

Abstracts

Regional Undergraduate Poster Competition

Jacobs Science Building

March 31, 2023

11:30am-3:30pm



University of Kentucky
Department of Chemistry
Lexington, KY 40508

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*Group A presents from 12:00pm to 1:30pm

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1

Retrospective Study of Nutrition and Diet in Children with Autism in Kentucky

Ashley Bates, Senior, Chemistry, University of Kentucky

Stephen Testa, Chemistry, University of Kentucky

David Toupin, Developmental Pediatrics, KY Children's Hospital

Laura Krueger, Hailey Mair, Emilie Touma, College of Medicine, University of Kentucky

Abstract

Autism Spectrum Disorder, or ASD, is a diagnosis of behavioral and communication deficits. It is characterized by difficulty in social interaction and communication and by restricted or repetitive patterns of thought and behavior. ASD affects approximately 1 out of 54 individuals in the United States, and its prevalence is continuing to grow. Children with autism have restrictive diets and are at risk for vitamin and nutrient deficiencies. To the best of our knowledge, this has not been studied in Kentucky patients. There is a lack of consensus guidelines on how vitamin deficiencies should be screened for in this population. This study will bring awareness to the dietary characteristics and risks of deficiencies in our specific population as well as assess the relationships between restrictive diets, nutritional deficiencies, and autism severity. Information on results and conclusions will be added once data collection is complete.



2

Investigating the Role of eIF5AhypK50 on TDP-43 Pathology and Brain Metabolism in TDP-43 Transgenic Animal Model

Rohan Desai, Sophomore, Chemistry, University of Kentucky

Patricia Rocha-Rangel, Sanders-Brown Center on Aging, University of Kentucky

Zainuddin Quadri, Molecular and Cellular Biochemistry, College of Medicine, University of Kentucky

Pete Nelson, Sanders-Brown Center on Aging, University of Kentucky

Ramon Sun, Neuroscience, College of Medicine, University of Kentucky

Abstract

The cytoplasmic accumulation and inclusions of TAR DNA-binding protein (TDP-43) are hallmarks of Alzheimer's Disease and Limbic-Predominant Age-Related TDP-43 Encephalopathy (LATE). Eukaryotic Translation Initiation Factor 5A (eIF5A) is the only eukaryotic protein that undergoes a post-translational modification: hypusination. This modification of lysine (K) to hypusine (hypk50) occurs through the enzymatic activity of deoxyhypusine synthase (DHS) and deoxyhypusine hydroxylase (DOHH). Our laboratory has reported that this pathway directly regulates TDP-43 accumulation in stress granules, phosphorylation and aggregation. We observed induced hypusine levels in AD and TDP-43 transgenic mouse brains. This study investigates the effects of induced eIF5AhypK50 via AAV-directed DHS/DOHH overexpression on TDP-43 pathology, neuroinflammation, and brain metabolism in a TDP-43 transgenic (TAR) mouse model.

Assessing the Impact of Antisense Oligonucleotide Therapy in a Lafora Disease Mouse Model

Laiken Griffith, Senior, Molecular and Cellular Biology, University of Kentucky

Katherine Donohue, Molecular and Cellular Biochemistry, College of Medicine, University of Kentucky

Bethany Fitzsimmons, Ionis Pharmaceuticals

Ron Bruntz, Peyton Coburn, Molecular and Cellular Biochemistry, College of Medicine, University of Kentucky

Abstract

Lafora Disease (LD) is glycogen storage disease that occurs in children and young adults, includes symptoms like seizures and neurodegeneration, and results in the death of the patient within about ten years of the onset of seizures (Akman et al., 2015, Gentry et al., 2005, Gentry et al., 2020, Lafora & Glueck, 1911, Minassian et al., 2001). LD results from mutations in either the EPM2A or EPM2B genes that encode for the proteins laforin and malin, and is driven by the formation of insoluble glycogen, which aggregates into Lafora Bodies (LBs) (Romá-Mateo et al., 2011, DePaoli-Roach et al., 2010, Duran et al., 2014, Gentry et al., 2005, Serratosa et al., 1999, Sullivan et al., 2017). This study examined an antisense oligonucleotide that targets glycogen synthase (Gys1) as a potential therapy with the goal of slowing the formation of LBs. We found that the Gys1 ASO resulted in a significant decrease in the formation of LBs, as well as fewer large LB aggregates.

Optimization of Fluorescent Labeling Conditions for Lithium Grease

Jacob Richardson, Senior, Chemistry, University of Kentucky

Jason DeRouchey, Chemistry, University of Kentucky

Jacob Bonta, Engineering, University of Kentucky

Abstract

Lithium grease is an important lubricant for a variety of applications whose properties depend on the formation of a complex microstructure. These grease systems exhibit mechanical degradation and recovery pathways. To study these reversible processes visually, we need a means to incorporate fluorescently labels in the grease structure. The objective of this project is to optimize the reaction conditions for creating a lithium grease structure containing a fluorescent tag. We reacted 7-amino-4-methylcoumarin with 12-hydroxysteric acid in chloroform, isopropyl alcohol, and methanol. We tested the effects of changing the reaction stoichiometry to minimize unreacted byproducts. We also experimented with different purification methods using liquid-liquid extraction. Fluorescence microscopy was used to assess the successful labeling of the grease structure. Different methods of evaporation were performed to determine their effect on the grease microstructure formation.

Utility of Exhaled Breath Condensate to Examine Spingolipids in Patients with ARDS

Ashley Trejo-Coke, Senior, Chemistry, University of Kentucky

Jeremy Allegood, Biochemistry and Molecular Biology, University of Kentucky

Peter Morris, Pulmonary, Allergy, and Critical Care Medicine, Heersink School of Medicine, University of Alabama at Birmingham

Stephen Testa, Chemistry, University of Kentucky

Jamie Sturgill, Microbiology, Immunology, and Molecular Genetics, University of Kentucky

Abstract

Acute lung injury (ALI) and acute respiratory distress syndrome (ARDS) are syndromes that are described by the acute onset of bilateral pulmonary inflammation and impaired oxygen. These syndromes are life-threatening, rapidly progressive illnesses that often occur in critically ill patients. In previous work done in our lab, it has been shown that sphingolipids play a significant role in lung inflammation and particularly ceramide has been of interest for its role in pulmonary disease. The presence of ceramide has been thought to be elevated in patients who develop ARDS/ALI and could be a potential biomarker for these syndromes. Exhaled breath condensate (EBC) is a non-invasive way to examine the pulmonary inflammation and potential biomarkers of the lung. Through this analysis, we can compare both EBC and plasma in mechanically ventilated patients in the ICU to determine if ceramide levels can be a possible contributor to pulmonary disease. Although this study is ongoing, of the patients we currently have data for it has been found that total ceramide seems to be a promising biomarker for patients with ARDS.

Synthesis of Chiral Organic Molecules for Potential Application in Hybrid Organic-Inorganic Light-Emitting Diodes

Dolan Whittle, Senior, Chemistry, University of Kentucky

Aron Huckaba, Chemistry, University of Kentucky

Abstract

Light-emitting diodes (LEDs) have become an everyday piece of technology utilized within the phone and television screens used today. Circularly polarized light-emitting diodes (CP-LEDs) are expected to be the display technology of the future. The aim of this project is to synthesize new chiral organic molecules that have a higher light emission efficiency compared to that of current molecules. Our strategy to synthesize the desired molecule is to add a carbonyl group to an indolizine heterocycle and then enantioselectively transform the carbonyl to an amine to create a chiral center. After confirmation of synthesis of the desired molecule's chirality, the organic cation will then be combined with an inorganic anion to create a hybrid organic-inorganic material.

Synthesis of Novel Organic Components for Organic-Inorganic Perovskite Cells

James McDaniel, Senior, Chemistry, University of Kentucky

Aron Huckaba, Chemistry, University of Kentucky

Alison Costello, Chemistry, University of Kentucky

Abstract

Organic semiconducting Perovskites (OSiPs) have applications in LEDs, Perovskite solar cells, field effect transistors, thermoelectric devices, and perovskite memory devices, and they have the structure ABX_3 . OSiPs have transition metals at the core with organic ligands. By incorporating isomeric organic ligands with different pi-stacking capabilities, differences in electron transport and material structure may be achieved. In this project, we synthesized two potential organic components for OSiPs and are seeking to test their application in OSiPs through crystallization with different transition metals.

Oxidative Catalysis of Alkanes Using Transition Metal Coordinated Ligands

Megan Hwang, Senior, Chemistry, University of Kentucky

Aron Huckaba, Chemistry, University of Kentucky

Abstract

Non-heme iron catalysis is a method of oxidizing alkanes. This field is important because it gives chemists access to untapped feedstocks for reactions. This experiment describes the production of transition metals coordinated to tribenzimidazole cyclohexane which act as a catalyst. The goal is to oxidize cyclohexene into its corresponding epoxy, alcohol, and ketone form. Gas chromatography showed that the nickel and cobalt catalyst accomplished this successfully, but the cobalt catalyst also reduced cyclohexene into cyclohexane. Additionally, a new alkane¹ (N-methylbenzene-1,2-diamine) was synthesized successfully and characterized using H N M R. It was then used to synthesize tripodal Me₃N₃TB (tris(N-methylbenzimidazol-2-ylmethyl) amine).

HFIP Promoted Hydrohalogenation using Aqueous HX Solution

Kyla Mitchell, Senior, Chemistry, University of Louisville

Yuhao Yang, Chemistry, University of Louisville

Carter Stinett, Zhou Li, Chemistry, University of Louisville

Bo Xu, Chemistry and Chemical Engineering, Donghua University

Gerald B. Hammond, Chemistry, University of Louisville

Abstract

Aqueous HX (X = Cl, Br, and I) solutions are the most ubiquitous HX source in the laboratories. However, the hydrohalogenation of an alkene or alkyne by an aqueous HX solution is difficult to perform under standard conditions. Because of the acid's high ionization potential in water, it is held in the aqueous phase and has a relatively low concentration in the organic phase; the alkene or alkyne, on the other hand, being highly nonpolar, exists primarily in the organic phase. Because the two reactants occupy different phases, their interactions with one another are limited, and, as such, aqueous HX is rendered a generally ineffective reagent. By introducing a hydrogen bond donor (HBD) such as 1, 1, 1, 3, 3, 3-hexafluoroisopropanol (HFIP), the nucleophilicity of water can be reduced such that HX is liberated from the aqueous phase and allowed to enter the organic phase where it may interact with the substrate; the result is an environment in which aqueous HX can serve as an effective hydrohalogenation reagent. Through this mechanism we have achieved high yielding hydrohalogenation of various alkenes and alkynes using aqueous HCl, HBr and HI, mediated by HFIP.

Synthesis and Preliminary Evaluation of a Potential Synthetic Opioid Rescue Agent

Grace McCarty, Senior, Chemistry, University of Kentucky

Lindsay Kornberger, Pharmaceutical Sciences, University of Kentucky

Dan Luo, Pharmaceutical Sciences, University of Kentucky

Stephen Testa, Chemistry, University of Kentucky

Thomas Prisinzano, Pharmaceutical Sciences, University of Kentucky

Abstract

Although fentanyl is utilized to treat acute and chronic pain and as an anesthetic, the misuse and abuse of the substance has led to rising overdose deaths in the United States. The primary cause of death is opioid induced respiratory depression (OIRD). The current treatment for OIRD is the opioid receptor antagonist naloxone. Recent findings suggest multiple doses of naloxone are often required to fully reverse fentanyl induced respiratory depression (FIRD). A more efficient and potent opioid rescue agent is needed to reduce the increasing rates of death caused by fentanyl. One approach to identifying a more efficient fentanyl rescue agent is modifying known opioid agonists into antagonists through structural modification. Analogues of bucinnazine and azaprocin were synthesized and characterized for their ability to activate opioid receptors or antagonize the effects of fentanyl in vitro utilizing a modified forskolin-induced cAMP accumulation assay. The information gained through these structure-activity relationship studies is expected to help identify a suitable lead molecule for further development of a more efficient and potent opioid rescue agent than currently available treatments.

Testing Stress Levels by Monitoring Electrodermal Activity

Kinley Jarvis, Senior, Chemistry, University of Kentucky

Stephen Testa, Chemistry, University of Kentucky

Victor Okuo, Chemistry, University of Kentucky

Abstract

There is very little research available concerning electrodermal activity (EDA) in regards to chemistry. EDA measures the change in an individual's skin conductance, and is also known as the galvanic skin response (GSR). GSR is used in professional lie detector tests to analyze the stress levels of the patient when answering questions. The aim of this research is to determine how an individual's stress level changes in response to finding elements on the periodic table. Along with EDA, eye tracking is used to determine when the subject has located the element they are prompted to find. The initial goal was to determine if stress levels increase when it takes longer to find an element on the periodic table. Since starting, this has been expanded to also see the overall stress level of the subject when finding elements on the periodic table, versus finding elements on a control, which is the periodic table with animals instead of elements. Currently, more research is needed to fully support the hypotheses.

Memorization and Learning Techniques in Chemical Courses

Kate Rogers, Senior, Chemistry, University of Kentucky

Stephen Testa, Chemistry, University of Kentucky

Abstract

In order to understand memorization and retention over time, specifically in chemistry courses, learning techniques were analyzed in this project. The first part of the project consisted of a baseline quiz followed by memorization of the periodic table for a two-week period. The second part of the project consisted of approximately seven weeks in which random quizzes were administered. After completion of the quizzes, memorization techniques along with the progression of memory loss were analyzed. The results were compared with other data to determine the best learning and memorization techniques for chemical topics and material.

Muscle Alterations and Functional Outcomes Following Critical COVID-19

Jonathan Starck, Junior, Chemistry, University of Kentucky

Kate Kosmac, Physical Therapy, University of Kentucky

Ahmed Ismaeel, Physiology, University of Kentucky College of Medicine

Kirby Meyer, Esther Dupont-Versteegden, Physical Therapy, University of Kentucky

Abstract

The global emergence of COVID-19 has resulted in a record number of hospitalizations. Given the substantial health burden, understanding the long-term impact of COVID on patient outcomes is an area in need of further investigation. Myalgia is commonly reported with COVID and skeletal muscle damage has been purported but remains largely unexplored. Additionally, symptoms of sustained fatigue, persistent weakness, and prolonged myalgia have been reported up to 10 weeks after infection. However, the contributions of changes within skeletal muscle to COVID recovery are unknown.

To determine whether skeletal muscle alterations contribute to prolonged COVID symptoms, we assessed muscle fiber type, fiber size, and mitochondrial activity in vastus lateralis biopsies and explored relationships of muscle features to strength, power, and function. Participants included three cohorts: COVID+ patients admitted to the intensive care unit (ICU), COVID+ individuals without hospitalization (mild COVID), and a community-dwelling control group.

Immunohistochemistry was used to determine muscle fiber type and size. Succinate dehydrogenase (SDH) histochemistry was used to determine fiber type mitochondrial activity. Cytochrome C Oxidase (CCO) and Citrate Synthase (CS) activity were also measured in muscle homogenate. Clinical testing for muscle strength (knee extension), power (leg press), and functional performance (six-minute walk, timed-up and go, chair rise) were performed. We found reduced muscle mitochondrial activity in COVID+ ICU patients, which was associated with lower function. Interestingly, those with mild COVID also displayed alterations in muscle mitochondrial activity. Understanding if muscle changes contribute to recovery following COVID could provide novel therapeutics to shorten recovery time.

Synthesis and Detection of a Probe for Covalently Modified DDAH

Tori Kinnamon, Senior, Chemistry & Biochemistry, Rose-Hulman Institute of Technology

Alfred Tuley, Chemistry and Biochemistry, Rose-Hulman Institute of Technology

Colin Beach, Michael Ryan, Chemistry and Biochemistry, Rose-Hulman Institute of Technology

Abstract

Self-labeling fusion protein tags can provide cellular imaging information, such as protein localization, in living and fixed cells. Creating new tags will diversify the options for labeling proteins. Dimethylarginine dimethylaminohydrolase (DDAH-1 or DDAH) has been chosen as a candidate to be a part of a fusion protein tag. A bump-and-hole strategy was utilized to test multiple R groups as side chains on the 4-chloropyridine based probe molecule. The fusion protein system will be visualized by click chemistry with the probe containing an alkyne and the tag containing an azide. To test multiple different R groups to determine what will bump with the modified DDAH hole protein, a matrix-assisted laser deposition/ionization (MALDI) system was designed. This system will hopefully be a beneficial addition to biological tools for research.

Stability and Functionality of Macrophage Engineered Vesicles

Nora Sypkens, Sophomore, Chemistry, University of Kentucky

Christopher Richards, Chemistry, University of Kentucky

Khaga R Neupane, Alina Dorosh, Isaac Chavez, Chemistry, University of Kentucky

Abstract

Current options for cancer treatment often include non-targeted therapeutics which can inflict damage upon healthy cells of the body rather than simply the affected, cancerous, cells. We believe that engineered immunomodulatory vesicles may be an alternative delivery platform that can specifically target the tumor environment. These vesicles can be loaded with chemotherapeutics or other therapeutics in order to properly treat such areas. Macrophages can also be utilized to approach this issue. Macrophage engineered vesicles (MEV's) can be generated by disrupting macrophage cellular membranes, and they can then be polarized to either pro-inflammatory (M1) or anti-inflammatory (M2) phenotypes. This study tests how temperature and time affect the functionality of these vesicles in order to determine the most appropriate storage strategy for maximum efficiency should they be applied immunotherapeutically. This study was first done for unloaded vesicles prepared by nitrogen cavitation, then repeated for MEV's which were polarized and prepared by sonication.

Characterization of 4-Pyrone Thermal Decomposition Products via Matrix-Isolation FT-IR

Khaled El-Shazly, Junior, Chemistry, Marshall University

Kathryn Narkin, Chemistry, Marshall University

Elizabeth Sparks, Tess Courtney, Heather Legg, Laura McCunn, Chemistry, Marshall University

Abstract

The characterization of the byproducts of biomass thermal decomposition is a critical part in the development of viable clean biofuels and renewable energy sources. 4-pyrone, (IUPAC name: 4-pyran-1-one) is one of the byproducts observed in the pyrolysis of many forms of biomass, such as wood chips, straw, and cotton husks, but little research exists on its own decomposition pathways. Using the technique of argon matrix-isolation Fourier-Transform Infrared (FT-IR) spectroscopy, the pyrolysis products of 4-pyrone were characterized by passing a diluted sample of 4-pyrone through a heated pyrolyzer tube onto a cold window that captures the products and allows for their analysis spectroscopically. Computational analysis using Gaussian 09 software was also utilized to predict relevant structures, transition states, reaction steps, and energies, and these results were compared to the experimental spectra for product identification. Data collected at temperatures ranging between 900 K and 1400 K indicate the formation of acetylene, vinylacetylene, propyne, carbon monoxide, ketene, and methylketene. The formation of formylketene is also likely, as some peaks have been observed that match computational predictions and experimental data on its pyrolytic precursor. The results of this project will be crucial in guiding the development of 4-pyrone-containing biofuels in industrial settings.

Synthesis of Pt Single Atom Catalysts on WS₂ Nanosheet Support for Hydrogen Evolution Reaction

Viraj Mistry, Junior, Chemistry, University of Kentucky

Doo Young Kim, Chemistry, University of Kentucky

Nadeesha Kothalawala, Chemistry, University of Kentucky

Abstract

Green Hydrogen is considered a promising clean energy carrier for replacing fossil fuels, and among the current technology for hydrogen production, electrocatalytic water splitting has shown promise in producing this environmentally friendly alternative. Platinum has been shown to be the most effective catalyst in this production, however, it is both expensive and rare. While many studies have attempted to replace platinum as a catalyst, there has been no data that suggests any compound works better than it. An alternative approach that has garnered much attention is transforming Platinum into single atoms, which improves its efficiency by increasing surface area. To do so, these single atoms must be on a stable surface for the durability of the platinum catalyst. In this work, we report the use of WS₂ as support to stabilize single Pt in enhancing the catalytic activity of Pt toward hydrogen evolution reaction (HER). Using our synthesis method, we were able to produce a mixture of Pt single atoms and grouped Pt atoms which are not combined in forming the nanoparticles (clusters) on WS₂ nanosheet support, Pt on WS₂ support showed excellent HER activity both in the acidic and alkaline media with a good durability. Hence this work paves the way for using alternative materials for hydrogen production in reducing the cost of green hydrogen.

Supplemental Nutrition Impacts on Viral Abundance of Local Honey Bee Pathogens

Elisabeth Rintamaa, Senior, Chemistry, University of Kentucky

Caroline Kane, Entomology, University of Kentucky

Stephen Testa, Chemistry, University of Kentucky

Clare Rittschof, Entomology, University of Kentucky

Abstract

Agricultural crops rely on pollinators, but native populations are decreasing. Honey bees are introduced to agriculture systems to improve local pollination. However, due to a number of biotic and abiotic factors, honey bee populations suffer from colony collapse disorder (CCD) around the globe. CCD is a rare condition that hasn't been observed in Kentucky since 2013. Colony death is nonetheless high nationwide, and caused by interrelated factors including poor nutrition, pesticides, pathogens, and parasites. Our understanding of how these factors work together is poor. There are over 30 viruses that transmit within and between colonies globally. A USDA national bee survey identified a higher frequency of Lake Sinai Virus-2 (LSV2) infections with Kentucky colonies as compared to the national average, which makes it important to study for the state. While there is no direct treatment for viral infection, adequate nutrition seems to help with a variety of issues like pesticide-induced mortality, and could decrease viral morbidity. The current focus of this study is to understand if beekeepers can improve colony health through management practices, such as nutrition supplementation, and if so, identify the best strategies. Management strategies often used include nutrition supplements which beekeepers can provide in the form of artificial pollen, protein supplements, carbohydrates, and local pollen to increase brood rearing and overwintering survival. This study focused on identifying if protein supplements can limit virus replication and improve overall colony survival with consistent feeding. LSV2 is a gut-associated virus which motivates its study with respect to nutrition. Samples from individual hives were collected before and after the experiment to measure changes in viral abundance. LSV2 was tested for viral abundance through quantitative polymerase chain reactions (qPCRs). The data collection is still ongoing, and analysis is incomplete.

Synthesis and Characterization of TIPS Pentacenopentacene for Potential Use as an Organic Semi-Conductor

Andrew Sturgis, Senior, Chemistry, University of Kentucky

John Anthony, Chemistry, University of Kentucky

Tanner Smith, Chemistry, University of Kentucky

Abstract

Organic semiconductors have been heavily researched in the previous few decades. Their importance in future biotechnology is heavily emphasized with their current use in photovoltaics, batteries, and other electronic devices. The materials used in the production of organic semiconductors tend to be more flexible and cheaper than their metal counterparts. Long, conjugated pi systems are a large focus of this research. This is because it mediates the transfer of charge throughout the molecule, increasing the capacity to transmit current. Previous literature has shown the production of an unstable and lowcharacterized pentacenopentacene. Through the addition of the triisopropylsilyl group to the pentacenopentacene, colloquially known as the TIPS group, it is believed to further stabilize the conjugated pi system. This further stabilization will allow further characterization of the compound and produce a wide array of possibilities the compound can be used for in future organic semiconductor research. The goal of the project is to produce further stabilized acenoacenes that can characterized and tested for their properties for future usage in organic semiconductors. The synthesis of TIPS pentacenopentacene begins with 1,5-dihydroxynaphthalene and uses processes of bromination, silylation, triflation, and Diels-Alder.

Synthesizing a Single-Atom Catalyst for Use in Clean Energy Conversion Technologies

Jenna Rector, Senior, Chemistry, University of Kentucky

Doo Young Kim, Chemistry, University of Kentucky
Prakhar Sharma, Chemistry, University of Kentucky

Abstract

The electrocatalyst is pivotal in determining the cost and efficiency of clean energy conversion technologies. Current noble-metal catalysts have certain limitations preventing them from being implemented on a global scale. First, these catalysts are not cost effective due to low metal utilization. Second, they involve a large wastage of metal due to the oxidation and dissolving of bulk metal during electrolysis. Third, the surface-level attachment of nanoparticles to the carbon support is unstable shown by the removal of the nanoparticle during electrolysis. We propose to combat these limitations by synthesizing a single-atom catalyst using common transition metals to replace noble-metal catalysts. In our experiment, we used bottom-up synthesis and two different heat stabilization techniques to synthesize the single-atom catalyst. Then we analyzed the structure and identity of our catalyst using XRD, STEM, TGA, and Raman spectroscopy. Our analyses confirmed the proposed catalyst structure, and thus we began to test the catalyst in two major electrochemical reactions: oxygen reduction and carbon dioxide reduction. While we are still gathering data, our results show promise of an effective and economically competitive catalyst to be used in a variety of clean energy conversion technologies.

Antimicrobial Efficiency of Rare Kentucky Mushroom

Isaac Huffman, Senior, Chemistry, University of Kentucky

Stephen Testa, Chemistry, University of Kentucky

Sylvie Garneau-Tsodikova, College of Pharmacy, University of Kentucky

Abstract

Antimicrobial resistance has been one of the most popular cataclysmic topics in science over the past decade. The rate at which novel drugs can be implemented is being seemingly outpaced by microbes' ability to resist antimicrobials. One of the best ways to prevent large scale resistance is to rotate our applications, to avoid creating a selective pressure. To do this, we must build a library of novel bioactive compounds and drugs. The secondary chemistry of plants and fungi have been well adapted to fight microbes in natural settings. This has caused much attention toward their potential for producing usable antimicrobial products. This project seeks to discover novel antimicrobial products from understudied species of Kentucky-native Basidiomycetes. Particularly, *M. opacus*, has shown the most promise. Field collection of *M. opacus* took place in Pulaski County Kentucky. The mushroom was grown, extracted, and tested for antibiosis. The components of the extract were separated by HPLC, and active fractions were subjected to NMR. The structural elucidation of the active compound is ongoing.

Computational Analysis of Possible SARS-CoV-2 Therapeutics

Akenpaul Chani, Junior, Chemistry, Centre College

Jennifer Muzyka, Chemistry, Centre College

David Toth, Computer Science, Centre College

Abstract

SARS-CoV-2 is the positive-sense RNA virus that causes COVID-19, a severe respiratory infection that has had a catastrophic impact on the daily lives of billions. SARS-CoV-2's non-structural protein 5 (NSP 5), otherwise known as the main protease (MPro) or 3Cl-like protease, is essential for its pathogenesis. As it processes 12 of the 15 nonstructural proteins in SARS-CoV-2's open reading frames (ORFs), inhibiting MPro will likely induce an antiviral effect in humans. Known inhibitors were docked with MPro and analyzed to qualitatively assess MPro's active site using computer software (PyMol for preparation and AutoDock Vina in AutoDock Tools for docking calculations). After a qualitative determination of MPro's active site in AutoDock Vina's coordinate system, MPro was docked to several million small molecules in the ZINC database, as well as a set of newly discovered chalcones. Multiple small molecules with binding affinities similar to those of potential inhibitors within the active site were identified.

Quantification of Hydroxyl Radical ($\cdot\text{OH}$) During the Ozonolysis of Syringaldehyde in Water

Mia Todd, Junior, Chemistry, University of Kentucky

Marcelo Guzman, Chemistry, University of Kentucky

Reagan Patton, Chemistry, University of Kentucky

Abstract

Phenolic aldehydes, commonly found in wastes from the production of bourbon can limit anaerobic digestion, causing harm to the environment when released. Ozonolysis is known to enhance the degradation of organics during wastewater treatment, but little is understood about the complex oxidation reactions taking place simultaneously. The production of hydroxyl radical ($\cdot\text{OH}$) has proven to be a driving reaction alongside the ring opening mechanisms of ozonolysis. To explore the effect that hydroxyl radical has on the degradation of wastewater, quantification of hydroxyl radical is conducted here using 4-hydroxybenzoic acid (4-HBAcid) scavenger reactions that produce 3,4-dihydroxybenzoic acid. Experiments used solutions containing 0.05-1 mM of 4-HBAcid and 1.0 mM of syringaldehyde (SA) at pH 8.0 ± 0.1 . An ozone generating system was used to deliver 1000 ppm of ozone gas through a coarse sparger into a 250 mL reactor containing the phenolic solution. Ultraviolet-visible spectroscopy was used to monitor the absorbance of the solution throughout the oxidation alongside high-pressure liquid chromatography (HPLC) analysis for the quantification of 3,4-dihydroxybenzoic acid. The work enabled a method for the quantification of 3,4-dihydroxybenzoic acid, and in turn to report the production of hydroxyl radical during the complex oxidations studied.

Tuning the Optical Properties of π -Conjugated Molecules Through Machine-Informed Design

Parker Sornberger, Senior, Chemistry, University of Kentucky

Chad Risko, Chemistry, University of Kentucky

Abstract

While organic π -conjugated materials demonstrate utility in energy generation and storage, lighting, transistors, sensors, and other optical and electronic devices, designing a new molecular material with precise properties for a specific application requires the exploration of a vast chemical space. Molecular generative models show efficacy for in silico property prediction and design of drug-like molecules. Given this success, these models have a natural extension to the design of π -conjugated molecules. Here, we discuss the development of generative normalizing flow models to tune the optical properties of π -conjugated chromophores. The models are trained on the more than 25,000 chromophores and points of optoelectronic data from the Organic Crystals in Electronic and Light-Oriented Technologies (OCELOT) database. The generative models focus on molecules that can be of interest for singlet fission and can quickly generate structures with the aim of tuning the energy gaps between low-lying singlet and triplet excited states. The model optimizes these gaps through sampling a learned chemical space and uses pretrained message passing neural networks trained on the optoelectronic data from OCELOT to predict the gap between a molecule's low-lying singlet and triplet excited states. Results from the generative models are verified via high-throughput density functional theory (DFT) and time-dependent DFT (TDDFT) calculations to obtain their optical transitions and frontier molecular orbital energies. Though the models here focus on robustly tuning optical transitions, the methods can be transferred to optimize additional electronic properties.

Retention of Periodic Table information over time

Carson Sims, Senior, Chemistry, University of Kentucky

Stephen Testa, Chemistry, University of Kentucky

Abstract

Memorization plays an important role in the education process, in many cases, it is the only way to retain certain information. However, mass memorization over a short time frame may not be the most effective for sustained knowledge retention. This strategy is often referred to as “cramming.” The purpose of this research project is to investigate the capacity at which students can retain the names and symbols from the periodic table over the course of a nine-week period. To accomplish this goal, a survey was prepared, and students were only allowed to study the names and symbols of the periodic table for the first two weeks. Weeks three through nine were spent taking periodic surveys to assess the retention of the information over time. From this project, it is expected to see a clear trend in the memorization capabilities of college students.

Impacts of Distractions on Heart Rate in Chemical Education

Sam Hillman, Junior, Chemistry, University of Kentucky

Stephen Testa, Chemistry, University of Kentucky

Victor Okuo, Kinley Jarvis, Chemistry, University of Kentucky

Abstract

Learning chemistry is a challenge to many students, especially in the day and age of endless distractions. However, as of today, there have been no published studies in the field of chemistry to determine the impact that distractions have on students.

Phones are an obvious distraction, which has been tested in the field of mathematics, but there are also others such as a sudden loud noise, talking nearby, and a change in lighting. As indicated in previous research, increased heart rate can be correlated with levels of distraction, so we effectively used an electrocardiogram heart rate monitor to quantitatively determine the heart rate of individuals completing a chemistry question set with and without being distracted. While the methodology is still in progress, our preliminary results will be shown on the poster.

Stabilization of Pentacene For Use in Photovoltaic Cells

Mason Reeves, Sophomore, Chemistry, University of Kentucky

John Anthony, Chemistry, University of Kentucky

Carl Thorely, Center for Applied Energy Research, University of Kentucky

Abstract

Moving into the future, it is vital that sources of energy alternate to fossil fuels be explored in order to both slow down global warming and decrease the over utilization of our dwindling natural resources. One method of improving our future energy generation capabilities is to improve the efficiency of solar panels via the addition of a photomultiplier layer. TES pentacene is a molecule with potential to be useful in this role, but the fact that it degrades upon exposure to light limits said utility. It is believed that this degradation is caused primarily by the formation of an endoperoxide. There is potential to stabilize TES pentacene through the addition of various functional groups. By synthesizing different pentacenes with various functional groups attached, exposing them to light and then examining them via UV-vis analysis at regular intervals in order to establish the rate at which they decay upon exposure, we are able to discover which functional groups serve to improve the stability of the pentacene. We also intend to design a means of conducting this same experiment under an inert nitrogen atmosphere, since, if the suspicion that endoperoxide formation is the primary means of degradation is correct, we should see greatly decreased degradation of the molecule when it does not have access to oxygen. We also will be testing these same materials at various temperature, both to help in establishing trends in their reactivity that may then inform future research and because temperature reactivity will inform the conditions under which it can be used as a photomultiplier layer for solar cells.

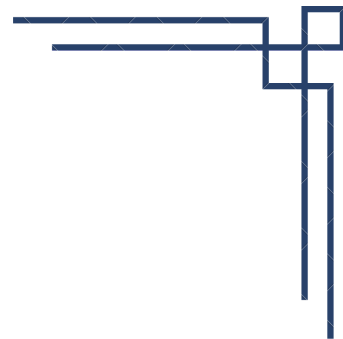
Cyclometalated Gold(III) Dithiocarbamate Complexes Elicits Potent Anticancer Activity in Cancer Cells

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Abstract

The design of stable metal-based complexes is central to the development of new anticancer drugs. In this work, we report on the facile synthesis of two classes of Au(III) dithiocarbamate complexes with differing degrees of cyclometalated frameworks; Au 1-4 have a phenylpyridine Au(III) framework while Au 5-6 bear a biphenyl Au (III) framework. The impact of cyclometalation on the pharmacodynamic properties of these classes of Au(III) complexes were determined using electrochemical, spectroscopic, and biological experiments. The electrochemical behavior coupled with LCMS stability studies in L-glutathione indicates that complexes with the biphenyl backbone demonstrate enhanced stability relative to complexes with phenylpyridine backbone. It was observed that the improved stability of the biphenyl Au(III) dithiocarbamate complexes altered their cytotoxicity as they showed reduced cytotoxicity compared to phenylpyridine Au(III) dithiocarbamate complexes. This result suggests that the cytotoxicity of phenylpyridine Au(III) dithiocarbamate complexes may result from its reduction to a more cytotoxic gold(I) complex in cells whereas the more stable biphenyl Au(III) dithiocarbamate is not subject to reduction and shows minimal cytotoxicity. Furthermore, the degree of cyclometalation affected mitochondria oxygen consumption rates. Seahorse data reveals that phenylpyridine Au(III) complexes inhibit OCR significantly in a concentration dependent manner compared to the biphenyl Au(III) complexes that show no inhibition. This work provides a basis for the development of future anticancer Au(III) complexes.



Quality Variations in Thyrotropin Alfa

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Abstract

Thyrotropin alfa is a prescription injectable drug containing human thyroid stimulating hormone (TSH). It's used with or without radioactive iodine to identify thyroid disease in patients with a certain type of thyroid cancer. Intra-lot and inter-lot variability in the spectra of Thyrogen® was detected in the Drug Quality Study (DQS) at University of Kentucky, as Fourier transform near-infrared spectrometry (FT-NIR) was used to scan through the bottom of the vials. 11 vials of 30 (36.7%) sampled from lot BY0484 appeared 31.7 multidimensional SDs from the others, suggesting that it represents a different material. Spectra of 30 vials from 4 lots in the spectral library contained 5 vials (16.7% of the total) that were outside the main group (79.6 SDs using a subcluster detection test), suggesting that the 5 library vials also contain differing materials.

Matrix Isolated FTIR Spectrum of 2,2,3,3,3-Pentafluoro-1-propanol

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Abstract

2,2,3,3,3-Pentafluoro-1-propanol (PFP) is used in many chemical reactions, including but not limited to, creation of unsaturated amines, detection of biochemicals like serotonin, and generate many different fluorinated compounds. PFP is composed of 5 fluoro-groups with a rotating hydroxyl group that can produce multiple conformers. Two conformers of PFP have been identified in gas phase by Xu et al.¹ using cavity and chirped pulse FTMW spectrometers, and conformational properties of PFP should affect the results of the reactions. In this study, matrix isolation FTIR and computational methods at both B3LYP/6-311++G(d,p) and MP2/6-311++G(d,p) levels were used to investigate the conformers of PFP.

1B. Wu, et al. 2,2,3,3,3-Pentafluoro-1-propanol and its dimer: structural diversity, conformational conversion, and tunnelling motion. *Phys. Chem. Chem. Phys.*, 2022, 24, 14975

The Thermoelectrical Performance of Blue-3 Polymer

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Abstract

The last couple of years have seen a significant increase in the amount of research conducted on organic semiconductor polymers. Some of the applications are towards converting heat to electricity or improving the performance of circuits with polymers. Polymers are known to exhibit different characteristic electrical performances based on the different counterions incorporated into the doped films. The experimentation of this presentation involves using blue-3, which the Jianguo Mei group makes at Purdue university. It is a poly(2,3 ethylenedioxythiophene,co-3,4-propylene dioxythiophene) derivative polymer. The objective is to understand how the counterions impact the electrical properties of doped blue-3 films. The counter ions that were used to increase the electrical performance of the film the polymer Blue-3 include Lithium bis(trifluoromethanesulfonyl)imide [LiTFSI], Tetrakis[3,5-bis(trifluoromethyl)phenyl]borate [BARF], and Lithium tetrafluoroborate [LiBF₄]. Sheet resistance measurements allowed for the electrical characterization of the polymer and afterwards thickness measurements were obtained of the doped films in order to determine how resistive the polymer was. Afterward, absorbance measurements were obtained to characterize the spectrum of blue-3 given the conditions of the counter ions. From this work, it was observed that the use of different counterions significantly improved the thermoelectric and conductive performance of blue-3 polymers.

Exploring Conformational Dynamics in Electron Transfer Flavoproteins from *A. Fermentans*

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Abstract

Electron bifurcation is an integral part of life, from Peter Mitchell's Q Cycle to the production of diatomic hydrogen in some methanogens. Bifurcation is exigent because it couples an endergonic reaction, such as ferredoxin in anaerobic bacteria, with exergonic processes, such as the reduction of much higher potential compounds. Fully understanding the process by which this occurs is important to our understanding of life, and as a potential means of creating more efficient industrial catalytic reactions. The goal of this research is to investigate conformational dynamics of the electron transfer flavoprotein found in *Acidaminococcus fermentans*, which gates flavin bifurcation and couples the reduction of ferredoxin with the more favorable reduction of Crotonyl-CoA. We are exploring various conformations of the ETF in solution via fluorine NMR. By replacing residues at key sites in the protein with a total of three fluorinated tryptophans and then using fluorine NMR, we will be able to observe and characterize the protein. So far, we have successfully demonstrated soluble production of the modified protein and are synthesizing it in larger quantities via NMR.

Leveraging Artificial Intelligence in the Characterization of Non-Small Cell Lung Cancer

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Abstract

Despite decades of research, lung cancer remains one of the world's deadliest afflictions, with a 5-year survival rate of only 28%. While recent advances in immunotherapy have offered hope to many, there is still a pressing need for additional treatment options. Epigenetic modulators, or drugs which alter the structure of chromatin in order to induce variations in gene expression, are one possible avenue for this advancement. In the case of non small cell lung cancer (NSCLC), it has been reported that a key epigenetic regulator, the EZH2 subunit of the Polycomb Repressive Complex 2 (PRC2), is overactive. Typically, EZH2 acts to catalyze the trimethylation (me₃) of lysine 27 loci on histone 3 tails (H3K27), which then renders the associated genes unavailable for transcription. Unfortunately, many of the molecules necessary for immune self-surveillance are influenced by H3K27me₃, causing EZH2 to take on a pathogenic role in tumor proliferation, though we do not fully understand the mechanisms involved.

In this experiment we utilized the HALO® artificial intelligence (AI) from Indica Labs to compare samples from 216 NSCLC patients. The tissue was stained for 6 markers, EZH2, H3K27me₃, B2M and HLA-DR,DQ,DP (representing the antigen presentation machinery MHC I and II, respectively), PD-L1 (programmed death ligand-1) and CBS (an upstream determinant of methyl availability), with the goal of determining how epigenetic regulators impact immune signaling status. Interestingly, we found no significant correlation between H3K27me₃ levels and EZH2 expression, and what's more, the other markers were discovered to have positive associations with H3K27me₃. This is in direct contrast to the expected model and strongly suggests that additional inquiry is needed. To that end, next steps include supplemental training of the AI to ensure accurate reporting and an exploration of gene expression patterns in public databases to further validate the activity of these molecules.

Coevolution of Histidine Kinase and Partner Response Regulator Amino Acid Residues Within the Two Component System

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Ryan Cheng, Chemistry, University of Kentucky

Abstract

Amino acid coevolution refers to the correlated amino acid identities between residue positions within a protein or protein complex. These correlations reflect the maintenance of residue interactions over the course of natural selection. In this work, we identify and quantify the coevolving residues between proteins from their sequence data (multiple sequence alignments) using a statistical approach called Direct Coupling Analysis (DCA).

We examine the well-studied bacterial two-component system (TCS), which consists of a histidine kinase and its partner response regulator. We build three separate coevolutionary models: (1) a model of the kinase sequences alone, (2) a model of the response regulator sequences alone, and (3) a model of the kinase and response regulator where the sequences of the partners are concatenated. We examine the differences when DCA predicts coevolution of individual proteins (1 and 2) compared to when a complete model of coevolution (3) is built. This would help us to better understand how robust the predictions of DCA are for individual proteins if knowledge of partner interactions are not known.

Optimization of Antigen Retrieval on Free-Floating PFA-Fixed Mouse Brain Tissue

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Chris Richards, Chemistry, University of Kentucky

Lydia Sanders, Ryan Shahidepour, Adam Bachstetter, Spinal Cord and Brain Injury Research Center, University of Kentucky

Abstract

Tissue fixation is necessary for preservation post-mortem to stabilize the structures of the cell and prevent protein loss through cross-linking. Even milder preservatives, such as paraformaldehyde (PFA), rely on cross-linking as the main mode of preservation across tissue. However, this limits the signal intensity when treating for antigens during immunohistochemical processes. Fortunately, this process can be reversed through heat induced antigen retrieval. Since antigen retrieval is not typically used for PFA-fixed tissue our goal was to optimize the process of antigen retrieval and determine which antibodies would benefit from the treatment. Free-floating sections of PFA-fixed mouse brain tissue were heated in a heat block at various temperatures and times to determine optimal conditions. Trials were run at 60, 65, 70, 75, and 80 degrees Celsius to determine an optimal temperature. At temperatures higher than 80 C the tissue wrinkled significantly. At temperatures higher than 90 C, the tissue started to dissociate completely and was unusable. At 75 degrees C, trials were run for 10, 15, 20, 25, and 30 minutes to determine optimal time. After determining preferable treatment conditions, trials were run on 5 common antibodies; IBA1, GFAP, 6E10, APP and CD45.