-PAGE). Additionally, datasets collected from *BoPDA* crystals soaked with ligands Co^{2+} and xylan were analyzed.

**(14) LIGHTS, DOTS, SYNTHESIS!
EXPLORING THE USE OF CARBON DOTS IN
[2+2] PHOTOCATALYTIC CYCLOADDITIONS**

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The use of photocatalysis in organic synthesis has continuously gained traction over the years due to its facile nature in elucidating chemically inert pathways towards target organic molecules. Widely studied is the [2+2] cycloaddition of alkenes that can undergo single electron transfers using photocatalytic conditions. Transition metals as photocatalysts have been at the forefront of said processes. The recent discovery of carbon-based quantum dots has opened a new door for the world of photocatalysis. Our research has taken a novel approach to the carbon dot reaction and photocatalyst index. The focus has been placed on utilizing blue-light mediated [2+2] reactions with nitrogen-doped carbon dots to produce four-membered rings. We report our recent findings in the preparation of carbon dots and photocycloaddition products. Synthetic studies, carbon dot characterization, and their function will be further discussed.

(15) ELECTROCHEMICAL CHARACTERIZATION OF POLYMER HYDROGEL COATED COMPOSITE SEPARATORS FOR REDOX FLOW BATTERIES

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Redox flow batteries (RFBs) meet the increasing demand for more effective and scalable energy storage technologies to implement renewable energy sources into the grid. The objective of this study is to determine the most effective combination of composite polymer separators within aqueous flow batteries. Through electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and chronoamperometry (CA) we can determine the charge transfer resistance, mass transfer resistance, and electronic and ionic conductivity in a custom flow cell hardware with various supporting and redox electrolyte chemistries at varying flow rates and at stagnant no-flow conditions within a single cell stack. Composite separators for electrochemical characterization including CelgardTM and DaramicTM coated with poly(acrylic acid) and poly(vinyl alcohol) hydrogels are studied. The electrolytic solutions for electrochemical measurements were 1.0 M, 0.5 M, and 0.1 M of H₂SO₄ and HCl. The results show an increase in resistance both with electrolyte concentration and in no flow conditions. The CelgardTM coated with PVA shows similar or lower resistance values compared to the DaramicTM. The uncoated Celgard CVs show higher resistance values with the PVA coating at very low frequencies, which is consistent with the EIS data. This will help inform the design of aqueous RFBs with cost-effective separators.

(16) SOLVATOCHROMISM AND AGGREGATION-INDUCED EMISSION ENHANCEMENT IN MOLECULES CONTAINING QUINOXALINE ACCEPTORS ATTACHED TO PHENYL-THIOPHENE DONORS

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Organic fluorophores are important for applications in biosensing, cellular imaging, photodynamic therapy, light emitting diodes, and solar cells. Depending on their structures, they can exhibit aggregation caused quenching (ACQ) or aggregation-induced emission enhancement (AIEE), as well as properties such as solvatochromism if they contain a donor-acceptor domain. Recently, our research group has synthesized several molecules containing electron-accepting quinoxaline rings that are either *ortho*-disubstituted (V-shaped) or monosubstituted (one-arm analog) with phenyl groups with various electron donors attached. Their donor-acceptor nature leads them to exhibit solvatochromism, which is a change in emission wavelength as a function of increasing solvent polarity. The V-shaped compounds have free rotation about the aromatic rings attached to the quinoxaline when dissolved, which means their fluorescence emission is weak due to non-radiative deactivation pathways. But when they aggregate, free rotation is no longer possible, so their emission increases and blue shifts. The one-arm analogs exhibit solvatochromism, not AIEE, as expected. In this work, solvatochromism and AIEE results will be presented for a one-arm analog containing a phenyl-thiophene donor, and comparisons will be made to its V-shaped analog and related structures. NMR and computational studies will also be presented.

(17) CHEMICAL IMMOBILIZATION OF URANIUM BY 2-2' BIPYRIDINE: A DFT STUDY

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Hydraulic fracking often results in uranium environmental pollution because of the way fracking fluid interacts with shale to release uranium. To combat this issue, uranium can be precipitated out of waterways using ligands. This project aims to use density functional theory to evaluate the potential of various ligands. First, the appropriate functional and basis set were selected by calculating the adiabatic ionization energy of UO_2 to try to reproduce experimental values. A range of hybrid and meta hybrid functionals were considered, as well as a range of basis sets of different sizes. The $\omega\text{B97X-V}$ functional best replicated previous experimental results and the 6-311+G* basis set provided sufficient accuracy to within 0.02eV when compared to the largest basis set. Thus, the $\omega\text{B97X-V}$ functional and the 6-311+G* basis set were selected for the calculations of the larger complexes. Next, we investigated the binding of 2-2' bipyridine with uranyl acetate and uranyl carbonate, optimizing their structures and calculating binding energies. These complexes were chosen because uranyl carbonate is the primary form found environmentally, and uranyl acetate is the form used in previous experiments. Comparing the results will validate the accuracy of the experimental model as being predictive of the efficacy of precipitation by ligands in environmental conditions. Additionally, these binding energies will be compared with those of other promising ligands, to identify the most promising ligand for the precipitation of uranium. These results can help minimize the negative environmental impact of hydraulic fracking.

**(18) EFFECT OF MODIFIED BETULINIC ACID ON
*DROSOPHILA MELANOGASTER***

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White Birch (*Betula papyrifera*) and American Sycamore (*Platanus occidentalis*) bark contain tannins, polyphenols, and lupane triterpenoids such as botulin, betulinic acid, and lupeol. In our lab, methanolic extracts of these barks have been found to be biologically active in assays on the common fruit fly (*Drosophila melanogaster*). The activity of purified fractions is divergent, demonstrating protection against oxidative stress, larval growth enhancement, larval growth inhibition, direct toxicity, or no activity as compared to a control. Extracts were characterized by GCMS, ¹H-NMR, and IR spectroscopy, and antioxidant activity was assessed by DPPH free radical scavenging assay. The most active component of these extracts in terms of increased growth and survivorship is betulinic acid, the main constituent of Sycamore bark extract. To investigate the mechanism of this novel activity, we have begun preparing a selection of synthetically modified betulinic acid derivatives to conduct a structure-activity relationship. Most recently, benzylation of an alcohol position on betulinic acid provided a derivative with twice the activity of betulinic acid. Results to be discussed.

**(19) STRUCTURAL AND FUNCTIONAL INVESTIGATION OF
MICROBIAL PROTEINS FROM *SALMONELLA*
TYPHIMURIUM AND *BACTEROIDES OVATUS***

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Characterization of essential microbial proteins can help with the development of novel antimicrobials. Two understudied bacterial processes are the spread of antibiotic resistance via conjugative plasmid transfer (CPT) in bacteria and the role of the gut microbes in disease states. We studied the relaxosome complex from *Salmonella* Typhimurium antibiotic resistant plasmid pCU1, and a polysaccharide deacetylase from gut microbe *Bacteroides ovatus*. The relaxosome is an essential protein complex that processes antibiotic resistant plasmids for transfer between bacterial cells during CPT. The *Salmonella* Typhimurium pCU1 relaxosome is thought to involve three proteins: TraI, TraK and IHF. Cobalt-His tag pull-down assays were used to understand binding interactions between these proteins. Analysis of the pull-down showed TraK bound to TraI, corroborating previous research. However, it remains unclear if IHF binds to TraI. To find the optimal molar ratio of TraK:DNA binding stoichiometry we used an electrophoretic mobility shift assay (EMSA). Results showed TraK fully binds at a 1:8 TraK:DNA ratio suggesting that TraK binds as two tetramers. To further investigate TraK protein-protein interactions, protein crosslinking was performed. Protein cross-linking is expected to improve the Cryo-EM results. Additionally, we plan to use isothermal titration calorimetry (ITC) to investigate the TraK-TraI-IHF binding interactions and optimize the EMSA. *B. ovatus*, a commensal gut microbe, helps in protecting humans from invading pathogens. Its cell surface capsular polysaccharides (CPS) are thought to contribute to this protection. However, CPS expression may also lead to autoimmune disease and studies characterizing CPS in *B. ovatus* are lacking. Our lab crystallized a CPS biosynthetic protein, *B. ovatus* PDA, bound to different metal cations to gain insight into its enzymatic activity. We refined two of the BoPDA metal-bound crystal structures, Co²⁺ and Ni²⁺, using the programs Coot and Phenix. This research helps to broaden our understanding of these important microbial processes, benefiting the ongoing development of novel therapeutics.

(20) QUANTIFYING DYE UPTAKE IN PRESSURIZED ENVIRONMENTS BY UV-VIS SPECTROSCOPY

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The effects of two different long-term storage methods were studied to determine the decomposition rate of the cold reactive dye, Procion Blue MX-R. The dye was examined over a four-week interval under both ambient and increased (0.7 bar) pressure conditions, with a sodium carbonate (soda ash) solution as a mordant for the dye. Over a 50% decrease was observed in dye binding for both pressurized storage methods, with the largest decrease observed at three weeks. The results indicate a proportional decomposition of the dye over the four-week storage period.

(21) CHARACTERIZING THE POLYMERIZATION AND STRUCTURAL PROPERTIES OF Δ 391 TAU

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The microtubule-associated protein tau is known for stabilizing and organizing microtubules in the central nervous system. However, abnormal tau aggregation into paired helical filaments (PHFs) and neurofibrillary tangles (NFTs) is a hallmark of Alzheimer's disease and related neurodegenerative disorders. Structurally, PHFs have a well-ordered core comprising tau's microtubule binding domain, which is surrounded by a disordered two-layer "fuzzy coat" established by the N- and C-terminals of tau. This study investigates the Δ 391 tau mutation, which truncates tau at Glu-391 and accelerates its aggregation into PHFs due to the loss of the C-terminus. We have interrogated three isoforms of the Δ 391 tau mutation—0N4R, 1N4R, and 2N4R—which differ in N-terminal length but share the same C-terminal deletion, and report on differences in polymerization kinetics and PHF structure compared to wild-type tau. Polymerization was assessed using a thioflavin S kinetics fluorescence assay, revealing immediate and rapid polymerization in the presence of arachidonic acid. To analyze polymer morphology, atomic force microscopy (AFM) was used to image polymers of all three variants. AFM imaging, conducted in dry environments and tapping mode, revealed the distribution of polymer lengths. Additionally, AFM imaging in fluid environments combined with quantitative nanomechanical mapping allowed us to measure the deformation and adhesion of the fibers, highlighting key differences between Δ 391 and wild-type isoforms. These findings will help guide future research on the C-terminal truncation's ability to aggregate into PHFs and NFTs.

**(22) INTERMOLECULAR [2 + 2] PHOTOCYCLOADDITION
REACTIONS OF INDOLE DERIVATIVES VIA VISIBLE LIGHT
PHOTOCATALYSIS**

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The efficacy of visible light mediated photocatalysis reactions, specifically the [2 + 2] cycloaddition of various indole derivatives and olefins coupling partners, is presented. [2 + 2] cycloaddition reactions, ubiquitous in molecular design, have been traditionally catalyzed by high-energy ultraviolet light. However, recent photochemical advancements have proven visible light as a more optimal energy source. Our work is centered on observing and understanding the regioselectivity and stereoselectivity of intermolecular [2 + 2] cycloadditions of 3-acyl indole with alkenes, yielding isomeric products. With the end goal of optimizing all procedures to be speedy, effective, and selective, we report the synthesis of various cyclobutane derivatives and the optimal conditions for such reactions, including molar ratios, solvents, and catalysts.

(23) THE IMPACTS OF HEAVY METALS ON PROTEIN PRODUCTION IN LICHENS

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Lichens are a symbiotic relationship between a fungal partner and either green algae or cyanobacteria and are incredibly sensitive to air pollution. This makes them very good bioindicators of air quality in a more local area. Lead and copper are both heavy metals and common environmental pollutants. Airborne lead pollution is primarily caused by metal processing and leaded aviation fuel. This pollutant can negatively impact plant growth and reproduction due to lead accumulation affecting the metabolic processes of plants. The same effect can be seen in lichens, alongside impacting their photosynthetic processes. While copper is not as common as an airborne pollutant, it is common as a water pollutant, typically caused by mining and manufacturing. Copper has been observed impacting the growth and pigment of *Trebouxia erici*, a lichen photobiont, as well as disrupting multiple other metabolic processes. Through proteomic analysis of lichens, identifying and quantifying the proteins within the lichen can aid in understanding the processes taking place within the lichen, and how certain variables can impact them.

(24) ETHANOL QUANTIFICATION IN LOCAL BEER SAMPLES

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We used the American Society of Brewing Chemists' Method "Beer 4: Alcohol" to determine the percentage of ethanol in beer samples. This method uses gas chromatography with flame ionization detection (GC-FID) to measure ethanol and uses n-propanol as an internal standard. The protocol demonstrates excellent linearity and precision with typical results having $R^2 = 0.995$ and $RSD < 1\%$. We have applied this method to samples of beer from local brewers in the Mid-Hudson area, which provides them with an actual measurement for comparison, as opposed to only the theoretical calculation.

**(25) ANALYSIS OF CATION-STABILIZED HYPF-N
OLIGOMERS TO STUDY THE STRUCTURAL
DETERMINANTS OF PROTEIN MISFOLDED OLIGOMER
TOXICITY**

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Misfolded protein oligomers, small aggregates of monomers intermediate to amyloid fibrils formed by aberrant protein deposition, play a critical role in neurodegenerative diseases such as Alzheimer's and Parkinson's diseases. To investigate the properties of oligomers, we leveraged a model amyloid system comprised of the 91-residue N-terminal domain of [NiFe]-hydrogenase maturation factor HypF (HypF-N) found in *E. coli*. By introducing K⁺, Na⁺, Li⁺, Ca²⁺, Mg²⁺, Cu²⁺ and Zn²⁺ to HypF-N monomer populations, we observed the formation of HypF-N oligomers with differential structural, chemical, and physical properties. Aggregation was assessed through ThT binding to analyze β -sheet content, ANS fluorescence to determine hydrophobicity, turbidity and AFM to analyze oligomer size, and SDS-PAGE to determine yield. Structural properties were then related to their ability to induce cellular dysfunction using MTT assays. These results elucidate the properties that enable protein misfolded oligomers to become cytotoxic to cells. Of the six metal ions studied, we note that Zn²⁺ stabilizes the most cytotoxic oligomers with products that are more hydrophobic and smaller than oligomers formed in the absence of ions. We found that oligomer size and hydrophobicity are indicators of cytotoxicity: smaller and more hydrophobic ion-treated oligomers induced higher levels of cytotoxicity.

(26) COMPARATIVE REACTIVITY STUDIES OF STYRENE AND 1,1-DIPHENYLETHYLENE WITH CHLOROSULFONYL ISOCYANATE AND ANTIMICROBIAL EVALUATION OF THE RESULTING PRODUCTS

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This research project aimed to synthesize β -lactams [via reduction of β -lactam N-sulfonyl chloride] from styrene and 1,1-diphenylethylene using chlorosulfonyl isocyanate (CSI). Several β -lactams were successfully produced with ease using this method including the styrene β -lactam. However, when 1,1-diphenylethylene was treated with CSI, a white foul-smelling crystalline product was obtained, and the NMR of the crude product was not consistent with the expected β -lactam N-sulfonyl chloride. The thin layer chromatography (TLC) of the white solid obtained by the reaction of 1,1-diphenylethylene with CSI revealed more than one product. The crude product was purified using column chromatography and the three products were analyzed by NMR. Bioassays were run on all three compounds using several gram-positive (*Enterococcus faecalis*, *Staphylococcus aureus*) and gram-negative bacteria (*Escherichia coli*, *Pseudomonas aeruginosa*). Results of this study will be presented.

(27) IN-VITRO ASSEMBLY OF TAU FIBERS WITH DISTINCT POLYANIONIC INDUCERS REVEAL DISTINCT MECHANICS OF THE “FUZZY COAT”

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Tau is a neuronal protein implicated in 20 neurodegenerative diseases, where it forms insoluble aggregates called neurofibrillary tangles (NFTs). These aggregates are comprised of tau filaments, which characteristically have a well-ordered core surrounded by a “fuzzy coat” formed by the protein’s unstructured termini. Distinct tau folds in the core of these filaments are unique to different diseases such as Alzheimer’s disease, Pick’s disease, and CTE, and while recent research has identified the presence of structural variations in fibrils induced by different polyanions, differences in structure and resulting mechanical behaviors of the fibrils have remained unexplored. This project examines how core structure variations affect disease-specific filament-filament interactions that ultimately lead to NFT formation. Two commonly used polyanionic inducers were selected to promote the in-vitro assembly of tau filaments: arachidonic acid and heparin sodium salt, and atomic force microscopy was used to collect high-resolution topographic images and quantitative nanomechanical maps. Tau filaments were imaged in fluid and their adhesive and deformation properties of the brush-like structure were simultaneously mapped. It was observed that distinct polyanionic inducers generated distinct mechanics of their “fuzzy coats”. These findings advance the understanding of tau aggregation in neurodegenerative diseases, paving the way for new avenues of intervention.

(28) OPTIMIZATION OF OLEFIN AZIRIDINATION VIA VISIBLE LIGHT PHOTOCATALYSIS: NITROGEN SOURCE AND REACTION EFFICIENCY

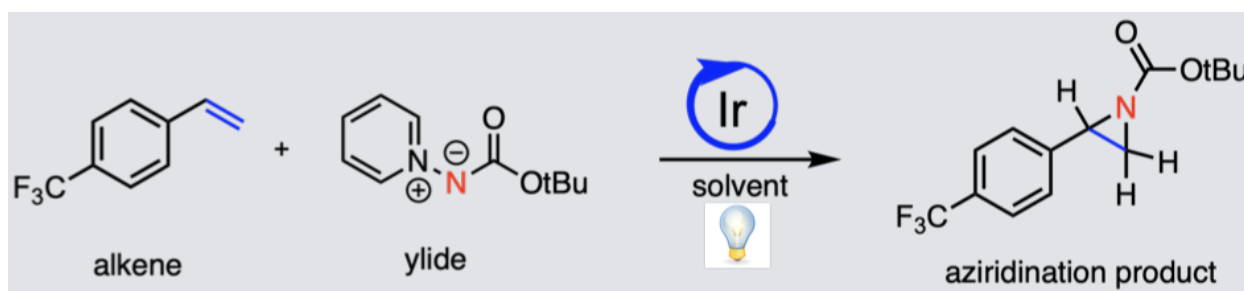
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Carbon-nitrogen (C-N) bonds are ever-present in both natural and unnatural small molecules. This work addresses the optimization of a relatively new methodology used to create two C-N bonds simultaneously using visible-light photocatalysis for the purpose of producing substituted aziridine products. Recently, visible-light photocatalysis has been shown to be an effective tool for small scale production of aziridines. Our research aims to improve the scalability of these reactions, the purification process, and examine electrophilic nitrogen sources such as bench-stable N-aminopyridinium ylides and related salts. In this presentation we report recent findings on the scope of the reagents and effects scale of our aziridination methodology, including under flow conditions.



(29) EVALUATING LIGAND STRATEGIES TO REDUCE HEAVY METAL CONTAMINATION IN SIMULATED HYDRAULIC FRACTURING INCUBATIONS

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Hydraulic fracturing (fracking) involves injecting pressurized hydraulic fracturing fluid (HFF) into shale formations to create fractures and release natural gas. During this process, chemical and physical alterations to the rock can lead to the dissolution of mineral phases, releasing heavy metals such as uranium into water that returns to the surface. These contaminants pose a serious risk to environmental and human health if not properly managed. This study investigated the potential of organic ligands such as 2-4 Bipyridine, Histidine, L-salicylic acid, Triethylene tetramine, Tetraethylene pentamine, and EDTA as additives to HFF to bind and stabilize heavy metals, thereby reducing their mobility and preventing their release into the environment. Batch experiments were conducted over a 21 day period with sampling at 15 minutes, 2 hours, 24 hours, 72 hours, 168 hours (7 days), and 504 hours (21 days). Metal concentrations were analyzed using Inductively Coupled Plasma Mass Spectrometry (ICP-MS) to evaluate the effectiveness of each ligand in promoting the immobilization of metals. Two experiments were performed: one using uranium salts, and another using ground shale. Across both setups, 2-4 bipyridine and tetraethylene pentamine showed strong efficacy in reducing metal concentrations, exhibiting approximately a 98% difference decrease in uranium levels compared to the HFF and water controls at the end of the experiment. While these ligands are highly effective, histidine represents a less toxic alternative that may be more favorable for applications where safety and environmental impact are critical considerations. Histidine itself showed a 88% difference decrease compared to the HFF control at the end of the experiment. However, significant variation was observed in ligand effectiveness depending on the specific metal, suggesting that a tailored ligand approach may be necessary for effective mitigation in fracking operations.

(30) EVALUATING THE POTENTIAL OF *SAUSSUREA LAPPA* AS A NATURAL INSECTICIDE

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Widespread concern over surmounting pesticide usage has augmented the appeal of plant-derived insecticides. *Saussurea lappa*, a plant indigenous to the Himalayan regions of India, Pakistan, and China, is a perennial herb of the family Asteraceae. For centuries, the root powder of *S. lappa* has been employed in the protection of crops and woolen clothes. This is attributed to the presence of two terpene derivatives: costunolide and dehydrocostus lactone. In this study, we conducted several assays to develop a multi-dimensional profile of *S. lappa*'s insecticidal activity. Phytochemical analyses of the crude ethanolic *Saussurea lappa* extract revealed the presence of flavonoids, carbohydrates, terpenoids and alkaloids. We found a strong dose-dependent correlation between *S. lappa* consumption and mortality of *Drosophila melanogaster* larvae (two days) and adults (fifteen days). In phago-deterrent studies, we observed retarded movements in flies exposed to 20% extract. To investigate whether a dose-dependent correlation exists between consumption of *S. lappa* and locomotion, we recorded how many times *D. melanogaster* crossed the midpoint of a closed tube with *S. lappa*-perfused diet of varying concentrations. This assay may elucidate the physiological mechanism through which *S. lappa* exerts its effects and thus enrich our understanding of its insecticidal potential. Results will be discussed.

**(31) FABRICATION AND APPLICATION OF MICROSCOPIC
PLATINUM–SILVER THERMOCOUPLES FOR
TEMPERATURE MONITORING DURING DIRECT LASER
WRITING**

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This study investigates the use of direct laser writing (DLW) to fabricate platinum–silver thermocouples. Accurately measuring temperature at the site of DLW remains a significant challenge in microfabrication, and this work aims to address that limitation. Using multiphoton absorption and photo-reduction techniques, micron-scale platinum and silver wires were fabricated to construct thermocouples. These devices were calibrated and employed to measure the temperature at the focal point of an 800 nm femtosecond laser and a 532 nm continuous wave laser, both of which are used for DLW of polymeric microstructures.

(32) SYNTHETIC METHOD FOR A 2-PHENYLINDOLE DERIVATIVE

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Serotonin and melatonin are both derived from endogenously secreted tryptamine. These molecules function as neurotransmitters and neuromodulators. However, many synthetic derivatives are used as recreational drugs and are therefore often categorized as controlled substances. Others have been prescribed for migraines or as antidepressants. In this project we wanted to focus on compounds that would bind to serotonin receptor 5-HT_{2A} with high selectivity as antagonists. Starting with a pool of 30 related compounds, we have narrowed down the potential targets to N-phenyl-2-phenyl (N-2-DPT) tryptamine through docking to 5-HT_{2A} receptor using Autodock Vina software. Our criteria were low K_d (high affinity) and feasibility of synthesis in our lab in terms of availability of equipment, safety requirements, and cost. Affinity was estimated to be between -6.7 kcal/mol to -7.9 kcal/mole, with N-2-DPT being predicted to be the highest in our set. N-2-DPT was also predicted to have higher affinity than several established 5-HT_{2A} receptor agonists such as LSD and bromo-benzofuranyl-isopropylamine. The presence of N-phenyl substituent is predicted to be more optimal than N-benzyl or N-isopropyl variants. Other variants included the methoxy group in the 5-position of the indole, halogens in meta position of the phenyl ring on the indole, and a 4-hydroxy on the indole. There was a structure-function trend observed trending towards bulkier groups attached to the amine increasing affinity that dropped off dramatically beyond a phenyl group. On the other hand, polar groups decreased affinity to the 5-HT_{2A} receptor.

(33) DIFFERENCES IN KINETICS OF TAU FIBER FORMATION REPORTED BY THIOFLAVIN DYES

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Tau is a microtubule associated protein that stabilizes and organizes microtubules. However, it has also been implicated in the progression of neurodegenerative diseases such as Alzheimer's disease, which are characterized by the presence of aggregated tau structures such as paired helical filaments and neurofibrillary tangles. To better understand the formation of these structures, tau fiber growth can be monitored using fluorescent reporter dyes that uniquely interact with the fibers. Two of the most commonly used dyes are thioflavin S (ThS) and thioflavin T (ThT); while both dyes have been previously reported to monitor tau polymerization, there have been few direct comparative studies. We assembled tau fibers *in vitro* and compared the resulting ThS and ThT fluorescence. Quantitative analysis of tau polymerization kinetics was accomplished by fitting growth curves to the Gompertz function. We compared a range of inducers, such as arachidonic acid, heparin, and polyphosphate, in the presence of ThS or ThT. In each case, we observed differences in how these dyes report tau polymerization, highlighting differences in how the two dyes interact with tau oligomers and polymers. This study provides the foundation for future comparative studies of fiber growth kinetics using other inducers, tau isoforms, and mutants.

**(34) INHIBITION OF *BDELLOVIBRIO BACTERIOVOROUS*
PREDATORY ABILITY BY TYPE A PROANTHOCYANIDINS**

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Bdellovibrio bacteriovorus, a gram-negative predatory bacterium, uses its Type IV pili to adhere to its prey which are other gram-negative bacteria. Cranberry juice can prevent the attachment of various types of bacterial pili, and the active component in cranberry juice has been documented as type A proanthocyanidins. Using optical density and plaque forming unit assays (PFUs), we investigate how neutralized cranberry juice affects *B. bacteriovorus* predation of *E. coli*. PFUs quantify viable *B. bacteriovorus* cells, whereas optical density reflects changes in growth and predation of *E. coli*, but both techniques rely on the larger *E. coli* cells scattering visible light while the smaller *B. bacteriovorus* cells do not scatter light effectively. We show that addition of cranberry juice prevents predation and explore how long this inhibitory effect lasts after removing the proanthocyanidins from solution.

(35) OPTIMIZING LION’S MANE YIELD: EFFECTS OF HARDWOOD SUBSTRATE AND MEDIA CHOICE

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Hericium erinaceus, commonly known as Lion’s Mane, is a mushroom of growing renown for its medicinal and nutritional benefits. As demand increases, optimizing cultivation strategies is essential for maximizing yield and efficiency. This study explores three key factors influencing *H. erinaceus* growth: (1) the efficacy of various hardwood species as fruiting substrates, (2) the role of different agar media formulations in promoting mycelial growth, and (3) genetic strain identity. To assess substrate influence, six hardwood formulations—poplar, beech, white oak, red oak, sycamore, and an equal-parts blend—were evaluated for their effects on fruiting yield. Additionally, mycelial growth was tested on potato dextrose agar (PDA), malt extract agar (MEA), and oatmeal agar (OMA), with and without yeast supplementation to enhance nitrogen availability. Three genetically distinct strains—a commercially cultivated strain and two wild strains isolated from oak trees—were evaluated for their influence on growth and fruiting performance. Across two replicates, strain identity emerged as a stronger determinant of yield than substrate composition. Second-generation clones exhibited enhanced yields when propagated on the same substrate as their parent strain, suggesting that *H. erinaceus* cultivation is best optimized by selecting strains adapted to specific substrates rather than modifying substrates for specific strains.

(36) COMPUTATIONAL INSIGHTS INTO POLYPHENOL-INDUCED BINDING AND CONFORMATIONAL BEHAVIORS OF MELITTIN

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Melittin, the primary peptide component of European honeybee venom, is a well-characterized toxin known for its ability to disrupt membrane permeability by catalyzing pore formation. In the search for protective agents against such toxic effects, epigallocatechin gallate (EGCG), a polyphenol, has been identified for its inhibitory activity against pore-forming toxins. EGCG may inhibit melittin's ability to interact with cell membranes. However, the precise mechanisms by which EGCG interferes with melittin's membrane binding and pore formation remain unclear. Our computational study investigates the molecular interactions between melittin and polyphenols using a combined approach of density functional theory (DFT) calculations and molecular dynamics (MD) simulations. We focus on how the introduction of EGCG influences melittin's binding interactions and conformational behavior, with particular attention to the physicochemical properties of this pore-forming peptide. DFT results show that binding energy is maximized when all phenol rings of the polyphenol directly interact with melittin's amino acid residues. Notably, an increase in the number of accessible phenol rings correlates with enhanced binding energy. These findings suggest that unhindered interaction between phenol rings and melittin residues is crucial for forming a stable melittin-polyphenol complex, thereby reducing melittin-induced cytotoxicity.

(37) ISOLATION, DNA BARCODING AND SCREENING FOR LIGNINOLYTIC ACTIVITY OF FUNGI COLLECTED FROM PARTS OF NORTHEAST AMERICA

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Many fungi express lignin-degrading enzymes such as Laccases and Manganese peroxidases. These enzymes break down lignin by oxidizing phenol hydroxyl groups of lignin. Our long-term interest is to study the application of laccases in the bioremediation of phenolic aromatic compounds, namely poly-fluoroalkyl substances (PFAS) or forever chemicals. We foraged nearly 30 mushrooms (Basidiomycetes) from various parts of Northeast America. Our immediate goals are to A) Identify the 30 different species of Basidiomycetes using DNA barcoding, B) Screen for ligninolytic activity from all 30 species, C) Study mRNA expression of Laccases and Manganese Peroxidases in these species and identify the specific isoforms of these enzymes. Our long-term goals are to clone, express, and purify some species-specific Laccases and decode Laccase activity against various PFAS compounds, serious contaminants in drinking water. So far, we have isolated and cultured mycelium from nearly 30 different fungi. Our current research focuses on DNA Barcoding and screening for the ligninolytic activity of these fungal species. In this poster, we will present data on screening several new fungi for ligninolytic activity. We have been optimizing polymerase chain reactions using fungal-specific ITS primers to identify the specific species of these fungi. We will present the results of PCR and our progress in optimizing the primers as a tool to identify species of Basidiomycetes.

(38) ALUMINUM CCC-PINCER COMPLEXES

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Catalysts are molecules that alter the mechanisms of chemical reactions to allow bonds to break and form selectively under more accessible conditions. Many catalysts are characterized as organometallic complexes that consist of one or more bonding interactions between a metal and carbon. Transition metals in particular have dominated the field of catalysis over the last 80 years due to their high activity and tunability. However, many of the most widely used transition metals are expensive and some are also toxic. Significant research has gone into developing catalysts based on more earth-abundant elements containing main-group (i.e., *p*-block) metals as potential alternatives to costly transition-metal catalysts. This work focuses on the synthesis of chelating CCC-pincer ligands and their corresponding aluminum complexes. These ligands featuring two N-heterocyclic carbenes and a central aryl group were used to create 5- and 6-coordinate aluminum complexes. The newly synthesized complexes were characterized by nuclear magnetic resonance spectroscopy and X-ray diffraction, and future work will test the reactivity of these aluminum compounds towards a variety of small molecules to determine possible catalytic applications.

(39) SYNTHESIS, PHOTOPHYSICAL PROPERTIES, AND STRUCTURAL CHARACTERIZATION OF ALKALI METAL COPPER(II) HALIDE NANOCRYSTALS

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Lead halide perovskite nanocrystals (LHP NCs) have garnered significant attention in optoelectronics due to their high color purity, tunable emission, and low-cost processing. While lead halide perovskites have achieved record efficiencies in red and green light-emitting diodes, their performance in the deep-blue region remains limited due to deep-level defects and phase instability. Moreover, lead toxicity poses a major concern for large-scale manufacturing. In response to these challenges, this project explores M_2CuCl_4 ($M=K,Rb,Cs$) nanocrystals as a promising lead-free alternative for blue light emission. Copper-based halide NCs are less toxic than LHP NCs, and exhibit strong, tunable visible light emission. A hot injection nanocrystal synthesis was optimized using alkali metal and copper (II) acetates dissolved in octadecene and oleic acid/oleylamine with benzoyl chloride as the halide source. The resulting nanocrystals are purified by precipitation with methyl acetate. Photophysical properties of the nanocrystals as a function of alkali metal composition were investigated and X-ray scattering was used to analyze their nanostructure. By optimizing precursor ratios, surfactant concentrations, and reaction conditions, this research contributes to the broader goal of developing stable and efficient lead-free materials for next-generation light-emitting applications, particularly in the blue spectral range, where current technologies fall short.

**(40) TRI(ETHYLENE GLYCOL) METHYL ETHER
ALKYLATION OF 2-HYDROXY-1,4-NAPHTHOQUINONE
TO IMPROVE SOLUBILITY**

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2-Hydroxy-1,4-naphthoquinone, or Lawsone, is a naturally occurring compound extracted from a plant, *Lawsonia inermis*, which is found in South Asia, the Middle East, and Northern Africa. It is traditionally used as a skin dye, but it has also been reported to have many therapeutic benefits, such as antioxidant, antibacterial, antitumor, and anti-inflammatory properties. Due to the rise in antibiotic-resistant strains of bacteria, natural compounds and their derivatives, such as Lawsone, are being considered as potential therapeutic candidates. One of the drawbacks of Lawsone is its low solubility and low bioavailability due to its hydrophobic character. The overall goal of this project is to increase the solubility of Lawsone by adding a hydrophilic alkyl ligand, triethylene glycol methyl ether (TEG), at the enol or carbon 3-position. A model reaction to study the alkylation reaction was initially carried out by reacting Lawsone with methyl iodide to determine the necessary conditions and product distribution. The results of the ^1H NMR, ^{13}C NMR, and TLC indicated methylation occurred at carbon-3 (13 %) and the enol (87%) sites. Current studies are underway to carry out the alkylation of Lawsone using TEG-Br.

(41) QUANTIFYING BISPHENOL A (BPA) IN REGENERATING PLANARIA

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BPA is a synthetic compound commonly used by chemical companies to alter polymer characteristics. Due to its ubiquitous uses in various industries, it has entered the environment as a contaminant, and recently there have been concerns regarding its potential adverse health effects. To understand how BPA can affect organisms in the environment, we have exposed regenerating planaria, a freshwater flatworm that can regrow/repair itself following transection, to specific concentrations of a deuterated form of BPA (d8BPA) where the eight non-exchangeable hydrogen atoms on the two aromatic rings have been replaced with deuterium, to distinguish BPA, the contaminant, from that used for controlled exposure studies. High-performance liquid chromatography (HPLC) was used to characterize the extracts from the d8BPA-exposed planaria. The intrinsic fluorescence from BPA and the altered retention time for the deuterated form were used to help quantify the amount of d8BPA in planaria exposed to controlled amounts of the substance in solution. Fluorescence signals were normalized to both an internal standard and the dry mass of planaria for accurate quantification. Planaria retained measurable amounts of d8BPA over their regeneration cycle of 14 days and showed decreased regenerative ability.

(42) DESIGN AND EVALUATION OF A POTENTIAL REDOX-ROBUST XYLANASE

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Xylanase plays a key role in the depolymerization of xylan, a major component of plant cell walls; thus, this hydrolytic enzyme has commercial utility in the biofuel, food, and papermaking industries. However, this enzyme is susceptible to oxidative inactivation under conditions often encountered in these industries. We therefore employed a combination of *in silico* and *in vitro* methods to study the interactions of assorted ligands with *Bacillus subtilis* xylanase (PDB ID 1XXN) and a tryptophan-to-phenylalanine mutant (W9F); AlphaFold Colab was employed to predict the structure of the W9F variant. Assessment of the affinity of ligand binding to both the reported wildtype and predicted W9F structures was conducted with Autodock Vina; this analysis included the ligand 1-hydroxybenzotriazole, a known oxidative inactivator of xylanase. Our computational findings were then compared to experimental data, using wildtype and W9F *B. subtilis* xylanase genes cloned into the pET-28a(+) expression vector with subsequent purification of His-tagged proteins via Ni-NTA affinity chromatography, followed by assessment of tolerance to oxidative conditions. The results enhance our understanding of xylanase structure and function for improved performance in the biomass processing industries. This integrated approach demonstrates the complementary strengths of computational and experimental methods in advancing enzyme engineering for industrial optimization.

(43) PALLADIUM (II) COMPOUNDS WITH N,S-THIOUREATE LIGANDS : SYNTHESIS, CHARACTERIZATION, AND USE AS SINGLE SOURCE PRECURSORS FOR PALLADIUM SULFIDE NANOMATERIALS

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Palladium sulfide nanomaterials have attracted attention for their unique electronic, catalytic, and electrocatalytic properties. Achieving phase-selective synthesis of various stable Pd_xS_y phases and controlling crystallinity are essential for elucidating structure-property relationships in these materials. In this study, we examined Pd(II) thioureate complexes as potential single source precursors for palladium sulfide nanomaterials. Homoleptic compounds bearing bis-chelate N,S-thioureate ligands were prepared by reacting N,N,N'-trisubstituted thioureas (N=butyl, N'=aryl) with bis(acetonitrile)dichloropalladium(II). Cationic heteroleptic thioureate complexes incorporating tetramethylethylenediamine (TMEDA) as a neutral N,N-chelate were prepared by reacting bis(acetonitrile)dichloropalladium(II), TMEDA, and trisubstituted thiourea proligands, and then isolated as tetraphenylborate salts. The newly synthesized bis-chelate N,S-thioureate palladium compounds were characterized with NMR spectroscopy, single crystal X-ray diffraction, UV-vis spectroscopy, and IR spectroscopy. The structure and bonding of these complexes was investigated with Density Functional Theory calculations. High-temperature thermolysis of these precursors in oleylamine produced Pd_xS_y nanoparticles which were characterized by UV-vis absorbance and photoluminescence spectroscopies. X-ray Total Scattering Pair Distribution Function Analysis was used to characterize the local atomic structure of the amorphous nanoparticles.

**(44) A COMPARATIVE ANALYSIS OF
MICROPLASTICS IN SOUTH KOREAN AND
AMERICAN SEAWEED**

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Microplastics are small fragments of plastic less than 5 millimeters in size, that are either intentionally added to products like cosmetics or formed by breaking down larger products over time. Microplastics have different forms, most often seen as shards, microbeads, and fibers. They can accumulate in the environment and present a risk to the health of humans and wildlife. Microplastics can leach their chemicals into the environment, disrupting ecosystems, and can be mistaken for food by marine animals. In this study, we compared the microplastic content of seaweed from Korea and Maine. Seaweed samples from two commercial brands were digested and filtered; filters were observed via microscopy, and an algorithm was used to estimate total particle counts of seaweed from both sources. Ocean's Halo Seaweed from Korea had an average of 59 ± 19 particles per gram, 31% of which were fibers and Maine seaweed had 44 ± 13 particles per gram, 70 % of which were fibers. A Student's t-test was used to compare the two seaweed brands, and there was no statistically significant difference between the total numbers of microplastic particles ($p = .14$).

(45) SYNTHESIS OF GROUP 4 METAL TETRAHYDROCARBAZOLE COMPLEXES

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This project investigated the synthesis of group 4 metal (Ti, Zr, Hf) tetrahydrocarbazole complexes. Tetrahydrocarbazoles (THC's) are widely used in pharmaceuticals (CAS RN: 942-01-8). This heterocyclic structure features two 6-membered rings, one aromatic and one saturated, which are bound together with a pyrrole ring. They have shown to be important to the development of pharmaceuticals due to their nature of having properties such as antibacterial effects, protein kinase inhibition, and tumor growth suppression. Previously in the Tanski Lab, THC's were successfully synthesized using a variety of substituents (CH₃, OCH₃, Cl). These THC's are formed *via* a borsche-drechsel cyclization. The specific method used to synthesize the variety of substituted THC's consists of a one pot synthesis of a substituted phenylhydrazine hydrochloride and a substituted cyclohexanone in the presence of antimony trioxide as a catalyst in methanol solvent at reflux temperatures. The formation of the metal complexes consists of adding a 1:1 or 2:1 molar ratio of THC to tetrakis(dimethylamido)M (M = Ti, Zr, Hf) using toluene as a solvent to synthesize the initial complex, [THC]M(NMe₂)₃(HNMe₂). Products were characterized by ¹H NMR, ¹³C NMR, GC/MS, IR, elemental analysis and X-ray crystallography.

(46) POLYSTYRENE CHARACTERIZATION AND DEGRADATION THROUGH EXPOSURE TO ULTRAVIOLET RADIATION

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Public concern regarding microplastics has led to increased research. Despite inconclusive effects on human health, studies link microplastic exposure to harm to endocrine, cardiovascular and gastrointestinal systems. This research aims to characterize the degradation of a common plastic, polystyrene, as well as carboxylate-modified and amine-modified derivatives. Polystyrene samples were exposed to ultraviolet (UV) radiation at 253.7 nm over a simulated period of 1.4, 3.75 and 9.375 weeks. The samples were characterized by attenuated total reflectance (ATR) Fourier transform infrared (FTIR) and fluorescence spectroscopy, scanning electron microscopy (SEM), wide-angle X-ray scattering (WAXS), and dynamic and electrophoretic light scattering (DLS/ELS). The degraded samples were analyzed using matrix-assisted laser desorption/ionization time of flight (MALDI-TOF) to determine how the microplastics were affected by the UV radiation. The characterization methods confirmed the identity of polystyrene and its derivatives, although SEM results showed significant agglomeration of polystyrene particles, which supported DLS results indicating large particles. MALDI-TOF analysis showed samples exposed to ultraviolet light for longer contained smaller fragments of polystyrene, although no samples contained polymers exceeding 800 m/z. Future research will analyze more samples exposed to ultraviolet light over different time periods.

(47) INVESTIGATING DNA AGGREGATION WITH FLUORESCENCE POLARIZATION

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The objective of this research was to study the binding between DNA and surfactant molecules to better understand the stability of the resultant aggregates that form between single strands of synthetic DNA and cationic detergents. Fluorophore labeled oligonucleotides of varying length were used to study the DNA aggregation process in the presence of alkyl ammonium halide salts using fluorescence polarization. Previous studies included the effects of surfactant length and structure on aggregation. The impact of an aprotic solvent (acetonitrile) and salt concentration on binding strength were the focus of this specific research project. Binding curves were fit to the Hill equation to obtain association constants, and these were compared to better understand the factors that affect the stability of the DNA-surfactant aggregates.

(48) EXPLORING RATE ENHANCEMENT WITH ZINC-ALGINATE BEADS: A GREEN CHEMISTRY-INSPIRED KINETICS EXPERIMENT

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This study integrates green chemistry principles into undergraduate laboratory experiments by exploring alginate beads crosslinked with zinc ions. Alginate, a biocompatible biopolymer, can form beads through crosslinking reactions with divalent metal ions, primarily calcium. We investigated zinc-crosslinked alginate beads as a system for enhancing the oxidative bleaching of Brilliant Blue dye using sodium hypochlorite. Zinc ions in solution significantly accelerated the reaction, demonstrating a rate-enhancing effect, with zinc-crosslinked beads showing comparable rate enhancements compared to calcium-crosslinked beads, which exhibited negligible activity. Introducing zinc-alginate beads in laboratory experiments provides students with a simple, non-toxic method to explore biopolymers, kinetics, and the influence of metal ions on reaction rates. The research highlights the potential of transition metal-alginate beads for sustainable chemistry applications, offering insights into their versatile rate-enhancing properties and potential environmental remediation strategies. Further investigation is warranted to elucidate the precise mechanism of zinc's influence on the reaction kinetics.

(49) QUANTUM AND KINETIC CHARACTERIZATION OF Ru80

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This project investigates the anticancer potential of Ru80, a ruthenium-based compound, through a combination of quantum modeling and experimental enzyme kinetics. Using Density Functional Theory (DFT) calculations in ORCA, the study evaluated Ru80s activation energy and thermodynamic properties during interactions with dihydrofolate reductase (DHFR), a key enzyme in folate metabolism. Complementary wet lab experiments employ Michaelis-Menten kinetics to quantify Ru80s inhibitory effects on DHFR by determining parameters such as K_m and V_{max} . By integrating computational and experimental results, this research intends to see how Ru80 acts independently and with other molecules. Insights gained from discrepancies between theoretical predictions and empirical data contribute to understanding the dynamics of ruthenium complexes.

**(50) CHARACTERIZATION OF TONB4 AND TONB6
PROTEINS IN *BACTEROIDES THETA* IOTAOMICRON
THROUGH GENERATION OF MULTIPLE GENE DELETION
STRAINS**

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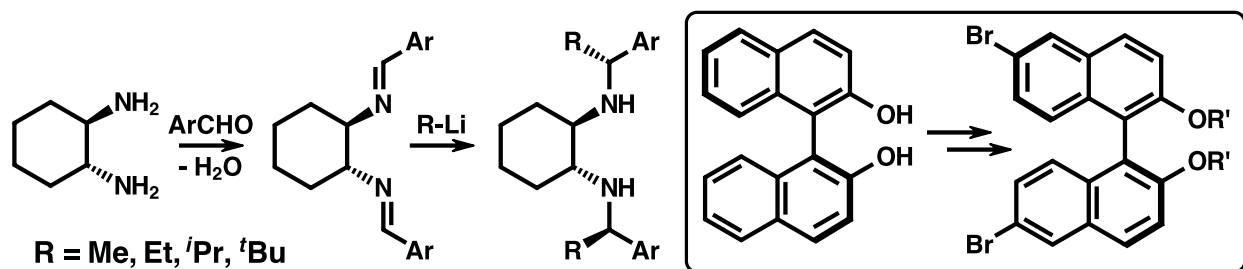
Bacteroides are vital members of the human gut microbial community that are primarily responsible for the utilization of polysaccharides. *Bacteroides thetaiotaomicron* (*B. theta*) is a model organism for the *Bacteroides* genus and transport of degraded oligosaccharides through TonB-dependent transporters (TBDT). These outer membrane transporters are powered by an inner membrane energizing complex composed of the TonB, ExbB, and ExbD proteins. Previous research has identified 11 homologous TonB proteins encoded in the *B. theta* genome. Analysis of *B. theta* strains containing single *tonB* gene deletions suggests that TonB4 is the primary protein used in the energizing complex associated with polysaccharide transporters but TonB6 has a redundant function. To further investigate the roles of TonB4 and TonB6, this work seeks to generate multi-deletion strains expressing only the TonB4 or TonB6 protein and a double deletion strain expressing all TonB proteins with the exception of TonB4 and TonB6. To make strains expressing only TonB4 or TonB6, we aim to conduct deletions of the other 9 *tonB* homologs and have successfully deleted *tonB1*, 2, 3, 5, 8, 9, 10, and 11 leaving *tonB* 4, 6, and 7. Previous work to produce a *tonB4* and *tonB6* double deletion strain have not been successful, perhaps because the double deletion results in a lethal phenotype. To address this limitation, we have produced *tonB4* and *tonB6* single deletion strains with the corresponding protein expressed under an inducible promoter at a third genomic site, allowing for the second *tonB* gene to be deleted. Though a double deletion strain has not yet been isolated, screening data suggests this is a viable approach. Generation of these strains will provide additional tools for understanding the role of TonB in polysaccharide utilization with the goal of differentiating between the energizing complexes in beneficial bacteria such as *B. theta* and closely related pathogenic species including *B. fragilis*

(51) TOWARDS SYNTHESSES OF NEW CHIRAL RECEPTORS

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We describe efforts to incorporate *trans*-1,2-diaminocyclohexane (DACH) and 1,1'-bi-2-naphthol (BINOL) into new molecules that may be useful as receptors for enantioselective sensing, catalysis, and separation. We hope this work will enable the precise tuning of steric and chiral environments about reactive DACH subunits, and the creation of shape-persistent macrocyclic motifs. Towards these aims, we are pursuing two synthetic strategies: First, we have extended a known diastereoselective reaction of methyllithium and simple DACH-derived diimines to include 1°, 2° and 3° alkyl lithium reagents. Our modifications required significant changes in solvent, temperature, and reaction time; and proceed with virtually complete and consistent stereoselectivity (confirmed in 2 of the 3 new cases by X-ray crystallography). We have also explored substrate scope with respect to the diimine, including attempted additions to macrocyclic diimines. Our second methodology involves creation of BINOL-derived diimines linked through 6,6' positions. This approach relies on a previously reported regioselective electrophilic aromatic bromination of BINOL, which we envision will provide access to rigid, BINOL-containing macrocyclic dimines.



(52) DIFFERENTIATED AMINO ACID SENSING BETWEEN WT AND AP-3 DEFICIENT CELL LINES

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Mammalian Target of Rapamycin Complex-1 (mTORC1) is an important protein complex that regulates cell metabolism and proliferation. It functions as a kinase and is active when cells are in a nutrient rich environment. One protein that is phosphorylated by mTORC1 is S6k, a kinase that controls the balance between promoting proliferation (when active) and inducing autophagy (when inactive). Previous work has shown that AP-3 deficient melanocytes (*mocha* or *mh* melanocytes) are more sensitive to starvation induced autophagy than their wildtype counterparts (WT) and have decreased nutrient sensing efficacy. This previous work has also shown that *mh* melanocytes do not sense an essential mix of amino acids compared to WT. Our goal for this project was to determine if there were any individual amino acids that were not being sensed by *mh* melanocytes but sensed normally in WT. We subjected *mh* and WT cells to starvation conditions and measured autophagy through Western blotting. We found that single amino acid treatments are not sufficient to provide the mis sensing response seen through treatment of the essential amino acid mix. These results indicate that multiple amino acids are being mis sensed or mis trafficked causing decreased nutrient sensing efficacy in *mh* melanocytes.

(53) SYNTHESIS OF ORGANOMETALLIC CHROMOPHORE LINKERS FOR THE DESIGN OF PHOTOACTIVE METAL ORGANIC FRAMEWORKS

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Transition metal chromophores (TMCs) have a wide variety of applications in fields such as photodynamic therapy, phosphors for organic light-emitting diodes, photoredox catalysis, and non-linear optics. TMCs with iridium(III) have garnered particular interest as cyclometalated iridium complexes exhibit emergent behavior when incorporated into self-assembled complexes like metal-organic frameworks (MOFs). This work explores the integration of iridium(III) chromophores into the structure of metal-organic frameworks (MOFs) to develop materials with enhanced photophysical properties. Two synthetic approaches were explored: (1) iridium(III) complexes functionalized onto NU-1000 type MOFs and (2) iridium(III) complexes as organic linkers bound to zirconium nodes in the synthesis of MOFs. While results suggested the successful functionalization of iridium(III) complexes onto NU-1000, additional optimization efforts are needed for the use of the iridium(III) complexes as organic linkers in designing new MOF structures.

(54) LIMESTONE FOR THE IMMOBILIZATION OF URANIUM POLLUTION

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Over the last several decades, hydraulic fracturing (fracking) has become a common process to extract oil and natural gas, but this process has led to many environmental problems including release of many elements to water that is returned to the surface. Uranium (U) is a toxic and radioactive pollutant brought to the Earth's surface during the fracking process. This study explores limestone for the immobilization of U. Batch incubations of U-salts or shale in solutions of different pH, including in simulated fracking fluid, were conducted. These incubations were sampled over time to monitor the mobility of U in the presence of limestone, Ca^{2+} and PO_4^{3-} additives. Aqueous phase samples were analyzed by Inductively Coupled Plasma Mass Spectrometry (ICP-MS) while the precipitates were analyzed by Scanning Electron Microscopy with Energy Dispersive X-ray Spectroscopy (SEM-EDS). Analysis indicates that the additives decrease the concentration of aqueous U within 48 hours by $> 99.6\%$ at pH 7-8 range and 91.2% at pH 3, which is more relevant to the context of fracking. These results suggest that a combination of limestone, Ca^{2+} , and PO_4^{3-} is a potential solution to decrease U pollution in produced and flowback waters as a result of fracking.

(55) THE REDUCTION OF CHALCONES USING HYDROGEN TRANSFER CATALYSTS

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Alkenes (C=C) and ketones (C=O) undergo addition reactions with molecular hydrogen, in the presence of a transition-metal catalyst, to produce alkanes and alcohols respectively. The reaction can also be performed using reducing agents such as LiAlH_4 and NaBH_4 . In transfer hydrogenation, reductions are performed without a source of hydrogen gas by employing a hydrogen-transfer catalyst. These catalysts remove hydrogen from one reagent, known as the hydrogen donor agent, and transfer it to the organic substrate. The goal of the project was to investigate whether chalcones can undergo similar reduction reactions via transfer hydrogenation. Chalcones are a family of organic compounds that contain both C=C and C=O bonds in a conjugated system. 2-propanol was used the H-transfer agent and $\text{RhCl}(\text{PPh}_3)_3$ was the catalyst. In this system, 2-propanol is converted to acetone upon donation of hydrogen. The results of transfer-hydrogenation reactions were monitored by Infra Red spectroscopy and Proton NMR.

(56) UNDERSTANDING THE BINDING POTENTIAL OF Ru80 TO DIHYDROFOLATE REDUCTASE ENZYME

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The folate pathway has long been studied as a target for anti-cancer research. This is due to the role of dihydrofolate reductase (DHFR) as an essential catalyst for the biosynthesis of purines, which is crucial for DNA production. Transition metal complexes may have the potential to inhibit the activity of DHFR, thereby slowing tumor growth. My research focuses on the anticancer potential of novel ruthenium compounds. The unique chemical properties of ruthenium compounds provide promising alternatives to traditional platinum-based drugs because of their potential for selectivity and reduced side effects. The ruthenium complex under study is Ru80 which consists of two ruthenium centers coordinated to phenformin, a known antidiabetic drug. In this project, I examine the efficacy of this compound through UV absorption assays, enzymatic activity assays, and ITC. These methods offer insights into how varying the drug's incubation time affects DHFR activity as well as the thermodynamic parameters of the Ru80 binding mechanism.

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