



The Mid-Hudson American Chemical Society

24th Annual

UNDERGRADUATE RESEARCH SYMPOSIUM

Friday, April 19, 2024



24th Annual Mid-Hudson ACS Undergraduate Research Symposium April 19, 2024

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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 Prof. Sean Brady, Rockefeller University
(*Coykendall Science Building Auditorium*)

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

Guest Speaker

Sean F. Brady, Professor Rockefeller University

NATURAL ANTIBIOTICS WITHOUT NATURAL PROCESSES

The characterization of small molecules produced by bacteria in laboratory culture has been a key step to developing diverse small molecule therapeutics. As successful as this approach has been for identifying novel bioactive small molecules, extensive sequencing of bacterial genomes and metagenomes has revealed that the bacterial biosynthetic diversity currently accessed in the laboratory represents only a small fraction of what is predicted to exist in nature. This shortcoming arises from both our inability to culture most bacteria in the laboratory and from the fact that most biosynthetic gene clusters remain silent under laboratory fermentation conditions. We have developed a new bioactive small molecule discovery pipeline that avoids the requirement for either bacterial culture or gene cluster expression. In this purely in vitro approach, which we have termed synthetic-Bioinformatic Natural Products (synBNPs), the structures of natural products encoded by biosynthetic gene clusters are predicted bioinformatically, and the resulting predictions are then chemically synthesized to generate libraries of bioactive small molecules that are inspired by nature. Contrary to other synthetic approaches, all of the structures we produce are inspired by natural selection and, consequently, are expected to exhibit bioactivities at a high rate. In this presentation I will discuss a number of antibiotics we have identified using a synBNP approach.



SEAN F. BRADY

Professor

Laboratory of Genetically
Encoded Small Molecules

Rockefeller University

New York, NY

Sean F. Brady graduated with a degree in molecular biology in 1993 from Pomona College in Claremont, California. He received his Ph.D. in organic chemistry from Cornell University in 2001. In 2002, he moved to Harvard Medical School as a fellow in the Institute of Chemistry and Cell Biology. He was named an instructor in the department of biological chemistry and molecular pharmacology at Harvard Medical School in 2004. In 2006 he moved to The Rockefeller University as an assistant professor. In 2015 he was promoted to Evinr Associate Professor at The Rockefeller University. In 2016 Sean founded Lodo Therapeutics. In 2018, he was promoted to Professor at the Rockefeller University.

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

(1) ADDITIVE MANUFACTURING (FDM) OF VITON-AMMONIUM PERCHLORATE-ALUMINUM(VAPAL)

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The purpose of this study is to investigate the compatibility of ammonium perchlorate and aluminum (AP/Al) with Viton (VAPAL) for use in additive manufacturing (AM). After compatibility testing to ensure safety, VAPAL of various solids loading was successfully formed into filaments using a Filabot extruder. The procedure developed for suspending AP/Al in Viton was effective, with a theoretical maximum density of over 90%. The results from both sensitivity testing and analysis showed that Viton is compatible with AP/Al as the stability of the product increased when compared to ammonium perchlorate by itself. Additionally, results from a differential scanning calorimeter (DSC) show that the decomposition of VAPAL occurs near the same temperature as ammonium perchlorate, indicating that VAPAL is safe to print at fused deposition modeling (FDM) temperatures. Lastly, samples taken intermittently along an extruded sample show uniform density of AP/Al, validating our filament extruding process. Further research will be done to explore the feasibility of VAPAL within 3D printing. Challenges we expect with the next phase of research include how VAPAL will behave in the extruder head, what definition we can print with this filament, and the variance in burn rate and deflagration rate of printed VAPAL.

(2) ADDITIVE MANUFACTURING (DIW) of ENERGETIC INKS

**Caleb Kwi, Chloe C. Sample, Ernest C. McVey,
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Additive manufacturing (AM), known as 3D printing, is widely used today to produce complex geometries quickly and cheaply. The ability to produce exact, repeatable, designs has intrigued the energetics community who would like the ability to rapidly produce explosive designs for wave shaping. Two main problems that occur when AM energetics, heat and density. Energetic performance is exponentially related to the density of material; discovering an AM technique that maintains high solids loading and density is required to be useful for military applications. Based on Pluronic F-127, we have developed a stackable, high solids loading, high density direct ink writing (DIW) ink that can be printed without the use of heat or UV-curing. Additionally, the DIW ink developed utilizes a water-based solvent which greatly increases the safety during the processing and printing of energetic materials. Currently, microgram and nanogram copper particles have been developed into printable inks which will be used to form the shape charge portion of our 3D model. Initial work incorporating the explosive pentaerythritol tetranitrate (PETN) into the DIW ink has been successful and future work will be conducted to characterize the energetic ink.

(3) EFFECT OF TYPE A PROANTHOCYANIDINS ON *BDELLOVIBRIO BACTERIOVOROUS* PREDATION ABILITY

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Cranberry juice contains type A proanthocyanidins, compounds that have been shown to inhibit various types of bacterial pili. Type IV pili, which are reportedly affected by these compounds, are used by the predatory bacterium *Bdellovibrio bacteriovorus* to adhere to its prey before inserting itself into the prey cell periplasm. Here, we explore the effects of neutralized cranberry juice on *B. bacteriovorus* predation of *E. coli*. Although predation is fully inhibited in the presence of cranberry juice, removal of cranberry juice from the bacterial media results in a resurgence of predation. This effect is observed through optical density measurements, fluorescence microscopy, and plaque forming unit assays. Moreover, we are using the AlphaFold Protein Structure Database to consider how type A proanthocyanidins might bind to different pili proteins, causing a reversible inhibition of pilus activity.

(4) SYNTHESIS & BIOCHEMICAL ASSAYS OF METAL COMPOUNDS WITH METFORMIN AND PHENFORMIN LIGANDS

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This study explores the synthesis and characterization of transition metal complexes, specifically ruthenium (II) and copper (II), incorporating metformin and phenformin as ligand and aims to contribute to the development of novel anticancer therapies based on metformin and phenformin derivatives. To elucidate the properties and potential synergistic effects of combining metal centers with metformin, a variety of assays/techniques were employed, including CRISPR, gel electrophoresis, UV-vis DNA melting, with the goal of investigating the mechanism of action of the compounds.

**(5) REVEALING HEAVY METAL COMPOSITION IN
DUTCHESS COUNTY: A STUDY OF SOIL IN OAKWOOD
FRIENDS SCHOOL WETLANDS**

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Contamination of soil with heavy metals presents a significant environmental concern due to its widespread occurrence and adverse effects on ecosystems and human health. The presence and toxicity of these metals underscore the urgent need for concerted efforts in research and remediation to protect environmental quality and public health. The proximity of the longstanding Dutchess garbage incinerator, located approximately one mile from the testing site at Oakwood Friends School, raises concerns regarding potential heavy metal contamination historically in this region. This study focuses on analyzing diverse depth profiles, particularly emphasizing mercury concentrations, obtained from soil samples collected in the wetland area of Oakwood Friends School in Poughkeepsie using ICPMS and DMA instrumentation. Preliminary findings indicate a nearly twofold increase in mercury concentration beyond the 3 cm depth, followed by stabilization. Looking ahead, our research aims to broaden its scope by investigating additional locations to gain a comprehensive understanding of heavy metal distribution in Dutchess County. In addition, leveraging the heavy metal results obtained from this study will enable us to establish correlations with historical cleanup measures by the incinerator, enhancing our understanding of the dynamics of soil contamination in the region.

(6) ALGINATE ENCAPSULATION FOR IMPROVED LACCASE PERFORMANCE

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Application of oxidative and hydrolytic enzymes to lignocellulosic biomass provides opportunity for lignin valorization and cellulosic pulp production with reduced demand for chlorine-based oxidants. We had previously reported that alginate encapsulation stabilizes the hydrolytic enzyme xylanase against the oxidative environment generated by the laccase mediator system. This study thus considered the utility of preserving laccase activity via encapsulation, assessed by following the oxidation of 2 mM veratryl alcohol, a lignin model compound, with 1 mM 1-hydroxybenzotriazole (HBT) as the mediator. The efficacy of encapsulation was investigated by measuring the yield of product veratraldehyde as a function of pH and temperature; residual laccase activity was also determined. Alginate encapsulation was found to protect laccase activity even at 50 °C. Further, residual activity of encapsulated laccase was enhanced in the absence of HBT or in the presence of veratryl alcohol. Importantly, a greater yield of veratraldehyde was observed for the alginate-encapsulated laccase ($26.9 \pm 2.3\%$) over the free enzyme ($7.6 \pm 1.2\%$) at pH 5.0. The yield enhancement was even greater for encapsulated laccase ($35.1 \pm 2.9\%$) over free enzyme ($0.91 \pm 0.43\%$) at pH 3.5. Such results demonstrate the benefit of employing encapsulated enzymes for biomass processing.

(7) GRAPHENE/SILVER NANOPARTICLE THIN FILMS FOR ELECTROCHEMICAL BIOSENSOR ELECTRODES

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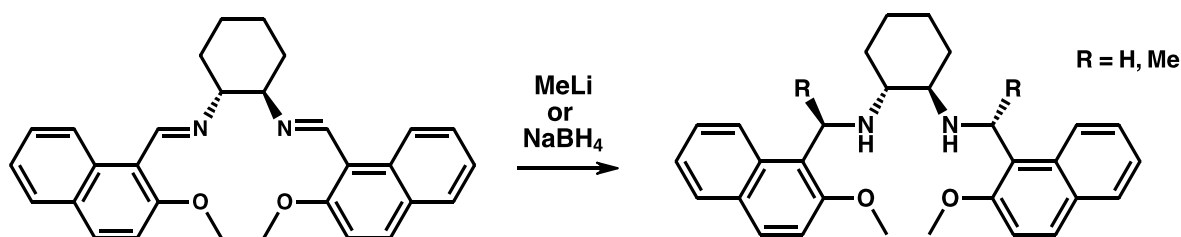
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The high surface area and conductivity graphene/noble metal nanoparticle films via galvanic displacement make it viable for charge transfer with surface analytes for catalysis or sensing in electrochemical environments. This sensitivity is critical to develop high performance electrochemical sensors for biological and chemical sensing. To achieve this, we demonstrate a scalable method utilizing a galvanic displacement technique for the formation of silver nanoparticles onto graphene supported copper substrates. Various concentrations of chloroauric acid and silver nitrate solutions from 10 mM to 100 mM were investigated. Copper supported graphene oxide films were produced via static spin coating. The noble metal salt solutions were casted onto the copper-supported graphene films to galvanically displace the noble metals with the underlying copper metal. The resulting films were dried in ambient and were immersed with poly (methyl methacrylate) (PMMA) to enable creation of a free-standing polymer film integrated with noble metal nanoparticle/graphene after etching the underlying copper. Therefore, utilizing our thin film process, nanocomposite electrodes with various noble metal nanostructures such as platinum, palladium, and ruthenium can be developed. The electrochemical performance of the Ag nanoparticle/graphene free-standing films for electrochemical activity and electrooxidation of glucose for biosensor applications were assessed using cyclic voltammetry and impedance spectroscopy.

(8) STERICALLY CROWDED DIAMINOCYCLOHEXANE-BASED RECEPTORS

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Our laboratory has a longstanding interest in the development of diamines derived from *trans*-1,2-diaminocyclohexane (DACH) in which both amines contain benzylic groups. These compounds are useful as stereoselective catalysts, sensors, molecular receptors. Recently, we sought to reduce conformational freedom in this system by introducing both 2-methoxy-1-naphthyl and methyl groups at the benzylic C atoms (see below, right). These modifications enhance steric demand about the vicinal diamine group, which is expected to modify the molecular recognition properties. The presence of methyl groups (R = Me, below) creates additional chiral centers which we have introduced stereospecifically by adding methyllithium to the corresponding diimine at -78°C . The assignment of the new chiral centers is tentative, and we hope to confirm the configuration by X-ray crystallography. Broadening of ^1H - and ^{13}C -NMR resonances of groups about the benzylic atoms in the methylated compound, but not in the hydrogenated compound (R = H), suggests that the presence of both methyl and 2-methoxy-1-naphthyl groups restrict conformational motion about the vicinal diamine group.



(9) DEGRADATION OF FLUOROPOLYMERS FOR PER- AND POLY-FLUOROALKYL SUBSTANCES (PFAS) THROUGH THERMOGRAVIMETRIC ANALYSIS-MASS SPECTROMETRY (TGA-MS)

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The Environmental Protection Agency (EPA) is pursuing ongoing research to develop methods to detect and quantify PFAS contamination and evaluate potential disposal mechanisms, to include incineration (EPA, February 2020). This technique disposes of chemicals by combustion at high temperatures, upwards of 1000 to 1400 °C. The persistence of any PFAS byproducts in the environment present a challenge due to the abundance of strong carbon-fluorine bonds. Research on the efficacy of incineration is limited, but recent models predict that the combustion of C1 and C2 PFAS results in the formation of the products of incomplete combustion (PICs) such as CF₂ and CF₃ radicals (Krug et al, Journal of the Air & Waste Management 2022). In our study, we analyze the thermal breakdown and degradation products from polytetrafluorethylene (PTFE) using Thermogravimetric Analysis from 20 to 1000 °C, coupled to Mass Spectrometry (TGA-MS). The TGA-MS data provides an understanding of the potential gaseous degradation products during the thermal breakdown of PTFE. The separation of individual byproducts and isolation of gaseous byproducts is a challenge. Ongoing studies aim to investigate potential reaction pathways leading to the degradation of PTFE to correlate with the DFT mechanistic modeling for kinetic and thermodynamic parameters.

(10) DIFFERENTIATING R5L AND WT TAU AGGREGATION

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The intrinsically disordered microtubule-associated protein tau functions to stabilize microtubules in neuronal axons. Aberrant tau aggregation into neurofibrillary tangles is highly correlated with neuropathologies such as Alzheimer's disease. The protein consists of three major regions: the projection domain, the microtubule-binding domain (MTBD), and the C-terminus. There are six naturally occurring isoforms of tau, which vary in their number of N-terminal (2N, 1N, or 0N) and MTBD repeats (3R or 4R). The MTBD and its mutations has been largely studied due to its important role in microtubule binding and in pathological aggregation, however the projection domain's function has remained more elusive. To further comprehend the projection domain's role, the present work focuses on the tau mutant R5L, which has been found in patients with progressive supranuclear palsy (PSP). This study aims to compare the three 4R N-terminal isoforms of R5L and wild type tau to understand how this mutation in the projection domain affects aggregation behavior. Tau aggregation is induced using arachidonic acid and analyzed using atomic force microscopy (AFM) imaging to compare.

(11) CONNECTION BETWEEN LIPID AND PROTEIN HOMEOSTASIS IN THE ENDOPLASMIC RETICULUM

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The yeast lipid phosphate phosphatase Scs3 (function conserved in human), a 6-transmembrane protein of the endoplasmic reticulum (ER), contributes to ER lipid homeostasis and prevents ER stress, a condition known to trigger cell death if unresolved. Follow up analysis in yeast allowed the identification of Die2, a key enzyme involved in protein glycosylation in the ER, as genetic interactor of Scs3. Intriguingly, SCS3 deletion has been previously shown to affect protein homeostasis in cells, suggesting a link between lipid and protein homeostasis in the ER. To further investigate this connection, my work was therefore 2-fold: 1. Confirming by growth test assays the genetic interaction between Die2 and Scs3. 2. Decipher Die2/Scs3 role in ER protein metabolism by performing a cycloheximide chase assay to track ER protein half-life by western blot analysis using cells deleted for SCS3 and overexpressing Die2.

**(12) CHARACTERIZATION OF AN AMINOSTEROL THAT
BOTH
INHIBITS A β ₄₂ AGGREGATION AND PROTECTS CELL
MEMBRANES FROM A β ₄₂ OLIGOMERS TO ATTENUATE
PROTEOTOXICITY IN ALZHEIMER'S DISEASE**

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Aggregation of the 42-residue form of the amyloid- β (A β ₄₂) peptide leads to the formation of oligomers, which play a key role in the development of Alzheimer's Disease (AD). Previous studies on the aminosterol "Trodesquamine" have shown its ability to reduce oligomeric toxicity despite increasing the rate of aggregate formation. We studied the effects of a different aminosterol compound and found it to decrease both the rate of A β ₄₂ aggregation and its cytotoxicity. Experiments were run with varying concentrations of the aminosterol and resulted in decreased aggregation rates by reducing predominantly the elongation microscopic step in A β ₄₂ aggregation. Reactive oxygen species (ROS) results showed that the aminosterol also suppressed A β ₄₂-induced toxicity towards human neuroblastoma cells. The ability of this aminosterol to reduce both aggregation rates and the toxicity of oligomeric species suggests a promising therapeutic approach against AD.

(13) EFFECTS OF BETULIN DERIVATIVES FROM BIRCH AND SYCAMORE BARK 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 betulin, betulinic acid, and lupeol. Methanolic extracts of these barks have been found to be biologically active in assays on *Drosophila melanogaster*. The activity of crude extracts and more purified fractions is divergent, demonstrating protection against oxidative stress, larval growth enhancement, larval growth inhibition, or no-activity as compared to a control. Extracts were characterized by GCMS, H-NMR, and IR spectroscopy, and antioxidant activity was assessed by DPPH free radical scavenging assay. Crude birch extracts, composed of betulin and lupeol, displayed no statistical difference from control. However, purified recrystallizations of > 85% betulinic acid from sycamore showed enhanced proliferative/protective effects compared to both crude extracts. Extraction of betulinic acid via methanolic preparation was conducted which was treated with activated charcoal in boiling methanol and recrystallized, providing a white solid with a betulinic acid content of 85 to 95+ % by mass. Further structure activity experiments are being conducted to gain insight on these effects, with a selection of esters derived from betulinic acid, including glycosylated versions, are being synthesized.

**(14) SYNTHESIS, PHOTOPHYSICAL PROPERTIES, AND
STRUCTURAL CHARACTERIZATION OF LEAD-FREE
Cs_xMnBr_y PEROVSKITE NANOCRYSTALS**

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Lead halide perovskites are a promising light absorbing semiconductor material for next-generation solar cells. However, there are multiple issues with using these lead-based materials, including exposure during the manufacturing process, the possible risk of lead coming out of the panels and contaminating the area where they are placed, and the exposure risk during the decommissioning of these panels. The main purpose of this project was to investigate lead-free perovskites which are energetically tuned to target the significantly contributing wavelengths within the solar light spectrum. Three phases of Cs_xMnBr_y nanocrystals were explored in this work: a red emitting phase (CsMnBr₃), a green emitting phase (Cs₃MnBr₅), and a blue emitting phase (Cs₂MnBr₄ · 2H₂O) from a hot injection synthesis using Cs⁺ and Mn²⁺ oleates and TMSBr as the Br⁻ source. Additionally, a red emitting phase of CsMnCl₃ was synthesized using TMSCl as the Cl⁻ source. Photophysical characterization of the colloidal nanocrystals including UV-Vis absorbance spectroscopy, photoluminescence (PL) spectroscopy, and photoluminescence excitation (PLE) spectroscopy was performed. X-ray scattering measurements were performed to confirm the local structure of the 1D perovskite materials. These results show that phase engineering of Cs_xMnBr_y nanocrystals allows for bandgap tuning across the visible spectrum of light.

(15) FIRST-PRINCIPLES STUDY OF CONFORMATIONAL CHANGE OF MELITTIN IN THE PRESENCE OF EGCG

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Melittin, a peptide forming the main component of European Honeybee venom, is a toxin that has been well documented for its ability to interact with and disrupt the permeability of membranes through catalyzing the formation of pores within the membranes. In looking for counteracting agents to protect cells against these toxicological effects, epigallocatechin gallate (EGCG) was identified as a polyphenol exhibiting protective effects against such pore-forming toxins. EGCG markedly exhibits the promotion of oligomerization in its interactions with other proteins, which decreases the membrane-binding activity of these proteins. In a similar manner, EGCG may decrease the activity of melittin to prevent its interaction with the cell membrane. However, the exact methodologies as to how EGCG inhibits the function of Melittin in binding to and forming pores within the membrane is not well understood. Our study explores into the intricate details of how melittin and EGCG bind, utilizing a combined methodology of density functional theory (DFT) calculations and molecular dynamics (MD) simulations. The focus of our research is on illustrating how the introduction of EGCG impacts the conformational change of melittin, delving into the physicochemical properties of pore forming agents.

(16) MAPPING THE MECHANICAL PROPERTIES OF TAU'S POLYELECTROLYTE BRUSH USING ATOMIC FORCE MICROSCOPY

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Tau is a neuronal protein best known for its role in microtubule stabilization and organization. In its pathogenic state, however, tau forms filamentous, insoluble aggregates called paired helical filaments (PHFs) that have been found within Alzheimer's disease-affected neurons, yet the details surrounding tau's role in neurodegenerative disease pathology remain unclear. This project studies the mechanical properties of tau that may affect its neurotoxicity. Tau's unstructured nature has allowed it to elude traditional protein structural characterization methods, but analysis with atomic force microscopy (AFM) offers a novel method to interrogate tau structure. This research focuses on a distinct aspect of tau: the brush-like structure it assumes in its fibrillar state. Predominantly comprised of the protein's unstructured termini, interrogation of this brush can offer valuable insights into critical aspects of tau aggregation. Applying an optimized protocol for high-resolution imaging and PeakForce-QNM AFM, tau fibers were imaged in fluid and their adhesive and deformation properties were simultaneously mapped. These characteristics of tau were modulated by changes in electrolyte concentrations and pH, indicating fiber behavior in the cellular environment. These findings hold the potential to advance our understanding of tau-related neurodegenerative disease and may pave the way for new avenues for intervention and treatment.

**(17) APPLICATION OF FTIR TO IDENTIFY MICROPLASTICS
FOUND IN DEPOSITS ASSOCIATED WITH STREAM
OUTFLOWS INTO LAKES AND ESTUARIES
OF THE HUDSON VALLEY**

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Microplastics represent a major form of sedimentary pollution in our waterways. The sediment at the bottom of aquatic areas becomes a sink for the denser plastic particles. By analyzing sediment from several tributary systems located in the Hudson Valley, the relationship between hydrology of stream-to-slack systems and the density of microplastics present in sediment was investigated. Sediment was collected from four different waterways (three creeks and a lake), with each site surveyed at multiple locations at variable distances between the stream head and open water. In all sites, the highest concentration of microplastics in sediment were found in spatial hotspots 600-700m downstream from the stream opening, and 150m downstream in the lake system. As an addition to the field work completed for this project, lab techniques including Fourier Transform Infrared Spectroscopy were applied to these samples to determine the specific types of plastics present. By measuring the absorption of infrared light by samples, and comparing the spectrum to a polymer database, the samples could be matched to specific types of plastic polymers. This work sought to qualify the types of plastics found in tributary waterways to the Hudson River and offer insight into their origins.

(18) ENERGETICS ANALYSIS OF MEDIEVAL BLACK POWDER

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Thermodynamic studies consisting of bomb calorimetry and differential scanning calorimetry (DSC) were conducted to empirically determine the energy output and pre-ignition conditions of medieval black powder recipes. The recipes were also used in a replica medieval cannon for live-fire trials. Using high speed imagery, cannonball velocities were measured and compared to the empirical work from the laboratory to see if the lab tests could provide predictive analysis of the black powder performance. In addition to varying the ratio of the three main ingredients (charcoal, sulfur, and potassium nitrate) the medieval gunners also used additives such as vinegar, brandy, and camphor. Ultimately, the purpose of the research is to aid historians in their interpretation of medieval texts and to determine if medieval artillery men empirically understood why certain additives and ratios of black powder increased performance.

(19) LATERAL FORCE MICROSCOPY OF MICROCONTACT PRINTED SURFACES FOR ADHESION STUDIES

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We are interested in modeling differences in adhesion between two surfaces and have turned to atomic force microscopy (AFM) to obtain experimental data to aid with our model. Lateral (or friction) force microscopy is a branch of AFM used to study differences in adhesion between an AFM tip and a surface. We have derivatized gold films (deposited on silicon surfaces) with self-assembled monolayers using thiols that contain either straight chain hydrocarbons (DDT) or carboxylic acid (MUDA) functional groups to quantify the differences in friction force between the AFM tip and the monolayer surface. Microcontact printing was used to transfer the thiol “ink” to select regions of the gold film and lateral force images were collected, which show contrast on the surface due to differences in friction between the AFM tip and either the MUDA or DDT stamped surface. We hope to use our experimental findings in a model to study lateral adhesion.

(20) TRANSIENT ABSORPTION OF ZnTPP USING A TWO LASER PUMP-PROBE SETUP

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Transient absorption spectroscopy is a time-resolved technique that can be used to study electron photoexcitation and to analyze photochemical reactions. Our system was created using two nanosecond-pulsed lasers, a pump and a probe, at wavelengths 520 nm and 450 nm respectively. The pump laser was used to excite the molecule zinc tetraphenylporphyrin (ZnTPP) while the probe laser was used to measure the change in absorption of the molecule, which is known as transient absorbance (TA). The time delay between the pump and probe is varied electronically allowing the TA signal to be monitored for several microseconds. The addition of C₇₀ fullerenes to the ZnTPP solution also enabled charge transfer kinetics to be studied.

**(21) PROCESS DESIGN AND MECHANISTIC MODELLING OF THE
PER- AND POLY-FLUOROALKYL SUBSTANCES (PFAS)
PRODUCED FROM THE THERMAL DEGRADATION OF
FLUOROPOLYMERS**

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Recently, the Environmental Protection Agency has expanded its Contaminant Candidate List to include several PFAS subtypes with thousands of distinct chemicals towards identifying additional PFAS that could potentially require future regulation under the Safe Drinking Water Act. (EPA, October 2022) In our study, we are modeling the thermal degradation of polytetrafluoroethylene (PTFE) and neat polymers hexafluoropropylene (HFP) and polyvinylidene fluoride (PVDF) through process modeling in Aspen Plus. The thermal degradation process is modeled in a Gibbs Reactor in atmospheric combustion conditions with varying oxygen flowrates and temperatures, ranging in temperatures of 250 to 1000 °C. The process feed stream to study the thermal breakdown of PTFE is modeled as its constituent monomer, HFP, perfluorobutyl ethylene (PFBE), chlorotrifluoroethylene (CTFE), and perfluoropropyl vinyl ethers (PPVEs) reacting with varying air flow rates of stoichiometric oxygen and nitrogen. Thermogravimetric analysis shows the degradation of PTFE initiates around 260 °C while the significant degradation occurs between 550 °C to 600 °C. (K. Ochi, Ehime University 2008) Overall, the aim of this study is to determine the mass and energy balance of PFAS products formed during the combustion of fluoropolymers.

(22) SOIL LEAD IMMOBILIZATION

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Childhood elevated blood lead (>5 mg/dL) in Poughkeepsie and Newburgh has been historically much higher than national and regional averages, with about 1 in 5 children being affected at its peak. To find major contributing sources of lead, samples of soil, water, and paint from these communities were collected at one case-study residential property in each city and analyzed by XRF and ICP-MS. Results indicate that the main lead source, paint chips, as indicated by the direct relationship between distance from the house and lead concentration. This study focuses on reducing bioaccessibility of the lead found in soil through various applications of phosphate rich fertilizers in solid phases – bone meal and zeolite – and the liquid phase – lawn food. The zeolite and bone meal were applied in two forms, top drizzle where it was sprinkled on top of the soil and as a homogenous mixture of soil and fertilizers. The preliminary results show up to a 10.97% reduction in bioaccessibility of lead based on the SBET method when applying top drizzle zeolite. Next steps include using additional standard bioaccessibility assays and to determine the chemical/mineralogical form this less bioaccessible lead is present in.

(23) COMPARISON OF SOLVATOCHROMISM AND AGGREGATION-INDUCED EMISSION ENHANCEMENT OF A V-SHAPED ORGANIC MOLECULE TO ITS ONE-ARMED ANALOG

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Light emissive organic molecules are of current interest due to their potential applications in fluorescent materials, biosensors, polarity probes, and detectors. Recently, our group has synthesized several “V-shaped” organic molecules with electron donor-acceptor units and studied their photophysical properties in various solvents. The donor-acceptor nature of these compounds leads them to exhibit solvatochromism, and their overall structure results in aggregation-induced emission enhancement (AIEE) behavior. When photoexcited, these molecules can relax non-radiatively in good solvents by free rotation around the single bonds. However, upon aggregation in poor solvents, a restriction of intramolecular rotation induces relaxation along radiative pathways. One synthesized V-shaped molecule features two bulky phenyl-fluorene donor units *ortho*-disubstituted on an electron-accepting quinoxaline ring. To fully assess the degree of AIEE and solvatochromism in the V-shaped molecule, a structural analog featuring only one phenyl-fluorene group was synthesized as a control to confirm that it exhibits solvatochromism but not AIEE since it lacks the steric bulk that prevents free rotation upon aggregation. Synthesis and characterization of the one-armed analog will be presented and compared with the results for the V-shaped molecule.

(24) INVESTIGATION OF $\text{NaNb}_{13}\text{O}_{33}$ AS AN ANODE MATERIAL IN FAST-CHARGE LI-ION BATTERY APPLICATION

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Stable Wadsley-Roth shear structures of $\text{NaNb}_{13}\text{O}_{33}$ facilitate the incorporation and diffusion of Li-ion. Investigating the insertion and intercalation of Li-ion into $\text{NaNb}_{13}\text{O}_{33}$ to form $\text{Li}_x\text{NaNb}_{13}\text{O}_{33}$ advances the growing need to investigate lithium anode materials for fast-charging battery capabilities. In fast-charging conditions, Li-ion deform the anode structure, which significantly reduces the charge and discharge capacity. At a slow cycling rate, $\text{NaNb}_{13}\text{O}_{33}$ reached a capacity of 233 mAh/g, indicating a greater than one-to-one transfer of Li-ion. The phase transition of niobium observed in the differential capacity plot support this evidence. $\text{NaNb}_{13}\text{O}_{33}$ was compared to the well-studied TiNb_2O_7 and was shown to have a greater lithium diffusion constant and capacity. With an average voltage of 1.6 V and higher rate capabilities, $\text{NaNb}_{13}\text{O}_{33}$ demonstrates potential use as an anode material for fast-charge Li-ion battery application.

(25) SYNTHESIS AND ANTIBACTERIAL POTENTIAL OF MONOBACTAMS AND MONOBACTAM N-SULFONYL CHLORIDES

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Beta lactams are specifically structured molecules distinguished by their four-membered cyclic amides. These compounds are the most widely used class of antibiotics and exhibit notable antimicrobial properties, including those found in common antibiotics such as penicillin. Beta-lactam antibiotics cause cell lysis and death by inhibiting bacterial cell wall synthesis. They bind and acylate catalytically essential serine leading to inhibition of the penicillin-binding protein and thus preventing it from catalyzing transpeptidation. With growing resistance to antibiotics, the synthesis of new synthetic beta-lactam compounds could prove to be quite invaluable.

The objective of this research was to synthesize beta-lactam N-sulfonyl chlorides from alkenes using chlorosulfonyl isocyanate and then reducing and purifying these N-sulfonyl chlorides to their corresponding beta-lactams so that their antimicrobial properties could be tested. Products were purified using recrystallization and/or column chromatography and meticulously analyzed with TLC and NMR. Disc diffusion bioassays were run against gram positive (*Bacillus cereus*, *Enterococcus faecalis*, *Staphylococcus epidermis*, *Staphylococcus saprophyticus*) and gram-negative bacteria (*Escherichia coli*, *Pseudomonas aeruginosa*, *Pseudomonas putida*) to evaluate the antimicrobial potential of these compounds. The results of the bioassays will be presented. Moreover, the mechanistic insights into the chlorosulfonyl isocyanate-mediated synthesis of beta lactams were investigated, shedding light on the reaction kinetics and key intermediates involved in the transformation of alkenes into valuable antibiotic scaffolds.

(26) QUANTIFYING DYE UPTAKE BY UV-VIS SPECTROSCOPY

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In collaboration with a local tie dye shop, a method was developed to determine the concentration of Procion Red MX-5B bonded to cotton fabric during the dyeing process. A series of MX-5B solutions in various concentrations was used to dye fabric. Using UV-VIS, the maximum dye uptake was determined to be 15.03 ± 0.02 g/L. A similar process was used to observe how aging dye solutions affects dye uptake. Over a four week period the dye uptake decreased 12.5% for the highest concentrated MX-5B solutions and a 29.7% decrease for the lowest. The method was effective in determining the concentration of dye uptake on fabric as well as analyzing the effects of time on dye uptake. This method can be applied to different colored dyes.

(27) A NEW METHODOLOGY FOR ANALYSIS OF ICE-RAFTED DEBRIS IN END-TRIASSIC SEDIMENTS

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Analysis of ice-rafted debris (IRD) and other dropstones in sedimentary rock is almost exclusively done using destructive techniques such as grain-size analysis, which requires the rock sample to be dissolved in acid or peroxide to reveal the original sediments locked within the carbonate. Techniques such as this not only destroy samples which are often in limited supply, but also are time consuming and reveal the presence of IRD in only small sections of sample cores at a time. The aim of this project is to discover a geochemical proxy for IRD, allowing for non-destructive and total analysis of individual samples and whole sample cores. Through X-ray fluorescence and X-ray diffraction we are able to find the relative abundance of elements within the sample and compare them against the relative amounts of IRD also present. Using this data and inputting it into computational programs, such as R, we have begun to narrow down on several potential proxies for IRD which can be explored in future experimentation.

(28) INVESTIGATION OF THE BIOPHYSICAL PROPERTIES THAT DRIVE CYTOTOXICITY IN PORE-FORMING AGENTS

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Pore forming agents attack cells through the formation of holes in the cellular membrane, leading to ion dyshomeostasis and cell death. In the search for the biophysical properties that drive cytotoxicity in pore-forming toxins, we investigated a series of polyphenols. Our previous work demonstrated that the polyphenol epigallocatechin gallate mitigates the harmful effects of melittin, a pore-forming agent intrinsic to bee venom, by decreasing the extent of melittin's solvent-exposed hydrophobicity and promoting its oligomerization into larger species that no longer bind the cell membrane. To further investigate this relationship, we studied the ability of structurally similar polyphenols to mitigate the toxicity of melittin. This research contributes to our understanding of strategies to combat the pore-forming mechanisms employed by specific biologically toxic agents and highlights the importance of physicochemical properties for these pore-forming substances in their ability to interact and disrupt cell membranes.

(29) EVALUATION OF NEW POWER SUPPLIES AND REACTION CONDITIONS FOR METAL NITRIDE CLUSTERED FULLERENES

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Madeleine Gaidimas initiated the synthesis of metal nitride clustered fullerenes (NCFs) project by constructing the Vassar arc-vapor deposition reactor in 2020. Christopher Triggs determined the optimal reaction conditions to produce NCFs in 2021. This work aims to address the difficulties in synthesizing NCFs by modifying the reaction system with new power sources. Experiments combined with HPLC analyses investigated the effects of current amperage and voltage and the effects of the reactor atmospheric composition on fullerene synthesis efficiencies. The results demonstrate that cured graphite rods with larger diameters are required at higher amperages and voltages, and atmospheric compositions are less important than the arcing quality. The low fullerene production efficiencies in the experiment reflect that further optimization of the hardware and reaction conditions is necessary.

(30) CARBON MONOXIDE AND ITS ANALOGS

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Carbon monoxide (CO) has garnered notable attention within the field of chemistry because of its bonding characteristics and reactivity. Along with theoretical interest, it has immense biological importance, as it can bind with oxygen in the bloodstream, leading to potentially fatal conditions such as carbon monoxide poisoning. Herein, we explore CO and its triply bonded diatomic analogs N_2 , P_2 , PN, SiS, CS, SiO, CN^- , NO^+ , PS^+ , SiP^- , CP^- , SiN^- , NS^+ , PO^+ , BF and BCl. All calculations were performed using the VBSCF method along with the cc-PCVDZ basis set. Valence bond methods allow for the determination of in situ bond energies and resonance energies for the separated σ and π systems. In this manner, we were able to determine the preference for coordinate vs. traditional and σ vs. π bonding in these molecules.

(31) SYNTHESIS AND CHARACTERIZATION OF NOVEL ENERGETIC STABILIZERS

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This research seeks to develop novel energetic stabilizers that will enhance the energetic performance and inhibit the decomposition of propellant formulations. These novel energetic stabilizers may serve as candidate additives in propellant formulations. We report the synthesis of 10 new nitrated aromatic building blocks which are substituted with several ring-strained cycloalkane amines (cyclopropylamine, cyclobutylamine and bicyclopentylamine) via nucleophilic aromatic substitution. Characterization of these compounds was performed via single crystal X-ray diffraction, nuclear magnetic resonance, Fourier-transform infrared spectroscopy, thermogravimetric analysis, and differential scanning calorimetry.

(32) SYNTHESSES OF DIAMINOCYCLOHEXANE-BASED RECEPTORS

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We are interested in using chiral molecular recognition to separate and/or analyze mixtures of enantiomeric substrates. By this method, a chiral receptor is used to selectively interact with one substrate enantiomer over another in a mixture, without covalently modifying either substance. Specifically, we have synthesized a series of six chiral receptors on gram-scale that use *trans*-1,2-diaminocyclohexane (DACH) as a common subunit. Our synthetic strategy involves nucleophilic addition of hydride and methyl anion equivalents to DACH-derived diimines. When methyl anions are used, the reactions produce additional chiral centers within the molecule, and we have achieved virtually complete stereocontrol in at least two cases (as determined by NMR measurements). Most of our target compounds have been purified by column chromatography, and/or recrystallization. In the future, we plan to study the stereoselective binding properties of our receptors towards various carboxylic acid containing substrates. Structural variations among the purified receptors will allow us to assess the influence of substituents at various sites within the DACH substructure on the selectivity of the chiral recognition process.

(33) SYNTHESIS AND CHARACTERIZATION OF Pt(II) COMPOUNDS WITH ISOCYANIDE LIGANDS

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Cyclometalated Pt(II) compounds with various isocyanide ligands were synthesized and characterized. Two C^N chelate imine ligands were utilized in order to facilitate C-H orthometalation with the tetramethyl platinum precursor Pt₂Me₄(μ-SMe₂)₂. Subsequently, the dimethylsulfide ligand was easily substituted for with various isocyanide ligands. The target Pt(II) compounds thus contain one chelate C^N imine ligand, a methyl ligand, and an isocyanide in the coordination sphere. The compounds' photophysical properties (absorbance, emission, excited state lifetimes, and photoluminescence quantum yields) were measured and studied as a function of their ligand architecture.

(34) SYNTHESIS AND CHARACTERIZATION OF ZINC OXIDE CORE SILICA SHELL NANOPARTICLES

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Zinc oxide core silica shell nanoparticles have been investigated for their medicinal properties. On their own, zinc oxide is a known antimicrobial and silica is known to accelerate blood clotting. The combination of these properties may advance studies in anti-infection wound healing. The nanoparticles synthesized in this research were silica coated ZnO nanoparticles. ZnO nanoparticles were synthesized then coated with silica facilitated by hexadecylcetyltrimethylammonium bromide (CTAB). CTAB served to direct the silica coating by binding the negatively charged silica to its positively charged group. CTAB was explored in different concentrations to optimize reagent ratios. The effectiveness of applying the silica coating on the ZnO nanoparticles was characterized using scanning electron microscopy (SEM) and dynamic light scattering (DLS). CTAB proved to be more effective in binding silica to the ZnO nanoparticles than without it. However, SEM results showed that the ZnO nanoparticles aggregated and were only partially coated with silica. This indicates that experimental conditions need to be further optimized.

**(35) PROGRESS TOWARDS THE CONCISE, METAL-FREE,
DIVERGENT TOTAL SYNTHESIS OF HERICERIN A,
ISOHERICENONE J, AND ISOHERICERIN**

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Hericerin A, isohericenone J, and isohericerin are three geranyl-resorcinol or tetraketide-based meroterpenoid natural products found in *Hericium erinaceus*, an edible mushroom commonly known as Lion's Mane Mushroom. Previous research identified these compounds to be cytotoxic against specific cancer cell lines—Hericerin A and isohericenone J against human leukemia cell lines and isohericerin against human melanoma cell lines. Hericerin A has never been synthesized before, while isohericenone J and isohericerin have been synthesized previously. However, the syntheses utilized reagents containing metals and accessed the structurally very similar natural products using different routes. Alternatively, we aim to synthesize all three geranyl-resorcinols using a concise, metal-free, divergent synthesis approach. Metal-free synthetic routes are cost-efficient and ensure that there is no trace metal contamination or toxicity in the final products. Divergent syntheses are time-efficient because all products are obtained from a common late-stage intermediate. Herein, we discuss our progress towards the divergent total synthesis of hericerin A, isohericenone J, and isohericerin. We succeeded in coupling a sterically hindered tertiary alcohol with a sterically hindered phenol under Mitsunobu conditions to form a geranyl ether—the bottleneck transformation of the route. Our work transcends the scope of the Mitsunobu reaction and inspires concise, metal-free syntheses.

(36) A INVESTIGATING LYSOSOMAL PROTEIN CHANGES IN AP-3 DEFICIENT MOUSE MELANOCYTES

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Adaptor Protein-3 (AP-3) is a heterotetrametric protein complex involved in the cargo-selective transport of materials in cells. AP-3 deficiency results in mistrafficking of proteins, including Lysosomal-Associated Membrane Protein-1 (LAMP-1) and tyrosinase. Previous research in our lab using an AP-3-deficient melanocyte cell line, *mocha*, has shown that LAMP-1 is over-expressed and has a lower molecular weight in these cells due to glycosylation changes causing it to be more sensitive to Endoglycosidase H. To determine if this change is seen in other AP-3 deficient cell lines, wildtype (WT) melanocytes were modified with CRISPR in hopes of knocking out AP-3; however, based on genetic analysis, this was unsuccessful. Instead, a second line of AP-3-deficient cells, *pearl*, was analyzed and showed the same change to LAMP-1. Other cellular proteins were investigated for size variations, including LAMP-2 and tyrosinase. LAMP-2 showed a decrease in molecular weight in both AP-3-deficient cell lines, but tyrosinase showed no change. Lysosomal hydrolase (cathepsin) activity was assessed by analyzing cathepsin D expression through Western blotting and cathepsin L distribution and activity using a florescent reporter monitored by microscopy. Overall, we found that AP-3 deficiency affects glycosylation in LAMP-1 and LAMP-2, modifies cathepsin L distribution, and may decrease cathepsin D expression.

(37) MECHANISTIC INSIGHTS ON DEGRADATION MECHANISM OF SARIN ON GRAPHENE-SUPPORTED SINGLE ATOM CATALYSTS

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Chemical warfare agents (CWAs) are highly toxic synthetic chemicals or their precursors that can be dispersed as gas, liquid, aerosol, or powder. A specific form of these neurotoxins is Sarin, a very potent organophosphate compound, which detrimentally disrupts an organism's neural impulses by inhibiting the degradation of neurotransmitter acetylcholine. For the detection and catalytic breakdown of sarin, several platforms including metal-organic frameworks (MOFs), graphene, and metal oxides have been investigated. Lately, there's growing interest in utilizing single metal atoms as active sites in heterogeneous catalysis, noted for their enhanced stability, reusability, and distinctive electronic and structural attributes, outperforming nanocluster analogs. Our study evaluates the effectiveness of single atom catalysts (SACs) for sarin decomposition, focusing on hydrolysis and dealkylation mechanisms using single metal atoms (Au, Pt, Rh, Ir, Pd) anchored on nitrogen-doped graphene oxide, analyzed through density functional theory (DFT) calculations. The BEP-type relationship can be seen between the energetic difference and activation energy associated with rate-determining step of both mechanisms. Overall, these metal-dependent changes in surface thermodynamics and kinetics offer a route to tuning and enhancing the catalytic efficiency of SACs towards sarin degradation.

(38) MEASUREMENT AND CHARACTERIZATION OF AGGREGATION IN SINGLE AND DOUBLE STRANDED OLIGONUCLEOTIDES WITH CATIONIC SURFACTANTS

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Single stranded oligonucleotides can aggregate or condense in the presence of lipids or lipid-like compounds; an important property of nucleic acids, which was used to aid in the delivery of mRNA into the cell in the SARS CoV-2 vaccine. We have studied this aggregation process using primarily the cationic surfactant cetyltrimethylammonium bromide (CTAB), as well as hexyltrimethylammonium bromide (HTAB) and decyltrimethylammonium bromide (DTAB), and both single- and double-stranded synthetic DNA. Oligonucleotide solutions were titrated with surfactants and changes in fluorescence anisotropy were recorded. Saturation binding curves were obtained using CTAB and showed a sigmoidal shape indicative of a cooperative process, which was used to obtain association constants and the extent of cooperativity. We found a critical length was needed for DNA aggregation in the hydrocarbon chain of the surfactant. We also found subtle differences in the extent of aggregation of dsDNA or ssDNA at a given surfactant concentration. To further characterize differences in aggregation, we have begun using atomic force microscopy to image aggregates formed from ssDNA and CTAB.

(39) DESIGN AND CHARACTERIZATION OF HYDROGEL MICROSTRUCTURES AS LOCAL THERMAL SENSORS

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Photopolymerization of acrylic monomers is often performed using UV light or by the nonlinear absorption of two-photons of near-IR light (e.g. 800 nm), which is known as two-photon polymerization (TPP). Recently, we showed that an acrylic resin with ethyl(2,4,6-trimethylbenzoyl)phenylphosphinate (TPO-L) as a photoinitiator can be polymerized by a 532 nm CW laser, which is unexpected because TPO-L has negligible absorbance at 532 nm. We hypothesize that the polymerization may be due to local heating from the focused laser. To test this, we created a temperature responsive hydrogel that shrinks when heated. After testing the thermal response of macroscopic (~1 cm) samples, microscopic cantilever-shaped structures were made using TPP. The TPP microstructures were then used as micron-scale local temperature sensors to probe the polymerization process using a 532 nm CW laser.

(40) WHICH CdSe NANOPARTICLE IS THE BEST DETECTOR FOR EXPLOSIVE VAPORS?

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Previous research has shown that the sizes of various CdSe nanoparticles fluoresce at different wavelengths. Also, it is known that when these particles are placed near explosive vapors, their fluorescence is quenched and thus their response to explosives could be used to construct a detector for soldiers and first responders. In efforts to optimize the use of these particles in this way, our research seeks to determine whether the size of the nanoparticle can be leveraged to provide the fastest and most efficient, as a detector of explosive vapors.

(41) WATER DESTABILIZES THE ADSORPTION OF BORONIC ACIDS ON THE TiO₂ RUTILE (110) SURFACE

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Solar energy is a potential solution to the ongoing energy and environmental crisis our planet is facing. Dye-sensitized solar cells (DSSCs) show great promise in their affordability and effectiveness. In DSSCs, anchoring groups facilitate covalent bonding between photosensitive dye and a semiconductor (TiO₂). We have introduced boronic acids, such as boric, methyl, phenyl, and 2,3,4-fluorophenylboronic acid as new anchoring groups on a TiO₂ rutile (110) surface. We have employed computational analysis using DFT to determine whether these boronic acids will adsorb more strongly than commonly used anchoring groups such as carboxylic or phosphonic acids. In previous work, a clean surface was examined, but to create a more realistic model, we examined a hydrated surface. Multiple configurations of boronic acids on a TiO₂ rutile (110) surface were examined. The doubly dissociated bidentate configuration was the most stable, which is consistent with previous work. Adsorption of boronic acids is less stable on a hydrated surface than on a clean surface, showing that water has a destabilizing effect when adsorbed on the surface. The adsorption of 4-fluorophenylboronic acid is the most stable boronic acid, which shows a means of further stabilizing boronic acid anchoring groups in DSSCs.

(42) AP-3 EFFECTS ON DOWNSTREAM PHOSPHORYLATION AND AUTOPHAGY

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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). Immune cells lacking Adaptor Protein-3 (AP-3) have been shown to be more sensitive to autophagic stimuli than WT cells, but it is unknown if this relationship holds in other cell types. Our goal for this project was to test the hypothesis that AP-3-deficient melanocytes (*mocha* or *mh* melanocytes) are more sensitive to starvation-induced autophagy than their wildtype counterparts (WT). We subjected *mh* and WT cells to starvation conditions and measured autophagy by biochemical and immunofluorescent analyses. We found that *mh* cells were seen to have a decrease in S6k phosphorylation – indicating decreased nutrient sensing efficacy. We also found that LC3-II and P62 – both markers of autophagosomes – accumulated in *mh* cells at higher rates than in WT cells. These results support our hypothesis that AP-3^{-/-} melanocytes are more sensitive to nutrient conditions than WT cells.

(43) ELECTROCHEMICAL CHARACTERIZATION OF COMPOSITE SEPARATORS FOR REDOX FLOW BATTERIES

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The increasing demand for better, more effective techniques of energy storage will always remain as one of the objectives within the future – flow batteries have the potential to do such. Redox flow battery operates by passing an electrolytic solution through the battery thus causing both oxygen and reduction reactions. The objective of this study was to determine the most effective combination of separators and electrolyte solutions within a flow battery – analyzing the most reactive and energy favorable combinations. The electrochemical characterization of separators can be analyzed to isolate the contribution of each functional component within a battery – the separator, ion solution attributes, charge transfer resistance, and mass transfer resistance. To characterize separators, a custom flow cell was used to run different ion solutions at 75 mL/min flow and at no flow with different combinations of separators in conjunction with electrochemical impedance spectroscopy (EIS), cyclic voltammetry plots (CV) and chronoamperometry (CA) plots. The composite separator tests for characterization include CelgardTM, coated CelgardTM with PAA and PVA (hydrogel coatings), and DaramicTM. The concentrations utilized for electrochemical testing include 0.5 M, 0.1 M, and 1.0 M of H₂SO₄, HNO₃, HCl, CaCl₂. The separators were also electrochemically studied in DI Water as a baseline. From analysis of the EIS plots, the pure resistive contribution of each test can be analyzed by identifying the x-intercept and semicircle diameters that align with the real impedance axis. A comparison of each test can isolate the positive contribution of the specific separator used, concentration of ions, type of ions, and the impact of flow. These extensive material characterization analysis for the conductivity of separators for their application in flow batteries identify the need to select the most advantageous material for battery characterizations. A fundamental understanding of the contributions of each component will also allow for further experimentation, using novel aqueous graphene oxide suspensions as a potential solution and electrode combination with advantageous electrochemical characteristics.

(44) QUANTIFICATION OF BISPHENOL A (BPA) IN REGENERATING PLANARIA

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BPA is a chemical compound commonly found in many plastics. It is considered a contaminant with concerns due to its adverse health effects. We used regenerating planaria, a type of freshwater flatworm, to study the effects of BPA on the process of planarian tissue growth and repair. To differentiate the BPA used for our controlled exposure studies, a deuterated form of BPA (d8BPA) was used where eight non-exchangeable hydrogen atoms were replaced with deuterium. From previous experiments, d8BPA had the same lethal effects as BPA. High-performance liquid chromatography (HPLC) was used to characterize the extracts from the d8BPA-exposed planaria to quantify the extent of retention. The signals from the worm extracts were normalized using the mass of the dried worm pellet, which was crucial for quantification since worm sizes varied.

(45) INVESTIGATING THE VISIBLE-LIGHT MEDIATED 2+2 PHOTOCYCLOADDITION OF 3-ACETYL INDOLES

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Photochemical reactions are fundamental in organic synthesis, valued for their functionality, efficiency, and reaction selectivity. Traditionally, UV light has been the preferred activation source for these reactions due to the way organic molecules absorb under it. However, visible light has recently emerged as a safer and more broadly applicable tool for organic photoreactions. The objective of this project is to explore the influence of differently N-protected on 3-acetyl indoles on visible light-mediated reactions of the C2-C3 pi bond. To accomplish this, we synthesized a group of 3-acetyl indoles bearing three unique protecting groups to gauge their reactivity in visible light mediated [2 + 2] photocycloaddition reactions. The resulting photoproducts were reported and characterized using ¹H NMR spectroscopy. This research considers the potential of visible light in photoreactions, and expands the knowledge of protecting groups in influencing reaction outcomes.

(46) SYNTHESIS OF IRIDIUM ORGANOMETALLIC CHROMOPHORES

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Transition metal chromophores have attracted the attention of a variety of fields, such as non-linear optics (NLO), photoredox catalysis, photodynamic therapy, biological sensing, and as phosphors for organic light-emitting diodes (OLEDs). Second and third row transition metal complexes, such as iridium(III), have garnered particular interest because they exhibit reverse saturable absorption (RSA) due to their large spin-orbit coupling constants and metal-to-ligand charge transfer. This work describes the synthesis of five novel variations of the 2-phenylbenzothiazole (pbt) integrated iridium cyclometallated complex $[\text{Ir}(\text{pbt})_2(\text{acac})]$ by substituting phenyl (Ph), nitro phenyl ($\text{NO}_2\text{-Ph}$), fluoro phenyl (F-Ph), and difluoro phenyl ($\text{F}_2\text{-Ph}$) on the pbth ligands.

(47) IDENTIFICATION OF BASIDIOMYCETES AND SCREENING OF LIGNINOLYTIC ENZYME ACTIVITY IN FUNGAL SPECIES FROM NORTHEAST AMERICA

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A significant proportion of fungi produce lignin degrading enzymes such as Laccases and Manganese peroxidases. These enzymes degrade lignin by oxidizing phenol hydroxyl groups. These enzymes have potential in bioremediation as they also oxidize various aromatic compounds such as substituted phenols and aromatic amines. We foraged 30 different Basidiomycetes from various parts of Northeast America. We have isolated and cultured mycelium from these fungi and are currently screening them for ligninolytic activity. We are culturing the fungi on media containing Guaiacol (2-methoxy Phenol) and ABTS (2,2'-azinobis 3-ethylbenzthiazoline-6-sulfonate); the color reactions serve as a screen for Ligninolytic activity. In this poster we will present the results of screening of 8 species with ABTS and Guaiacol. We are also optimizing protocols for culturing, isolation of fungal genomic DNA and DNA barcoding. In this poster we present our detailed protocols and early results. Immediate goals are A) Identify the 30 different species of Basidiomycetes using DNA barcoding, B) Screen for ligninolytic activity in all species, C) Study mRNA expression of Laccases in these species and identify specific isoforms. Our long-term goals are to clone, express, purify specific Laccases and decode Laccase activity against Polyhydroxy aromatic hydrocarbon (PAH's)-a serious contaminant in drinking water.

(48) NOVEL FLUID ADDITIVES FOR ENHANCED URANIUM IMMOBILIZATION IN HYDRAULIC FRACKING

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Hydraulic fracking is well-known for its negative environmental impacts, which include the leaching of toxic heavy metals into local water sources. One such metal is Uranium (U), which is harmful to humans and decays into the radioactive and dangerous element, Radon. This study investigates less-toxic and cost-effective alternatives to bi-pyridine, previously recognized as an additive to Hydraulic Fracking Fluid (HFF), to stabilize U within the shale, thereby mitigating environmental contamination risks. Through rigorous experimentation involving uranyl acetate, various organic ligands, and HFF, the average percentage of residual U in the solution was calculated across four testing dates and two replicate incubations. ICP-MS analysis indicated that none of the incubations approached complete removal, indicating approximately 75% of U remained insoluble, settling at the incubation bottle bottom throughout the experiment. Among the organic ligands studied, histidine and salicylic acid exhibited the most effective U removal, with less than 10% of U remaining in the solution. These disparities in precipitation may stem from distinct bonding capacities of the organic ligands with U. The marked reduction of U in ligand-present incubations compared to ligand-absent ones denotes the success of this preliminary experiment, suggesting histidine and salicylic acid's ability to precipitate U from aqueous solutions containing HFF.

(49) LIPID ENZYME FIT2/SCS3 AND ENDOPLASMIC RETICULUM HOMEOSTASIS

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The acyl coenzyme A diphosphatase FIT2 has proven to be a crucial actor in mammalian endoplasmic reticulum (ER) lipid homeostasis. Using yeast as a model organism, the FIT2 orthologue SCS3 was utilized to investigate how exactly this ER resident enzyme preserves homeostasis. To accomplish this, yeast cells were deprived of the enzyme and a genetic screening was conducted to determine key genetic interactors that work with SCS3 to maintain ER lipid homeostasis. The candidate genes identified in the screen were confirmed and subsequently expressed into both wildtype and SCS3 deprived yeast cells. In this study, two specific genes were focused on, *Izh1* and *Die2*. The genetically modified cells were evaluated through several means such as growth assays and ER homeostasis tests. In addition, numerous stressors were employed to compare the wildtype and engineered cells resultant ER stress response. With the suppression of a normally lethal phenotype, *Izh1* and *Die2* proved to be essential components in ER regulation through zinc metabolism and protein folding respectively; a suggestion that SCS3 has a more intricate role than initially theorized.

(50) HYDROLYSIS KINETICS of OPIOID-LIKE COMPOUNDS

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Non-lethal opioid-like ester derivatives revealed unexpected differences in rates of hydrolysis with slight variations in molecular structure. These moieties can be found in other biologically active substances. Our research goal is to examine the effects of various methyl 3-(piperidin-1-yl) propanoate analogs on the rate of ester hydrolysis. Throughout the course of this research inquiry, various analogs were used to identify alternate factors such as substituent identity, substituent placement, the presence of a piperidine, pH, and concentration that may impact the ester hydrolysis of methyl 3-(piperidin-1-yl) propanoate. ¹HNMR and GCMS allowed for the determination of half-lives and kinetics of ester derivatives. Going forward, modeling the chemical reactions using density functional theory will provide insight into other reaction factors, including thermodynamic barriers. This will aid in the understanding of substituent effects to elucidate the mechanism.

(51) SOLVENT-FREE 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, among them a very strong antibacterial activity. We want to understand how the chemical structure influences the antibacterial ability of these compounds. A small library of chalcones substituted with various electron-donating and electron-withdrawing substituents on either aromatic ring or both rings have been synthesized via the Claisen-Schmidt condensation in order to contribute to a structure-activity relationship study. Although most aldol condensation reactions are run in organic solvents at elevated temperatures, solvent-free 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.

**(52) CHARACTERIZING THE ATTACHMENT OF
BDELLOVIBRIO BACTERIOVORUS TO THE PREY CELL
*ESCHERICHIA COLI***

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Bdellovibrio bacteriovorus is a unique Gram-negative bacteria that preys upon many other Gram-negative bacteria and has potential applications in medicine, industry, and agriculture. Once it identifies prey, *Bdellovibrio* attaches to the outer membrane of the prey cell, enters the prey cell periplasm, and seals the opening behind itself. *Bdellovibrio* feeds and divides before finally bursting out from the host cell to continue this cycle and leaving behind a lysed prey cell. This research aimed to characterize the attachment phase of this cycle using atomic force microscopy. Specifically, *Escherichia coli* was adhered to a cantilever using Cell-Tak and pressed into a glass slide of similarly adhered *Bdellovibrio* for one second or five minutes before being retracted. While the 1-s dwell time resulted in minimal adhesion forces between the two sets of cells, the 5-min dwell time yielded a strong adhesion force (8-15 nN) over a relatively short pull-off distance (0.2-0.5 mm). These results were distinct from control force curves. We also looked into deterring this attachment phase by using cranberry juice, which is known to contain type A proanthocyanidins that inhibit cells' pili. In the presence of pH-neutralized cranberry juice, the 5-min dwell time did not generate force curves with substantial adhesion forces. To determine whether cranberry juice inhibited *Bdellovibrio* predation on a more macroscopic scale, *Bdellovibrio* growth on *E. coli* was monitored by UV-Vis spectroscopy in the presence and absence of neutralized cranberry juice. A higher optical density at 600 nm suggested more *Escherichia coli* in solution and less *Bdellovibrio*, as *Escherichia coli* is large enough to substantially scatter light, unlike *Bdellovibrio*. Results thus far suggest that cranberry juice cuts off but does not completely inhibit *Bdellovibrio* proliferation.

(53) THEORETICAL INVESTIGATION INTO THE THERMAL DEGRADATION OF POLYTETRAFLUOROETHYLENE

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Synthetic fluoropolymers, notably poly- and perfluorinated alkyl substances (PFAS), are widely utilized in various industrial applications, such as kitchenware, textiles, and flame-resistant materials. The presence of C-F bonds endows many fluoropolymers with significant wettability, along with thermal and chemical stabilities, and distinctive friction characteristics. However, there are growing concerns regarding the toxicity of fluoropolymers in living organisms, attributed to their strong affinity for proteins and their persistence in the environment. A combustion-based methodology has been proposed to mitigate the concentrated presence of fluoropolymers in open-air conditions. However, identifying the key decomposed compounds produced from combustion process is not a trivial task. Therefore, atomistic simulations have been used to forecast the potential products formed during experimental thermal decomposition. In this study, the degradation mechanism of polytetrafluoroethylene (PTFE) has been investigated via the combination of density theory (DFT) calculations and molecular dynamics (MD) simulations. Additional analysis of the enthalpic and entropic contributions to the production of key reaction intermediates, including perfluorocyclobutane (C₄F₈), was considered. Overall, such theoretical data may serve as a reference to identify key products of the thermal degradation processes of various fluoropolymers.

(54) SYNTHESIS, CHARACTERIZATION, AND REACTIVITY OF THE PAsP ANALOG OF A HIGHLY ACTIVE PPP-PINCER IRIDIUM ALKANE DEHYDROGENATION CATALYST

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Goldman et al. recently reported the most active homogeneous catalyst for dehydrogenation of n-alkanes known to date. Based on experiments and calculations, this iridium complex, bearing a triphosphorus “PPP” pincer ligand, owes its enhanced reactivity over related PCP pincer complexes to a destabilization of the square-planar Ir(I) resting state common to both systems, as well as lowering the activation energy of the rate determining β -hydride elimination step. While having many similarities, such as nearly identical electronegativities and only about 10 picometers difference in radius, arsenic and phosphorus have not been studied equally in the field of organometallics. Relatively few examples of complexes/catalysts with organo-arsenic ligands have been reported as opposed to the ubiquitous phosphines. We aim to answer if the incorporation of arsenic into this ligand scaffold will promote or poison catalysis. The PAsP ligand (bis(2-di-t-butylphosphinophenyl)arsine) was successfully synthesized with slight modifications to Goldman’s procedure, and was metallated with $[\text{Ir}(\text{COE})\text{Cl}]$, providing the PAsPIrHCl complex. The structure of the iridium complex was characterized via x-ray crystallography and C, H, and P NMR spectroscopy. Coordination of CO was achieved by exposing solutions of the complex in aromatic solvents to 1 atm of carbon monoxide, yielding the octahedral PAsPIrHCl(CO) adduct. Addition of potassium triethylborohydride resulted in a mixture of the square planar PAsPIrCO complex and the PAsPIr(H) CO complex (ostensibly due to oxidative addition of the H gas produced), which completely converted to PAsPIrH₂CO after further exposure to 1 atm of H₂. Analogously to Goldman’s work, the PAsPIrHCl complex was reacted with potassium tertbutoxide in the presence of H₂ gas to form an $[\text{Ir}]\text{H}$ complex. However, at room temperature little reaction occurred and reactions using lithium superhydride were also unsuccessful. A structural comparison between the PPP and the PAsP complexes will be discussed as well as further reactivity and catalysis studies.

(55) INVESTIGATING FRACKING FLUID ADDITIVES FOR THE REMOVAL OF ARSENIC FROM FLOWBACK WATER

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In response to rising global energy demands, hydraulic fracking has emerged as a predominant form of natural gas energy production.

Fracking requires the injection of hydraulic fracking fluid (HFF) at high volumes and pressures into shale rock formations; chemical additives to fracking fluids react with shale, releasing trace metals, metalloids, and radioactive material into returned water. One such metalloid that is a water contaminant of concern is arsenic. The primary goal of this study is to assess possible ligand additives to HFF that could form complexes with As(III) and As(V) and thereby remove arsenic from flowback water. Two trials of arsenite and arsenate salt incubations have been completed so far, the first using four bipyridine isomers, and the second using salicylic acid, EDTA, L-cysteine, dibenzylthiocarbamate, methylimidazole, and diphenylimidazole. Incubations were sampled on 4-5 dates over 20 days, and total arsenic concentrations were determined by ICP-MS analysis. All ligands tested proved ineffective in arsenite removal, and while all ligands in trial 2 removed about 40% more arsenic from arsenate incubations than the control, results were still inconclusive. A third trial will use aspartic acid, cysteine, histidine, triethylenetetramine, and tetraethylenepentamine, selected based on research on the binding of arsenic by common functional groups.

**(56) INHIBITION OF DHFR ENZYME AND BINDING OF DHFR
RNA BY RUTHENIUM (II) AND COPPER (II) METAL
COMPLEXES WITH PHENFORMIN AND METFORMIN**

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An important target in cancer has been the folic acid pathway in which the enzyme dihydrofolate reductase (DHFR) catalyzes the reduction of dihydrofolate to tetrahydrofolate using NADPH, an essential cofactor for the biosynthesis of purines, thymidylate, and several amino acids. Our project focuses on (i) the binding of ruthenium and copper complexes with DHFR enzyme and subsequent evaluation of DHFR catalytic activity and (ii) direct binding of ruthenium and copper complexes with the mRNA of DHFR gene and subsequent evaluation of RNA function in a translation assay. The in vitro binding affinity of Phenformin, Metformin, Ru79, Cu65 and Ru-cymene were investigated using DHFR enzyme activity assay. Methods included seed cultures, plasmid extraction, restriction digestion, isoamyl:phenol:chloroform purification, transcription, incubation with metal complexes, translation, analysis with a DHFR activity assay, gel electrophoresis and mobility shift assays. It was concluded that there is serious potential of phenformin and metformin based drugs to better hinder the enzymatic activity of the DHFR enzyme and to eventually become successful anti-cancer drugs. Future work will revolve around more studies with additional Ru(II) and Cu(II)metal complexes from the Anderson laboratory and binding studies with DHFR mRNA.

(57) MONOBACTAMS AND THEIR CORRESPONDING N-SULFONYL CHLORIDES AS POTENTIAL ANTITUBERCULAR AGENTS

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β -lactams are currently the most widely used antibiotic compounds, but widespread use has led to a rise in bacterial antibiotic resistance. There are several bacterial diseases which, even with current antibiotics, continue to be a problem globally. Tuberculosis, which is caused by the bacteria *Mycobacterium tuberculosis*, is one such disease. The mycobacterial ClpP enzymes play a critical role in protein turnover and are essential for the viability of *M. tuberculosis*. It was found that appropriately substituted β -lactones were able to perturb the activities of these enzymes. Due to their structural similarity to β -lactones, various monobactams and their corresponding β -lactam N-sulfonyl chlorides were synthesized to evaluate their antitubercular potential. For this study, *Mycobacterium phlei*, a non-pathogenic bacterium in the same genus as *M. tuberculosis*, was used. Cultures of *M. phlei* were grown in brain-heart-infusion (BHI) media and disc diffusion bioassays were run on the various monobactams and monobactam N-sulfonyl chlorides. Zones of inhibition were measured to quantify antibiotic activity. The results of this study will be presented.

(58) EPOXY ALCOHOL REARRANGEMENT OF 2-NAPHTHOL TO ACCESS PHARMACEUTICALLY RELEVANT SCAFFOLDS

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In an attempt to design a novel non-metal synthetic pathway for (+)-Brazilin via an acid-catalyzed rearrangement-cyclization reaction, we recently discovered an unprecedented reaction mode of 2,3-epoxy alcohols derived from 2-benzylidene-1-indanones. Treatment of these epoxy alcohols with trifluoroacetic acid triggers a skeletal rearrangement/aromatization reaction which affords substituted 2-naphthols in high yield. Overall, we have identified a high-yielding, 4-step synthetic route to 2-naphthols which does not require chromatographic purification until the final step. We are currently using various analogs of 1-indanone as precursors in the synthesis of 2-naphthols to further expand the scope of this reaction. These 2-naphthol products are a common structural feature of many biologically active compounds, including 2-arylpyrrolidines and TPY- β . Given the operational simplicity and low cost of this synthesis route, we will easily be able to prepare libraries of TPY- β analogues for biological evaluation.

(59) INVESTIGATING THE BINDING POTENTIAL OF RUTHENIUM BASED METAL COMPLEXES TO DNA-RNA HYBRIDS

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This study investigates the interactions between ruthenium-based compounds, namely LM5400, LM3000, and Compound B, with DNA:RNA hybrids—an area of the human genome primed for exploration. Building upon the Jain lab's insights into Cisplatin's effects on hybrids, our research aims to uncover the therapeutic potential of these compounds. Employing a multidisciplinary approach integrating advanced techniques and assays such as radiolabeling, CRISPR, gel electrophoresis, and UV-Vis melting studies, we seek to decipher the underlying molecular mechanisms of these interactions. This study may potentially represent a significant advancement in nucleic acid chemistry, with implications for reshaping biomedical research and clinical interventions aimed at diseases where DNA:RNA hybrids play a critical role.

**(60) COMPARATIVE STUDY OF AMERICAN AND UKRAINIAN
PROPOLIS: COMPONENT IDENTIFICATION AND
ANTIOXIDANT ANALYSIS**

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Propolis, also known as “bee glue”, is a resinous substance produced by *Apis mellifera* honeybees for sealing cracks and protecting the hive against intruders. Propolis has been gaining attention as a functional food due to its remarkable biological activities such as antioxidant, antibacterial, and anticancer. This work is a chemical characterization and antioxidant assessment of two distinct propolis samples: one sourced from Wappingers Falls, NY, and the other from Odesa, Ukraine. Acetone and methanol extracts of propolis were subjected to GC-MS and HPLC analyses to identify their chemical constituents. A total of 21 chemical constituents were identified across both samples, with many of them being bioactive compounds such as phenolic acids and flavonoids. The Wappingers Falls propolis is more rich in flavonoids whereas the Ukrainian sample is more rich in esters and long alkane chains, underscoring regional variations in propolis composition. Antioxidant activity was evaluated using a novel method of hydrodynamic voltammetry at a rotating ring-disk electrode (RRDE). Both propolis samples demonstrated comparable and significant antioxidant capabilities, as evidenced by their steady drop in collection efficiency. This study hopes to add more knowledge to existing literature on propolis chemical constituents of different regions and their associated antioxidant activity.

(61) REPRODUCIBILITY OF ATOMIC FORCE MICROSCOPY MEASUREMENTS ON TAU PROTEIN

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The microtubule-associated protein tau is an intrinsically disordered protein responsible for the regulation and stabilization of microtubules in neuronal axons. Its positively charged domain binds to microtubules, while the N-terminal projection domain extends from the surface. The aggregation of tau into neurofibrillary tangles is believed to play a role in neurodegeneration. Tau variants, which have been identified as potentially pathogenic, include hyperphosphorylated proteins as well as proteins with N- and C-terminal mutations. It is hypothesized that measurable changes to the projection domain in these variants may be correlated to differences in aggregation. Atomic force microscopy (AFM) was used to interrogate a single layer of monomeric tau bound to mica, which mimics the microtubule surface. Long-range repulsive forces were observed as the probe approached the surface, indicating the presence of the negatively charged projection domain. The focus of this study is to improve the reproducibility of these force-distance curves. Previous work has measured forces between the tau layer on the probe and the tau layer on the mica surface. Ensuring that the curves were taken asymmetrically, where the protein is present on only the mica surface and not the probe, seems to be crucial to achieving consistency. Once quantitative differences in the force-distance curves of different variants are observed, it will be possible to characterize the conformational changes in the N-terminal tau isoforms.

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Special Thanks

The SUNY New Paltz Chemistry Department thanks:

- Mid-Hudson chapter of the American Chemical Society
- School of Science and Engineering, SUNY New Paltz
 - New Paltz student and faculty volunteers
 - Tanjore Indian Cuisine, Fishkill, NY