18th Herty Medalist Undergraduate Research Symposium

Poster Presentation Abstracts

September 22, 2023

1:30-5:00 pm

Georgia Gwinnett College

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Georgia Gwinnett College welcomes presenters and attendees from over 15 institutions with regional, national and international representation.

ANALYTICAL CHEMISTRY (AC 1)

Presenter: Callie Goins
PI: John Reynolds (Georgia Institute of Technology)
Co-Authors: D. Eric Shen, Austin L. Jones and Anna M. Österholm
Title: Investigating User-Controlled IR Switching Capabilities of Dioxythiophene-Based Conjugated Polymers

Electrochromic materials that can dynamically switch between a highly transmissive and a highly absorptive state in response to an applied voltage in the visible, near-infrared, and mid-infrared regions of the electromagnetic spectrum are of interest due to their potential application in military camouflage, transportation, and traffic visualization. Specifically, developing materials with large optical contrasts in the 3-5 µm and 8-12 µm wavelength ranges would allow for on-demand switching at wavelengths where IR detectors operate. Conjugated polymers are examples of organic materials whose absorption properties in the visible wavelength range can be modulated electrochemically; however, few have been studied to exhibit large optical contrast in the mid-IR region. Here, we explore the mid IR-switching capabilities of a series of dioxythiophene-based conjugated polymers divided into three classes: donor-acceptor, alkyl side chain, and oligoether side chain. While these polymers have been widely explored for their visible color switching properties, little existing work has been done to investigate their mid-IR switching properties. These systems were selected based on their strong and stable electrochromic performance in the visible range and reversible switching for hundreds to thousands of switches, both of which are important properties as mid-IR switching materials.

First, we studied the IR spectra of the oxidized and neutral states of polymer thin-films (200-500 nm) spray-coated onto gallium arsenide. These thin-films demonstrated strong contrast in both the 3-5 µm range and the 8-12 µm range. Here, the donor acceptor polymers had the smallest contrast, followed by those with alkyl side chains, with the polymers with oligoether side chains having the largest contrast. Next, prototype reflective devices were constructed, demonstrating significant contrast up to around 60% in the 3-5 µm range at low voltages (± 1 V). We propose that these materials are promising candidates for applications requiring on-demand and user-controlled adaptive mid-IR switching.

ANALYTICAL CHEMISTRY (AC 2)

Presenter: Joseph Paul
PIs: Vivian Mativo and Thaer Almashikee (Georgia State University)
Title: Determining the Nitrate Ion Content in Green Leafy Vegetables

The nitrate ion (NO_3^-) is abundantly found in green, leafy vegetables like arugula, spinach, and cilantro. This naturally occurring ion offers health benefits by enhancing oxygen uptake and blood circulation when consumed. However, caution is required during the preparation of nitrate-rich foods, as excessive heat can trigger the conversion of nitrates into nitrosamines, potent carcinogens associated with tobacco products. Notably, this concern predominantly pertains to processed meats rather than vegetables. Thus, embracing a diet rich in fresh vegetables is paramount due to their multifaceted advantages.

Efficient quantification of nitrate concentrations is facilitated by an ion-selective electrode designed for nitrate ions, employing a polymer membrane sensor. The sensor's liquid membrane comprises ion exchangers with sensitivity to nitrate ions, enabling precise detection. Alternatively, in cases where initial equipment malfunction occurs, Beer's Law emerges as an alternative method. This principle establishes a direct relationship between absorbance and concentration. By employing solutions of known nitrate concentrations and measuring absorbance through spectrophotometry, the nitrate content of vegetable solutions can be estimated.

The overarching aim of this research is to ascertain the nitrate concentrations in diverse green vegetables. Moreover, the study delves into potential variations in nitrate concentration between organic and standard samples of the same plant species. This investigation contributes to a more profound scientific understanding of the nutritional composition of vegetables and underscores the importance of informed dietary choices.

ANALYTICAL CHEMISTRY (AC 3)

Presenter: Ben Kittleson
PI: Cassandra Quave (Emory University)
Co-Authors: Isabel Daher, Lewis Marquez and Sunmin Woo
Title: Isolation of Anti-Acne Compounds from *Callicarpa americana* Leaf Extracts

Cutibacterium acnes is a Gram-positive bacteria that causes the skin infection known as acne vulgaris, which is common in teenagers. Antibiotic-based methods of treating such infections have led to increasing rates of resistance in *C. acnes*, and new methods of treating such infections are increasingly needed. *Callicarpa americana L.* is a shrub native to the Southeastern US that has documented uses in Native American traditional medicines. This project aims to continue previous work that investigated the antibacterial properties of extracts from *C. americana* leaves and identified a fraction with strong inhibitory properties against *C. acnes* and low cytotoxicity against human keratinocyte cell lines, which was yielded from a 95% ethanol maceration and modified Kupchan partitions in ethyl acetate. Further fractionation of this partition previously identified a novel clerodane diterpene compound (12(S),16ξ-dihydroxycleroda-3,13-dien-15,16-olide) which demonstrated an ability to re-sensitize methicillin-resistant *Staphylococcus aureus* to beta-lactam antibiotics. Impure extract 649C-F13-PF4-SF5-sF4 was identified from previous work using a combination of NMR, GC-MS, and growth-inhibition assays as an impure fraction with potential anti-acne activity containing the clerodane diterpene compound. This fraction is currently being purified using a mixed-solvent crystallization method to isolate the pure compound for antibacterial testing. Here, we present the findings of continued isolation studies on 2745C-F2, 2745C-F4, and using preparatory HPLC, NMR, and mass spectrometry towards the identification of bioactive compounds to target *C. acnes* infection.

ANALYTICAL CHEMISTRY (AC 4)

Presenter: Alexander Smiarowski
PI: Isaac Agyekum (University of North Georgia)
Title: Catalyst-Free Gas-Phase Esterification of Fatty Acids *via* GC-MS

GC-MS analysis of fatty acids necessitates the conversion into their corresponding esters. However, typical esterification methods require various catalysts. This work presents evidence for the gas-phase catalyst-free esterification of fatty acids, further validated by characterizations of methyl and butyl esters of saturated fatty acids from Joro Spider web extracts.

ANALYTICAL CHEMISTRY (AC 5)

Presenter: Grant Williams
PI: Kevin Bucholtz (Mercer University)
Title: Portable Spectroscopies as Next Generation Non-Destructive Inspection of Advanced Aerospace Materials

With advanced materials such as bismaleimide (BMI) / carbon fiber composites paving the way for aerospace engineering of next-generation aircraft – effective protocols are needed for the determination and analysis of the performance of these materials in corrosive or heat-stressed environments. New reports suggest that some of the newest air frames produced contain at least 32% graphite / BMI or epoxy resin-based materials. The complexity and breadth of these advanced materials demand development of advanced non-destructive inspection (NDI) methods to prevent, monitor, and identify degradation. Handheld portable spectroscopic analysis is beginning to be examined as a Next Generation NDI technique for advanced materials and composites. Infrared (IR) and Raman spectroscopies have been used to examine heat treated BMI / carbon fiber samples and thermoplastic urethanes after UV accelerated weathering. Our results show that mobile IR spectroscopy is a reliable approach as an accurate, portable, NDI method for chemical analysis of advanced materials and demonstrates the potential for application of portable spectroscopies as next-gen NDI technologies.

ANALYTICAL CHEMISTRY (AC 6)

Presenter: Farah Haddad
PIs: Nicole Hollabaugh & Andrew Thomas (University of North Georgia)
Co-author: Haley Menees
Title: Cloud Chasing: Capturing E-Cigarette Vapors for GC-MS Analysis

E-cigarette usage continues to increase among middle and high school students, despite public health efforts and market regulations set forth by the FDA. As a result, vaping-associated pulmonary injuries have also risen sharply, demonstrating the dangers posed to the growing population of young users. Studies have shown that acetals are present in e-liquids and e-vapors, though not listed as ingredients, and have been linked to certain respiratory and cardiovascular toxicological effects. E-liquids are comprised of three main components: (1) a solvent system containing a mixture of propylene glycol (PG) and glycerol (GL), (2) fragrant aldehydes that serve as flavorants, and (3) salt-based nicotine. The flavorant aldehydes and solvent system undergo acetalization upon addition, yielding a unique set of PG- and GL-aldehyde acetals that can be transferred from the e-liquid into its aerosol form. Previous stages of this project evaluated the reaction dynamics in simulated e-liquids among cherry and tangerine e-liquids. Time-lapsed studies suggested that significant acetal formation occurs within 24 hours following addition of several different aldehyde flavorants. As the next step in the project, vapor puffs from an e-cigarette will be collected into an air-tight modified flask setup designed for this experiment, in order to assess the presence in these vapors of the aforementioned acetal products. These collected vapors will then be injected into a GC-MS for content analysis. The initial method development will entail the development of the modified flask for collection of the sample; the development of the experimental conditions; and preliminary results of the study.

ANALYTICAL CHEMISTRY (AC 7)

Presenter: Xavier Simpson
PIs: Zach Kennedy and Michelle Fenn (Pacific Northwest National Laboratory)
Title: Fused Filament Fabrication Using Metal Additive Material

In an effort to investigate viable options for low-cost Metal Additive Material, a few dozen trials were conducted to determine reliable formats to follow when producing filament. Filament is the combination of inorganic and organic materials fused together and then manufactured as a thin flexible strand.

All trials were conducted using a micro-compounder. Metal-infused filament requires a handful of ingredients and proper conditions in order to produce a printable strand of material. Adjusting the ingredients and conditions for filament can change the overall performance of a strand. Altering methods of extrusion is often the best way to determine a batch's reliability.

ANALYTICAL CHEMISTRY (AC 8)

Presenter: Lucas Brewer
PI: Shahab A. Shamsi (Georgia State University)
Co-Authors: Glen Murray, Claude D. Mbemba, Young B. Kim, A. Mezencevova and M. Henary
Title: Introducing a Forensic Chemistry Hub at Georgia State University

This project aims to develop a forensic chemistry program at Georgia State University (GSU) that focuses on collaborative, cross-discipline initiatives between the Department of Criminal Justice, and the Department of Chemistry at GSU as well as with the Georgia Bureau of Investigation (GBI). The students and faculty at GSU are currently engaged in beta-testing studies to design the Forensic Chemistry lecture and lab courses that we plan to offer in Spring 2024.

Forensic chemistry is the application of chemistry in the study of evidence in criminal or civil cases. The designed 3-credit hours lecture and 2-credit hours laboratory courses provide an opportunity to present, discuss, and integrate chemical science with forensic. We intend to develop a forensic hub to provides opportunities for students on accurate, reliable, cost-effective, and rapid methods for the identification, analysis, and interpretation of forensic evidence. The developed lecture and laboratory course assumed that students have completed their basic learning in organic, physical, and organic chemistry and have their basic math skills. After reviewing metrology, statistics, and significant figures, the students will apply their learning of foundations in chemical separations, mass spectrometry, and molecular and atomic spectroscopy in forensic evidence cases. In addition, the students will apply both basic analytical methods (such as planar chromatography, and UV-Vis spectrophotometry) as well as modern analytical methods such as gas chromatography-mass spectrometry (GC-MS), liquid chromatography-mass spectrometry (LC-MS), as well as capillary electrophoresis-mass spectrometry (CE-MS) for analyzing athlete poison, alcohol, and drug overdose, quality of gasoline and essential oils as well as arson investigations.

The format of the two courses is based on classroom lectures, e-videos, laboratory exercises, case study discussions, and several guest speakers on select topics in forensics science. This poster presents some representative examples of course content and beta-testing of the laboratory content. We present data that was recently obtained by engaging a group of four chemistry juniors and senior students who participated in eye-tracking studies in the forensic chemistry laboratory. Our proposed program is expected to attract a lot of interest among students who intend to begin their careers in forensic science, criminal investigations, and laboratory analysis of forensic evidence, as well as those who plan to pursue graduate study in forensic science.

ANALYTICAL CHEMISTRY (AC 9)

Presenter: Benjamin Shepard
PI: Simon Mwongela (Georgia Gwinnett College)
Co-Authors: Ajay Mallia and Neville Forlemu
Title: Novel Method Development for Separation of Cyclotides Using Capillary Electrophoresis

Method development and optimization of elution parameters for the separation of three cyclic peptides (Vancomycin, Gramicidin C and Cyclosporin A) was performed using capillary electrophoresis (CE). Currently to the best of our knowledge there is no reported CE method for the separation of cyclic peptides or cyclotides. The development of such a method would be beneficial for investigating the aggregation properties of individual cyclotides or a mixture of cyclotides in various separation media such as micellar and lipid bilayer environments. Some promising preliminary results have been obtained. However, the methods developed so far are not robust. Data reproducibility has remained a challenge which we have attributed to the ability of the cyclic peptides to adhere on the capillary wall and also the strong interactions that exist between the macromolecules. Further studies are being carried to addresses these challenges.

BIOCHEMISTRY (BC 1)

Presenter: Blaise Williams
PI: Mohammed Abdul Halim (Kennesaw State University)
Co-Authors: Md Ackas Ali, Kaylee Stone and Cole Bourque
Title: Multiple Ion Monitoring (MIM) Mass Spectrometry Based Protease Assay for Peptide Inhibitors Targeting the Main Protease of SARS-CoV-2

The deadly SARS-CoV-2 virus continues to represent a significant threat to the health of people across the globe, with 6.95 million deaths and 769 million infections caused by the virus. SARS-CoV-2 is a single-stranded RNA (ssRNA) virus translating 16 non-structural, 4 structural and 9 accessory proteins. Any of these proteins can be targeted for drug development, however, researchers have identified main protease (Mpro) as an important protein for viral replication. Various effective methods were developed to screen small molecules and peptides inhibitors targeting the 3CLpro. Mostly fluorescence resonance energy transfer (FRET) based assay is used to measure inhibitor affinity for the main protease. However, fluorescent assays present a shortcoming of providing false positive readings due to the background fluorescence of fluorogenic substrate interfering with the optical signal. Besides FRET, multiple ion monitoring (MIM) coupled with LC-MS can be employed as an alternation option because it provides excellent sensitivity and reliability due to its confidence on mass-to-charge ratios and does not require any chromophore. In this study, MIM based LC-MS method was used to compare substrate degradation and product formation to obtain the 50% inhibitory concentrations (IC_{50}) values for the known inhibitor, GC-376, of 3CLPro and the result was compared with FRET assay. The estimated IC_{50} of GC-376 obtained in LCMS assay was 116 nM which agreed with the IC_{50} value measured by FRET assay (180 nM). The developed MIM-LCMS method was applied for various linear and staple peptides of Temporin L which acted as the peptide inhibitor of 3CLpro. The estimated IC_{50} values of the Temporin L and its stable analogues TLP-1, TLP-2, TLP-3, and TLP3S1 obtained from LCMS assay were 18.39 μM, 6.673 μM, 2.589 μM, 22.17 μM and 304.6 nM which are comparable with FRET assay (38.80 μM, 11.4 μM, 11.5 μM, 7.4 μM and 574 nM).

BIOCHEMISTRY (BC 2)

Presenter: Mahdi Ghasemi
PI: Mohammed Abdul Halim (Kennesaw State University)
Title: Green Solid Phase Peptide Synthesis Using Deep Eutectic Solvents

Solid-phase peptide synthesis (SPPS) offer many advantages as it is faster due to fewer steps, easy separation of excess reagents and by-products, and very cost-effective compared to the liquid-phase peptide synthesis. To synthesize a peptide in SPPS, three key steps need to be fulfilled: i) resin swelling, (ii) deprotection of the protected group, and (iii) coupling reaction to form the amide bonds. The whole process significantly relies on the usage of sizable amounts of solvent for filtration and washing of the resin after each step of deprotection and coupling. The solvent plays a pivotal role on swelling of resin, dissolving deprotection reagents, Fmoc amino acids, and coupling reagents and removing excess reagent and by-products through extensive and repetitive washing. The most common solvents used for solid phase synthesis are N,N-Dimethylformamide (DMF), N-Methyl-2-pyrrolidone (NMP) which have reproductive toxicity. As hazard solvents represent 80−90% of the total waste mass in SPPS process, hence, using green solvents or alternative ways to diminish or recycle solvents are of great interest.

Deep eutectic solvents (DESs) have emerged as green solvents with superior properties over conventional solvents. DESs are more synthetically accessible with negligible vapor pressure, typically nontoxic, biodegradable, economical, and suitable for biological applications. Moreover, DESs can provide a superior reaction medium resulting in numerous advantages, including minimizing waste formation, improving the atom economy. In this study, various DESs were used to synthesize tripeptides. Our preliminary results showed that
Choline Chloride:Glycerol DES was successful for swelling, deprotection, coupling but not for amino acid dissolving and washing. This replaced 50 mL of toxic DMF and makes it 48% green. On the other hand, Menthol:Thymol DES was able to dissolve amino acids as well as swelling, deprotection, washing, and partial coupling. This replaced 100 mL of toxic DMF and makes it 95% green. This study showed that DESs have potential to replace the toxic DMF solvent in SPPS.

BIOCHEMISTRY (BC 3)

Presenter: Zetao (Tommy) Pan
PI: Hai Dang Nguyen (University of Minnesota)
Co-Author: Benjamin Hanson
Title: Functional Impact of RNaseH1 Phosphorylation on R-Loop Resolution

Myelodysplastic syndromes (MDS) are a group of heterogeneous disorders that affect the production of red blood cells. Over half of MDS patients carry splicing factor mutations that cause an increase in R loops, a three-stranded nucleic acid structure containing a DNA:RNA hybrid and a ssDNA. While R-loops are a part of normal cellular function, an accumulation of R-loops can lead to genomic instability and promote cell death. The goal of this project is to characterize regulatory mechanisms of RNaseH1, a R-loop specific hydrolase.

Previous experiments determined that Replication Protein A (RPA) enhances RNaseH1 R-loop recognition and stimulates RNaseH1 activity. We hypothesize that RNaseH1 phosphorylation promotes its interaction with RPA. To investigate this, human RNase H1 purified from *E. coli* was used to evaluate its function in biochemical assays. Cy3-Quencher fluorescence assay revealed that both RNase H1 phospho-dead and phospho-mimetic mutants have similar rates of enzymatic activity on degrading synthetic DNA:RNA hybrids *in vitro*. However, preliminary data remains inconclusive of the role RNaseH1 phosphorylation plays with its interaction with RPA.

Future experiments will further detail the role of phosphorylation in the regulation of RNaseH1 activity with the intention of investigating the therapeutic potential of targeting RNaseH1 to treat MDS patients harboring splicing factor mutations.

BIOCHEMISTRY (BC 4)

Presenter: Kevin Li
PI: Yong Wan (Emory University – School of Medicine)
Co-Author: Junlong Chi
Title: Development of MGAT1 Inhibitors Based on a Novel High-Throughput Screening System to Promote Breast Cancer Immunotherapy

Triple-negative breast cancer (TNBC) is a highly aggressive subtype of breast cancer that presents high metastasis rates and poor survivability. Although immune checkpoint blockade (ICB) therapy sheds light on TNBC treatment, only a small fraction of TNBC patients can benefit from it and the drug resistance has become a growing concern. Therefore, there is an urgent need to develop novel targeted therapies synergizing with ICB therapy. Accumulating evidence has demonstrated that N-glycosylation plays a critical role in the anti-tumor immune response. However, very few specific glycosyltransferase inhibitors have been successfully developed due to the structural complexity associated with the glycosylation process and the lack of specific methodologies to study it.

This project aimed to develop a novel *in vitro* functional-based high-throughput screening system to discover specific inhibitors targeting MGAT1, a glycosyltransferase strongly correlated with cancer progression, metastasis, and immunotherapy unresponsiveness in cancer patients.

This system incorporates four key components: (1) biosynthesized Man5GlcNAc2Asn glycans specifically recognized by MGAT1; (2) the UDP-N-Acetylglucosamine sugar donor; (3) the UDP-Glo Glycosyltransferase Assay kit which includes UDP detection reagent; (4) functional MGAT1 protein. Under *in vitro* conditions, MGAT1 will attach the N-Acetylglucosamine sugar onto the substrate glycan and release UDP into the solution. The UDP concentration will be characterized with UDP detection reagent in the form of luminescence as an indicator of MGAT1 function. However, when an inhibitor interferes with MGAT1 function, less UDP will be freed, and less luminescence will be detected. By detecting the amount of UDP released from the enzymatic reaction, this system can quantify MGAT1 enzymatic efficacy with high sensitivity.

Based on initial dose- and time-dependent experimental data, we have determined the ideal reaction conditions and confirmed that our system is able to convert enzymatic MGAT1 function into luminescence. Utilizing our validated conditions, we conducted a primary screening with 400 compounds and discovered a leading compound (#72) with an IC_{50} value of 0.64 ± 0.095 μM that may serve as a potential MGAT1 inhibitor.

We have developed a high-throughput screening system that can characterize the catalytic function of MGAT1 with quantifiable luminescence. The preliminary screening has discovered a leading compound that may inhibit MGAT1 enzyme function. The efficacy of leading compounds will be further validated with *in vitro* and *in vivo* studies. On the one hand, this system incorporates a novel functional-based approach to discover more promising inhibitors compared to traditional protein-protein or protein-drug interaction systems. On the other hand, this system will be applied to target numerous therapeutic targets found across N-glycosylation pathways.

BIOCHEMISTRY (BC 5)

Presenter: Amani Talbert
PI: Deva Chan (Purdue University)
Co-Authors: Dhulika Ravinuthala, Aritra Chatterjee and Janice Evans
Title: Development and Application of Atomic Force Microscopy (AFM) and Imaging Tools Towards the Measurement of Oocyte Mechanical Behavior

The mechanical properties of cells contribute to several different aspects of cell physiology, including cell shape, cellular morphogenesis, orientation for cell division, and the sensing and transducing of signals associated with mechanical forces. Additionally, the measurement of cortical tension of cells is a readout of actomyosin-mediated contractility. Previous studies assessing cortical tension in mammalian oocytes using micropipette aspiration revealed changes with progression through meiosis and the egg-to-embryo transition. Our work aims to develop and apply atomic force microscopy (AFM) and imaging tools towards the measurement of mammalian egg mechanical behavior, to elucidate how determining the interactions of calcium signaling and cytoskeletal dynamics during the egg-to-embryo transition to modify the egg plasma membrane to a state that is unreceptive to sperm, resulting in a block to fertilization by additional sperm (known as polyspermy). This project will involve the collection and culture of egg cells from mice, development of methods for immobilizing these cells for AFM measurements (*e.g.* anchoring on coverslips or embedding in agarose), and testing a spherical indenter for analyses of unfertilized eggs. With these experimental parameters in place, our goal is to perform these measurements to compare unfertilized and fertilized eggs, and then fertilized eggs that have been experimentally manipulated in ways that are known to alter calcium signaling, actomyosin dynamics, and events of the egg-to-embryo transition such as the membrane block to polyspermy.

BIOCHEMISTRY (BC 6)

Presenter: Katlyn Xiong
PI: Misael Romero Reyes (Georgia Gwinnett College)
Co-Authors: Amalia Barron and Nabil Ahmed
Title: Are K-Pods/K-Cups the New Water Purifiers?

Science equipment can be quite expensive and hard to access outside of a research lab, so to make water purification more accessible to everyone, we explored low cost and efficient filtration methods. We explored everyday use items such as the K-pod coffee filter that can be found at almost any store. The purpose was to compare a variety of filtration methods using pulverized wood as the decontamination media. We observed that K-pod filtration performed better than their laboratory counterparts at removing contaminants from water.

BIOCHEMISTRY (BC 7)

Presenter: Vishrut Thaker
PIs: Angela Mabb and Dina Yakout (Georgia State Neuroscience Institute)
Title: The Effects of Conformational Changes in Tau Protein on Dendritic Spines in Primary Hippocampal Neurons

The Tau protein is critical in cellular structural regulation through microtubule stabilization. Mutations in Tau lead to neurodegenerative diseases, such as Frontotemporal dementia (FTD) and altered conformations of Tau are seen in Alzheimer's (AD). Existing mutations in the Tau protein induce conformational changes that contribute to the pathogenesis of FTD. Tau is also linked to synaptic plasticity and learning, which are negatively impacted by FTD. The aim of this study was to elucidate the impact that structural changes in the microtubule binding domain of Tau have on neuron morphology and receptor expression. Specifically, we explored the impact of a Tau mutant form (P301L) found in FTD. Spine analysis was manually conducted by measuring spine density in hippocampal neurons overexpressing GFP, GFP-tau, and GFP-P301L-tau. Additionally, we determined receptor expression by quantifying the AMPA subunit, GluA1, utilizing immunocytochemistry. Unexpectedly, our findings reveal that mutations in Tau's microtubule binding domain do not affect dendritic spine density but do diminish GluA1 levels in the dendrites and soma of hippocampal neurons.

BIOCHEMISTRY (BC 8)

Presenter: Peter Chapman
PI: Aditi Das (Georgia Institute of Technology)
Co-Author: Tiffany (Yi-Chien) Tang
Title: Elucidating the Metabolism of Lipidated Serotonin and Selected Drugs by Cytochrome P450 2U1 (CYP2U1) in Nanodiscs

Cytochrome P450 2U1 (CYP2U1) is an intriguing orphan lipid-metabolizing enzyme abundantly expressed in the thymus and brain. CYP2U1 is involved lipid metabolism that includes substrates such as long-chain polyunsaturated fatty acids, arachidonic acid and docosahexaenoic acid, as well as lipidated neurotransmitter such as N-arachidonoylserotonin. Its involvement in various diseases and pathological conditions has drawn significant attention. Mutations in the CYP2U1 gene have been linked to hereditary spastic paraplegia (HSP), a genetic neurodegenerative disorder. Additionally, altered expression of CYP2U1 has been observed in specific cancer types, such as breast cancer. Unraveling the biochemistry of CYP2U1 in terms of its role in lipid and drug metabolism holds great promise for potential therapeutic interventions in these disease states.

Our hypothesis is that there is a potential interaction between CYP2U1 and drugs used for thymus cancer treatment and antidepressants, which may modulate endogenous CYP2U1-mediated lipid metabolism. This hypothesis is motivated by the substantial expression of CYP2U1 in the thymus and brain. To investigate this, we recombinantly expressed and purified CYP2U1 in a bacterial expression system and incorporated them into nanoscale lipid bilayers called Nanodiscs. By employing UV-Vis spectroscopy, fluorescence spectroscopy, and liquid chromatography coupled with mass spectrometry (LC-MS/MS) methodologies, we explored the metabolism of lipidated serotonins and selected drugs such as sorafenib and sunitinib (targeting thymus tumors) as well as amitriptyline and fluoxetine (antidepressants).

Our findings reveal that CYP2U1 metabolizes lipidated serotonins into multiple bioactive products. Furthermore, we demonstrate favorable interactions between CYP2U1 and the different drugs using spectral binding titrations and LC-MS/MS analysis. Through modeling of CYP2U1 in Nanodiscs, we identify key residues involved in its interactions with lipidated serotonin and the selected drugs. These findings shed light on the intriguing interplay between CYP2U1 and lipidated serotonin and specific drugs, offering valuable insights for further exploration.

BIOCHEMISTRY (BC 9)

Presenter: Gabriel Perez-Perez
PI: Misael Romero-Reyes (Georgia Gwinnett College)
Co-author: Ericka Tinajero
Title: Comparing Water Technologies for Water Filtration

Louis Pasteur opened many doors for immunology and vaccinations with the idea of using resources that are more readily available. We use this theory and apply it to water filtration using wood applications. The pores of the wood act as a canal for the water to filter through while the fibers of the wood are interacting with impurities in water that is being filtered.

BIOCHEMISTRY (BC 10)

Presenter: Tong Wu
PI: Jenny J. Yang (Georgia State University)
Title: Development of A Novel Protein Based MRI Contrast Agent, hProCA32.collagen1

The overexpression of collagen is a molecular biomarker for diagnosis of chronic diseases including liver, heart, kidney diseases and multiple types of cancers. The Yang lab has pioneered a new class of protein Magnetic Resonance Imaging (MRI) contrast agent for early detections of these diseases. hProCA32.collagen1 is a Magnetic Resonance Imaging contrast agent designed from scaffold protein with a strong binding affinity to collagen. Compared to other contrast agent, hProCA32.collagen1 has high stability and binding affinity for Gd^{3+}, and also has high relaxivity values, low dose efficiency and high binding affinity to collagen. To perform biophysical characterization and preclinical applications, we need to produce large amount of this protein. The purpose of this study is to obtain and optimize expression and purification conditions of hProCA32.collagen1.

The hProCA32.collagen1 protein was expressed in *E. coli* cells and induced with rhamnose *via* the liquid LB media based on the standard operation protocols. To purify the proteins, different methods such as lysis, heating, PEI, dialysis and FPLC were used to separate other kinds of proteins. Finally, to detect desired proteins; SDS-PAGE was used to visualize the results; Bradford assays were used to determine the concentration of the proteins and ELISA and relaxometry analysis were used to determine characteristics such as binding affinity and relaxivity of the proteins.

The protein expression was successful based on the result of SDS-PAGE with an average yield of 5.33 g of cell pellets per Liter LB liquid media. The purification showed the yield of
14.21 μg of hProCA32.collagen1 protein per cell pellet. An optimal pH of 6.0 was used to purify the protein through cation exchange. The SDS-PAGE result for purification indicated the dimer and trimer of the target protein (caused by disulfide bonds) was only observed in the non-reducing gel. The proteins obtained also showed a high binding affinity of collagen and relaxivity compared to the previous reference values.

BIOCHEMISTRY (BC 11)

Presenter: Yushan Zhang
PI: Jenny J. Yang (Georgia State University)
Title: Optimized Purification of hProCA32.collagen1 for Early Diagnosis of CLDs

Liver fibrosis, characterized by the excessive accumulation of collagen and extracellular matrix proteins, is a common outcome of chronic liver diseases (CLD). Early detection of liver fibrosis is pivotal for potential reversibility and improved patient outcomes. This study addresses the pressing need for early diagnosis and noninvasive detection methods, focusing on liver fibrosis and related liver diseases.

Magnetic Resonance Imaging (MRI) is a powerful tool for assessing internal organ status, yet its effectiveness is hampered by the limited performance of existing contrast agents. To address this challenge, researchers previously developed hProCA32.collagen1, a human collagen type I-targeting protein-based contrast agent. This agent exhibits high collagen I affinity and promises enhanced efficiency in tissue targeting, allowing for reduced dosage.

This investigation centers on refining the purification process of hProCA32.collagen1, aiming for stability and purity improvements. The step SP column protocol was employed for purification. The HiTrap Capto SP ImpRes column featuring strong cation exchange chromatography resins, played pivotal role. The fractions obtained from the SP column were dialyzed for effectively removing impurities evident on gel analysis.

The study conducted purification, yielding insights into the protein's structure and quality. SDS-PAGE and Mass Spectrometry revealed the presence of the target protein at 14.5 kDa, albeit with some dimeric forms and a notable impurity at 15 kDa. ELISA results further confirmed cleavage of the targeting moiety, with decreased collagen I binding affinity in specific elution fractions. This research advances the purification protocol for hProCA32.collagen1, a promising contrast agent, offering improved prospects for early liver fibrosis detection and the broader application of enhanced protein-based contrast agents in medical imaging.

BIOCHEMISTRY (BC 12)

Presenter: Kenneth Wingate, Jr.
PI: Vincent Conticello (Emory University)
Co-Authors: Jessalyn Miller and Andrés Gonzalez Socorro
Title: Investigating the Structure and Assembly of Cannula A and Hyper2

Cannula A (CanA) is a supramolecular peptide structure that forms nanotubes. This self-assembling structure is formed by the archaea extremophile, *Pyrodictium abyssi*, as they undergo binary fission. The two resulting archaea are connected by this nanotube comprised of CanA and other components. In this work, we set out to recreate the assembly conditions for the self-assembly of CanA into nanotubes and to characterize this supramolecular structure.

The peptides that form the linkages between these hyperthermophile archaea are hyperthermostable. Protein expression was completed with *E. coli*. After protein isolation, purification, and establishing assembly conditions, the structure was characterized and imaged by transmission electron (TEM) and cryo-electron microscopy (Cryo-EM). Sequence alignment of CanA yielded the protein Hyper2 from another archaea species. Its structure showed a similar assembly mechanism as CanA.

BIOCHEMISTRY (BC 13)

Presenter: Xiaofang Ke
PI: Jenny J. Yang (Georgia State University)
Title: Advancements in Hepatic Fibrosis Detection: A Deep Dive into hProCA32.collagen1 Enhancement and Its Implications

Hepatic fibrosis, characterized by the extravagant accumulation of matrices like collagen, is rampant in a plethora of persistent liver disorders. This pathology arises from an imbalance where collagen synthesis overshadows its decomposition. Detecting such fibrosis in its nascent stage, when amendable, holds colossal therapeutic implications. While Magnetic Resonance Imaging is an esteemed modality for internal anatomical visualization, several contemporary contrast agents display tepid efficacy due to their sluggish relaxation rates, necessitating increased dosages and igniting trepidations over metallic ion toxicity. A fresh formulation from Dr. Yang's workshop, hProCA32.collagen1 - a collagen type I-focused contrast agent, offers an edge in the early recognition and evaluative study of ailments underscored by collagen type I hyperproduction, thanks to its enhanced predilection towards collagen I, warranting minimal dosage.

To enhance hProCA32.collagen, an intricate protocol was pursued. This blueprint involved rejuvenating cellular clusters, obliterating cells, instituting thermic procedures to discard unwanted proteins, expelling deoxyribonucleic acid with Polyethylenimine, molecular restructuring through redox mixtures, filtering, culminating with a dualistic Fast Protein Liquid Chromatography operation using SP and Fractogel column purifications.

Grasping the crux of protein purification is pivotal to comprehend its functional, structural, and interactive subtleties. Our exploration centered around honing the purification procedure for hProCA32.collagen1, a contrast agent. Post-optimization, the Sodium Dodecyl Sulfate Polyacrylamide Gel Electrophoresis and Mass Spectrometry analysis revealed a protein band around 14.5 kDa with intermittent dimer bands and a noticeable impurity band at 15 kDa. Enzyme-linked Immunosorbent Assay insights identified specific elutes containing fragmented protein, displaying a 12 kDa molecular weight, along with attenuated collagen I binding capability. The Fractogel SO3-M column demonstrated adeptness in partitioning these impurities.

BIOCHEMISTRY (BC 14)

Presenter: Haonian Zhou
PI: Jenny J. Yang (Georgia State University)
Title: CaSR Treated with TNCA and Its Property

Calcium (Ca^{2+}) acts as a universal messenger, assisting many organisms and cells in their biological and pathological processes. Intracellular Ca^{2+} stores, membrane channels, pumps, and/or receptors all influence Ca^{2+} levels. The Calcium-Sensing rReceptor (CaSR) is well-known for its role in calcium concentration regulation in both signaling pathways and diseases. The research presented was designed to interpret the presumed role of CaSR in the regulation of calcium homeostasis and to gain a better understanding of how cell pathways work. Multiple *in silico* and *in situ* methods were used to create a working CaSR model with several Ca^{2+}-binding sites with endogenous ambient amino acids within the CaSR-ECD that cooperatively activate the receptor.

During the presentation, efforts were made to develop new CaSR therapeutics using structure-based drug design. L-TNCA, a novel allosteric modulator discovered co-crystallized in the CaSR ECD, was used as the primary compound to make TNCA- derivatives tested in this study CaSR-mediated intracellular Ca^{2+} response was studied using fluorimetry on cell populations. To investigate the effects of the drug targets on CaSR, we modified the cell population functional assays, and the results showed that a three-ring compound was preferable for increasing CaSR activity.

BIOCHEMISTRY (BC 15)

Presenter: Jaylen Watson
PI: Juana Mendenhall (Morehouse College)
Co-Authors: Jonathan Banks and Jordan Turner
Title: Determining the Mechanical Properties of 3D Hyaluronic Scaffolds Using the Flexcell Compression System

Osteoarthritis is a degenerative joint disease that breaks down the articular cartilage in the joint, causes pain, and also affects the bone structure in the diseased area. There are costly treatments for this disease such as medication and surgery. A solution has been found in utilizing hydrogel scaffolds, which is a product of tissue engineering. The hydrogel is injected into the diseased area and begins regenerating loss tissue. But as hydrogel scaffolds are injected into the human body, it is important to make sure that these scaffolds can withstand the pressures that can be experienced by the human body. This study aims to assess the mechanical properties of the 3D printed hydrogel scaffolds and observe if they can retain their form while undergoing pressure from the human body.

Six different hydrogel samples were made, including a control sample, out of biomaterials used for tissue regeneration. After mixed and stored 24 hours, the Allevi 3D bio-printer was utilized to print hydrogel scaffold constructs for each hydrogel sample. Once dried, the scaffold constructs were loaded into the Flexcell Compression System to undergo compression testing. A structural analysis was performed on the hydrogel scaffold constructs to observe how they fared under compression.

The results showed that the hydrogel scaffolds did have the characteristic of low degradation at a certain level of compression. It was also observed that the water in samples may have caused faster degradation speeds when compared to those samples without water. To conclude, the hydrogel scaffold constructs do show potential to be able to withstand the pressures of the human body but further study is needed.

BIOCHEMISTRY (BC 16)

Presenter: Jace Lee
PI: Ajay Mallia (Georgia Gwinnett College)
Co-Authors: Joel Suazo, Byron Fisher, Neville Forlemu, Simon Mwongela and Sairam Tangirala
Title: Microwave-Assisted Extraction of Cyclotides and Purification Using HPLC

Cyclotides are plant-based cyclic peptides containing six cysteine residues that form three disulfide bonds. The present study describes the optimization of the microwave-assisted extraction of cyclotides from Australian violet (*Viola hederacea*) using water as the sole solvent. Purification of cyclotides using preparative HPLC, as well as the determination of their thermal properties using DSC and TGA, will be discussed.

PHYSICAL CHEMISTRY (PC 1)

Presenter: Jonathan Lawton
PI: Aimée Tomlinson (University of North Georgia)
Title: In Search of Non-Fullerene Acceptors Using Density Functional Theory

Narrow-band gap organic solar cells (OSCs) are an emerging interest for use in bulk heterojunction (BHJ) organic photovoltaic (OPV) active layers because OSCs have a strong absorption extending into the near-IR region. These systems are comprised of a BHJ-OPV which consists of an electron acceptor and an electron donor. Typically, fullerenes are used as electron acceptors in OSCs. However, fullerene acceptors (FAs) have weak absorption in the visible region and have a tendency for molecular aggregation which can hinder device efficiency. To combat this issue, non-fullerene acceptors (NFAs) are emerging electron acceptors that are intended to replace fullerene acceptors. These acceptors tend to have extended absorption into longer wavelengths and can form intermixed domains, giving them an advantage over their FA analogs. Here, we used density functional theory (DFT) and time-dependent density functional theory (TDDFT) at the mPW3PBE/SV level to analyze a set of systems which possess a benzo(*bis*)oxazole nucleus with a variety of aryl groups along the two axes. From our results we identified several systems which satisfy the criteria for use as an NFA in an organic solar cell device.

PHYSICAL CHEMISTRY (PC 2)

Presenter: Oliver Hvidsten
PI: Rampi Ramprasad (Georgia Institute of Technology)
Co-Author: Rishi Gurnani
Title: Li-ion Conductivity in Solid Polymer Electrolytes: Simulation-Experiment Data Fusion and Multi-Task Machine Learning

Lithium-ion batteries are the current industry standard for rechargeable batteries. These devices can be found in personal electronics, medical equipment, and electric vehicles. Recently, there has been a push to switch the commonly used liquid-state electrolyte for a solid-state electrolyte. Solid polymer electrolytes (SPEs) are one such solution for this change, but finding a chemistry that can compete with the ionic conductivity of the current liquid-state electrolytes has proven to be a complex task. In this work, we developed a machine learning model to predict lithium ion conductivity in solid polymers. Two datasets were used in this work. The first, containing 9118 data points for 169 polymers and 41 salts, was gathered from experimental research. The second, containing 6270 data points for 6042 polymers and one salt, was produced by molecular dynamics simulations. Using multi-task learning, these datasets were combined and used to train a neural network model that was able to leverage the breadth of chemistries found in the simulation dataset and the accuracy of the conductivity values in the experimental dataset. Additionally, the Arrhenius equation was encoded into the neural network's architecture to aid in learning the temperature dependence of ionic conductivity. By employing multi-task learning and encoding a known physics equation into the algorithm, we were able to develop a model that approaches experimental-level accuracy in broad chemical spaces.

PHYSICAL CHEMISTRY (PC 3)

Presenter: Shea Baldwin
PIs: Ian Krouse and Benjamin Shepler (Georgia Gwinnett College)
Title: Calculation of the Electron Affinity of Arsenic - Three Schemes

The experimental electron affinity of arsenic has been recently measured with high precision. Described here are three thermochemical schemes used to calculate the electron affinity of arsenic with the free demo server on Web MO (webmo.net). The wall time on Web MO is limited to 1 minute, thus calculations must be fast enough to complete, but also comprehensive enough to get appropriate and meaningful results. The computations were done with Gaussian 16.

Scheme 1 was a direct EA calculation $^4As + e^- \rightarrow {}^3As^-$ $\Delta E = -EA(As)$

Poor results were observed for most methods/theory. CCSD(T)/aug-cc-pVTZ, the highest method/theory obtainable under the circumstances, gave results ~20% lower than literature.

Scheme 2 was a hybrid approach

$$^4As + e^- \rightarrow {}^3As^- \quad \Delta E = -EA(As)$$
$$^3P^- \rightarrow {}^4P + e^- \quad \Delta E = EA(P)$$
$$^4As + {}^3P^- \rightarrow {}^4P + {}^3As^- \quad \Delta E = EA(P) - EA(As)$$

Since EA(P) is well established, this scheme uses both computational and experimental values to calculate EA(As). Because of its isogyric nature (same spins on both sides), this scheme appeared to 'cancel out' spin-related errors and gave good results for most methods/theory. B3LPY methods gave excellent results (within 3% of literature).

Scheme 3 involved reaction with the arsenic cation and arsenic anion to form neutral arsenic

$$^3As^- \rightarrow {}^4As + e^- \quad \Delta E = EA(As)$$
$$^3As^+ + e^- \rightarrow {}^4As \quad \Delta E = -IP(As)$$
$$^3As^- + {}^3As^+ \rightarrow 2\ {}^4A \quad \Delta E = EA(As) - IP(As)$$

This approach is also a hybrid model using both calculations and literature IP(As). Although thermochemically sound, this scheme also gave poor results. Only the B3LYP/6-31+G* result was within 10% of literature.

All calculations were completed within the 1 minute wall time, making this activity highly accessible for anyone with an internet connection. Because the calculations are completed using only atoms, input is easy and may even be done *via* smartphone. Scheme 2 has been applied to calculate other EAs of representative elements near arsenic (Ga, Ge, Se) with satisfactory results. To obtain better results, more advanced calculations that include spin-orbit coupling may be applied to correct spin-related issues involved with Schemes 1 and 3 giving improved results.

PHYSICAL CHEMISTRY (PC 4)

Presenters: Dorothea Tecar and Ethan Cook
PIs: Brynna Quarles (University of North Georgia)
Co-Authors: Rosi Gunasinghe and Nicole Hollabaugh
Title: Computational Modeling of Terpenoid, Phenol, and Benzaldehyde Derivatives as Tyrosinase Inhibitors

Tyrosinase is the rate-limiting enzyme in the production of melanin, which is responsible for skin pigmentation. Overactivity of tyrosinase can lead to increased melanin synthesis, which causes, among other things, skin hyperpigmentation. Examining the interaction between various inhibitors and tyrosinase can enhance our comprehension of how these inhibitors can be effectively employed to hinder both melanogenesis and enzymatic browning. Molecular docking investigations offer insights into the strength of binding between the inhibitor and the enzyme, the identification of enzymatic binding sites, and the affinity of different functional groups. Inhibitors exhibiting a strong binding affinity are more likely to effectively impede enzymatic activity. Although tyrosinase inhibitors are a widely studied group, this research primarily concentrates on the exploration of potential binding sites and different functional groups as inhibitors of tyrosinase, determination of their inhibition constants, assessment of the binding energies associated with each site, and analysis of the intermolecular interactions specific to each inhibitor-binding site pair. AutoDock software was utilized in this study to pinpoint binding sites and evaluate the intermolecular interactions between the inhibitors and tyrosinase.

PHYSICAL CHEMISTRY (PC 5)

Presenter: Sebastian Chu
PI: Joseph Chaiken and Paul Dent (Syracuse University)
Co-Author: Daniel Porreca
Title: Non-Invasive *in vivo* Continuous Monitoring of Real-Time Response in Peripheral Plasma Volume During a Passive Leg Raise Maneuver: Potential Method for Diminished Cardiac Output Detection

The cardiovascular system is continuously adjusting its processes to maintain homeostatic equilibrium. During congestive heart failure, the heart has an incredible ability to adjust its heart rate and signal the sympathetic nervous system to release hormones that compensate for its decreasing output. In the beginning, the heart and body compensate well enough to keep the patient's condition unnoticed, but over time, this ability does degrade and eventually cardiac output decreases. FRD/PVOH, a Raman spectrometer, focuses an 830 nm laser in the capillary beds of the fingertip using a fiber optic probe. FRD/PVOH separates scattered light as elastic or inelastic emission. FRD/PVOH takes its algorithm and calculates real-time fluctuations in red blood cell and plasma volume.

Medical practices today conduct passive leg raise maneuvers (PLR) as a fluid responsiveness test on patients for cardiac output. We are not able to modulate our heart's cardiac output on command, but we are able to adjust the blood fluid velocity of the arm as a function of external pressure. By comparing the differences in fluid responsiveness, the study hopes to link the differences as a model when comparing real patients with a diminished cardiac output versus healthy patients.

PHYSICAL CHEMISTRY (PC 6)

Presenter: Alexander Merryman

PI: Tae Song Lee (Georgia Gwinnett College)
Co-Authors: Charles Pibel, Seungjin Lee and Ying Guo
Title: The Theory and Construction of Laser-Induced Breakdown Spectroscopy (LIBS) Utilizing a Cosmetic Pulse Laser

Laser-induced breakdown spectroscopy (LIBS) has greatly increased its presence in research in recent years due to its elemental analysis capabilities. These abilities come from the laser exciting the substance, which creates a plasma cloud that can be analyzed. This plasma contains excited electrons that emit certain light wavelengths. Similar to density or the atomic number of elements, each element has unique wavelengths that can almost be used as a "fingerprint" to determine what is present in the substance. However, professional LIBS systems require resources that are neither abundant nor readily available, such as lasers built specifically for LIBS. A more accessible option is the use of a cosmetic pulse laser. Cosmetic pulse lasers are common in tattoo removal and utilize a Q-switched Nd:YAG laser with a dual wavelength of 1064 nm or 532 nm. Because the laser pulse has an energy of about 100 mJ and only lasts a few nanoseconds, the laser has high power (Power = energy/time). Similar to a professional LIBS system, certain structural elements are needed for experimentation. An enclosure that houses the laser, sample, and fiber-optic cable is needed to ensure the plasma's wavelength is measured and not that of the surrounding light. The light emitted from the excited substance is captured by the fiber optics and sent to the spectrometer (Aurora 4000) for analysis. The great thing about this LIBS system is that many trials can be completed in a short amount of time. With many trials, the objective is to determine whether or not a LIBS system utilizing a cosmetic pulse laser is effective in identifying elemental substances. The cosmetic pulse laser LIBS system should accurately classify pure substances as long as the set-up and procedure are completed correctly.

PHYSICAL CHEMISTRY (PC 7)

Presenter: Kate Moody
PI: Cynthia Woodbridge (Georgia Gwinnett College)
Title: Making Physical Chemistry Particle In a Box Experiment Green and Sustainable

The current particle in a box lab (PIB) uses conjugated dyes that have many hazards. Key principles of green chemistry used in this work include waste prevention, design safer chemicals, and safer solvents and auxiliaries. First the remaining dyes must be used before making the final switch to the greener experiment (minimize waste). Stock solutions will be shared amongst the class; this lowers the E-factor from 6.53 to 0.4 (minimize waste). A greener alternative to the dyes are the everyday compounds experiment that will be implemented (design safer chemicals and safer solvents and auxiliaries). The everyday compounds used are paprika, carrot, spinach, and turmeric. The pure compounds responsible for the colorings of these spices are capsanthin, β-carotene, lutein, and curcumin. These pure compound spectrums are used as a guide to determine the appropriate wavelength of the compounds. The everyday compounds provide a comparable learning experience while allowing a safe and inexpensive experiment. Thus, exposing students to chemistry in relation to the real world.

PHYSICAL CHEMISTRY (PC 8)

Presenter: Edin Osmanbasic
PI: Chayan Dutta (Georgia State University)
Co-Author: Diyali Sil
Title: Transport of Polystyrene Nanoparticles on Supported Lipid Bilayer Surfaces: Effects of Increasing Ionic Strength

Plastic nanoparticles (PNPs) have grown under the scrutiny of physical chemists due to their potential adverse effects on biosystems. Their minuscule size and high surface-to-volume ratio let them interact with lipid membranes, modifying the membrane's structure. This leads to long-term accumulation and internalization of the PNPs, which induces functional changes in membrane properties. Despite this, it is difficult to understand the specific effects PNPs exhibit on biosystems due to their physiochemical heterogeneity. Therefore, nanoscale single-particle measurements are required to comprehend PNPs effects on biosystems and their fates by analyzing their transport properties on the surfaces of supported lipid bilayers (SLBs). For our research, we studied PNP transport on SLB surfaces under differing ionic strengths, using single particle tracking (SPT) analysis. We operated a home-built total internal reflection fluorescence (TIRF) microscope to probe PNP transport on model lipid surfaces. We compared the transport of fluorescently labeled carboxy-functionalized polystyrene (PS) particles on SLBs made up of 1-palmitoyl-2-oleoyl-sn-glycerol-3-phosphocholine (POPC) and 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) under various ionic strengths to understand if and how PS adsorbs to the surface of SLBs. We correlated changes in diffusion properties and surface residence times of PNPs to alterations in the electrostatic interactions and hydrophobic effects between PS nanoparticles and the SLB surface. This early phase of research will aid in uncovering the physiochemistry of PNPs and begin to help us understand their adverse effects from a single-particle point of view.

PHYSICAL CHEMISTRY (PC 9)

Presenter: Karen Lin
PI: Ajay Mallia (Georgia Gwinnett College)
Title: Synthesis, Purification, UV-Vis Absorption, Steady-State Excitation, and Emission Properties of 4-(1-Naphthylazo)phenol

In the present study, 4-(1-naphthylazo)phenol was prepared from the diazotization reaction between 1-aminonaphthalene and phenol. The purification of the synthesized compound using column chromatography and its characterization will be presented. Additionally, the photophysical properties of the compound will be discussed.

PHYSICAL CHEMISTRY (PC 10)

Presenter: Himuni Gurung Kunwar
PI: Ajay Mallia (Georgia Gwinnett College)
Title: Effect of Alkyl Chain Length on Gelation Studies of Ammonium Alkanoates as Low Molecular Mass Gelators

Ammonium alkanoates with varying alkyl chain lengths (C12, C14, C16, and C18) were synthesized from the corresponding alkanoic acids by bubbling ammonia. The gelation properties of ammonium alkanoates were investigated in various polarity liquids. Gel melting temperature and critical gelator concentration of the gels will be presented. Ammonium alkanoates with varying alkyl chain lengths (C12, C14, C16, and C18) were synthesized from the corresponding alkanoic acids by bubbling ammonia. The gelation properties of ammonium alkanoates were investigated in various polarity liquids. Gel melting temperature and critical gelator concentration of the gels will be presented.

PHYSICAL CHEMISTRY (PC 11)

Presenter: Joshua Leonora
PI: Ajay Mallia (Georgia Gwinnett College)
Co-Author: Nguyen Le
Title: Synthesis of Alkoxy Coumarin Derivatives as Low Molecular Mass Gelators

Coumarin derivatives have been reported to have applications in medical imaging. In the present study, a series of four alkylated coumarin derivatives were prepared from 7-hydroxycoumarin and 4-hydroxycoumarin by varying alkyl chain lengths (n = $-C_8H_{17}$, $-C_{10}H_{21}$, $-C_{12}H_{25}$, and $-C_{18}H_{37}$). The synthesized compounds were characterized using spectroscopic and thermal analysis. The gelating ability of the synthesized compounds in various polarity liquids, as well as their steady-state fluorescence and thermal properties, will be presented.

INORGANIC CHEMISTRY (IC 1)

Presenter: Lexi Atilano
PI: Virginia Montiel-Palma (Mississippi State University)
Co-Author: Carlee Secrist
Title: Exploring the Catalytic Capabilities of a NU-1000 Catalyst Grafted with a Ni Organometallic Complex

In previous work by our lab, $PSi^{(iPr)}$ and $PSi_2^{(iPr)}$ (*i*Pr = *i*-propyl) ligands have been bonded to several metals including Ni, Ir, and Rh. Some of those metal complexes were grafted onto NU-1000, a metal-organic framework (MOF) material, to act as a catalyst for silicon and boron functionalization of organic substrates, popular reactions used in many industries. Recently, a Ni complex derived of the $PSi^{(iPr)}$ ligand was synthesized and proved to be active for hydroboration of aldehydes and ketones. The complex is thought to retain its catalytic activity once grafted onto the NU-1000 MOF and comparisons can be drawn between the homogeneous and heterogeneous systems highlighting the advantages of MOF grafting. Post-synthetic modification of the NU-1000 MOF with the aforementioned Ni complex led to a new material characterized by techniques including ICP-MS, SEM-EDX, and ^{1}H-NMR. The ability of the new Ni material to catalyze hydroboration reactions is herein presented.

INORGANIC CHEMISTRY (IC 2)

Presenter: Ziyan Wang
PI: Cora MacBeth (Emory University)
Co-Authors: Ailing Yu and John Bacsa
Title: Development of First-Row Transition Metal Complexes with Redox-Active Catecholamine Ligands and Their Corresponding Reactivities

Over the decades, various research has reported the potency of organometallic complexes as efficient catalysts to put previously unachievable reactions into practice. Second and third-row transition metals are predominantly used from the outset as they exhibit high catalytic activity in multi-electron transformations, yet the scarcity and extractability of such metals makes mass industrial production and subsequent waste treatment fraught with limitations. With the goal to design environmentally friendly, low-cost, efficient catalysts; chemists begin to use first-row transition metals, far more abundant in nature, to synthesize catalysts. The major challenge for this is that first-row transition metals exhibit a relatively low reactivity to promote multi-electron catalytic reactions under natural conditions. This research aims to approach this conundrum by developing ligands that can modify and enhance reactivities of the first-row transition metals through coordination. Specifically, the research focus is on the development of first-row transition metal complexes that incorporate redox-active catecholamine ligands along with close examination of the corresponding catalytic activity. Two types of ligands, N,N'-(azanediyl-*bis*(2,1-phenylene))*bis*(2,3-dihydroxybenzamide) (H_7L^{CAT})
and 2,3-dihydroxy-N-(2-(phenylamino)phenyl)benzamide (H_4L^{CAT}) have been designed, synthesized, and characterized through NMR spectroscopy. Both ligands contain nitrogenous and catechol systems with the objective to enable a versatile coordination and further enhance the reactive performance of the metal-ligand complexes. Metalation has been performed to synthesize bimetallic complexes with Fe(II)|Co(II) and Co(II)|Cu(II). The metal-ligand complexes were characterized by X-ray crystallography and would be subsequently employed in O-atom transfer and hydrazone oxidation to evaluate corresponding catalytic activity (monitored *via* UV-Vis spectroscopy).

INORGANIC CHEMISTRY (IC 3)

Presenter: Mary Beth Johnson
PI: Michael Morton (Georgia Gwinnett College)
Title: Exploring the Photophysical Properties of Cobalt(II) and (III) Complexes to Create a Spectrochemical Series

This experiment studies the photophysical properties of several cobalt(II) and (III) coordination complexes using various ligands. Compounds were synthesized and analyzed using UV Spectroscopy to gather the maximum wavelengths of absorbed light which were used to calculate the crystal field splitting energy. Using this splitting energy, the synthesized compounds were ranked within a spectrochemical series and compared to the universally accepted series. Many of the ranked ligands complemented the known series with some deviation occurring with chlorine, cyanide, and nitrite ligands. It was concluded that chemical structure, synthesis methods, and analysis error could be the cause of these discrepancies.

INORGANIC CHEMISTRY (IC 4)

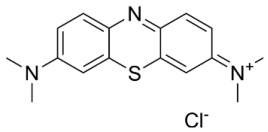
Presenter: William Dougherty
PI: Simon B. Blakey (Emory University)
Co-Authors: Harry Ung, Patrick Gross and Ethan Heyboer
Title: Understanding Reactivity of Rhodium Naphthindenyl Catalysts

The ability to modify the steric and electronic parameters of cyclopentadienyl (Cp) ligands has made them a privileged ligand class in the design of transition metal catalysts capable of diverse reactivity. The indenyl scaffold is a Cp-ligand derivative known for its enhanced reactivity resulting from an η^5-η^3 ring slip by preserving aromaticity in the fused, aromatic backbone. In this work, the effect of extending the indenyl ligand's aromatic framework is investigated through the synthesis of various linear and bent "naphthindenyl" rhodium complexes. Characterization of these rhodium naphthindenyl complexes by IR, NMR, and X-ray crystallography reveals different ligand coordination modes depending upon the nature of the naphthindenyl backbone. This work expands current Cp catalyst data sets, improving the prediction of catalyst reactivity.

ENVIRONMENTAL CHEMISTRY (EC 1)

Presenter: Derick Medina
PI: Misael Romero-Reyes (Georgia Gwinnett College)
Title: Dye Be Gone!

Contamination of water sources can come from various pollutants but one of the most prominent classes are dyes. Methylene Blue is one of the most common dyes found in water sources due because of the clothing industry. This research project focuses on the efficient removal of this dye using sustainable resources, such as wood. Moreover, we emphasize the use of affordable, common and environmentally friendly components.



Methylene Blue

ORGANIC CHEMISTRY (OC 1)

Presenter: Isabella Darwish
PI: Jeremy Olson (University of North Georgia)
Title: Cope Rearrangement Experiment for Undergraduate Students

The Cope rearrangement is an important reaction in the organic chemistry world, unfortunately there are not many experiments that have been simplified enough to be performed in an undergraduate setting. The following synthesis has been developed in order to demonstrate a Cope rearrangement along with other essential skills for an advanced organic chemistry student. The method involves a three-step process, first tigloyl chloride is subjected to Suzuki cross-coupling with phenylboronic acid. The resulting product is combined with allyl bromide to form a 1,5-diene to be used as the substrate for the Cope rearrangement. The rearranged product is then formed using the constant heat and pressure of a microwave reactor for 1 hour at 195 °C. This experiment not only demonstrates a Cope rearrangement but also produced a high yield of product without the need of column chromatography.

ORGANIC CHEMISTRY (OC 2)

Presenter: Riley Rowland
PI: Rahul Shahni (University of North Georgia)
Title: Furan-Based Semi-Rigid Diol: A Biomass-Sourced Monomer Prepared by Photocyclization

Semi-rigid diol monomers can replace hazardous BPA in the production of polyesters and polycarbonates with exceptional thermal and mechanical properties due to their flexible aliphatic chains and aromatic ring structures. These versatile furan-based monomers derived from biomass have garnered increased interest due to their potential as an alternative to petroleum-derived compounds. In this study, bioadvantaged compounds furfural and malonic acid are utilized to synthesize 2-furanarylic acid (FAA) *via* Knoevengal condensation, followed by a [2+2] solid-state photoreaction to produce rctt-3,4-di-2-furanyl-1,2-cyclobutanedicarboxylic acid (CBDA-2). The CBDA-2 is reduced using sodium borohydride and subsequent addition of an electrophile, either I_2 or BF_3•$(CH_3)_2O$, to produce the semi-rigid diol *cis*-1,2-(furan-2-yl)cyclobutane-3,4-dimethanol (CBDO-2). Characterizations of FAA, CBDA-2, and CBDO-2 structures were conducted using spectroscopic methods.
CBDO-2 displays promise as a semi-rigid building block for bioadvantaged polymers with outstanding mechanical and thermal characteristics.

ORGANIC CHEMISTRY (OC 3)

Presenter: Sebastian Cruz
PI: Maged Henary (Georgia State University)
Title: Modification of Perimidine-Based Squaraine Dyes for Biomedical Applications

Squaric acid-based dyes are a class of compounds composed of a 3,4-dihydroxy-3-cyclobutene-1,2-dione core connected to two aromatic heterocyclic structures showing absorbance in the near infrared region. The NIR region includes wavelengths from 650 nm to 1500 nm. This region is optimal for biological applications as light scattering and absorbance from biologically active molecules are limited. This characteristic allows for deeper penetration and higher resolution of the contrast agent. Squaraine dyes are unique in that they show high molar absorption, and high photobleaching thresholds. These dyes also have rotatable bonds which may promote energy relaxation through the vibrational pathway resulting in thermal expansion, this characteristic may imply that squaraines could be optimized for optoacoustic imaging.

Squaraine dyes typically incorporate indolium heterocycles which delocalize electrons in the squaric acid core and result in absorbance maximums typically below 700 nm. Herein, we synthesized squaraine dyes using a larger aromatic heterocycle to red shift the absorbance deeper into the NIR region. 2,3-dihydro-1*H*-perimidine molecules have optimal electron properties and promote further delocalization of electrons along the squaraine core which promotes the red shift in absorbance. The perimidine based squaraine dyes have shown absorbance above 800 nm. We have explored the photophysical properties of modified perimidine sporting symmetrical squaraine molecules.

ORGANIC CHEMISTRY (OC 4)

Presenter: Audrey Conner
PI: Christopher Newton (University of Georgia)
Co-Authors: Geeta Goyal and Marshall Liss
Title: Quadruple Diels–Alder Approach to Biaryl Systems

Asymmetric catalysis, a type of catalysis in which the formation of one stereoisomer is favored over others, is particularly useful in the synthesis of biologically active molecules, as different stereoisomers have different biological activities. 1,1'-Bi-2-naphthol (BINOL) and its derivatives are a well-studied group of chiral catalysts and ligands used in asymmetric catalysis. The goal of this project is to atropo-enantioselectively synthesize BINOL derivatives through the implementation of a synthetically novel quadruple Diels–Alder/retro-Diels–Alder (DA/rDA) reaction on a dimeric tetrazine moiety. The DA/rDA reaction is a well-established, synthetically efficient reaction used throughout organic chemistry. Through its use, we hope to find a simple, efficient method to build polycyclic aromatic systems which may be used in asymmetric catalysis. Recently, we have successfully synthesized the dimeric tetrazine moiety through the homocoupling of a monomeric bromo-tetrazine species and are currently working to optimize the reaction. Once the dimeric species has been synthesized in sufficient quantities, we will begin employing the quadruple DA/rDA reaction sequence to build the desired polycyclic aromatic systems.

ORGANIC CHEMISTRY (OC 5)

Presenter: Joshua Thorpe
PI: Margaret Meadows (Mercer University)
Co-Author: Komal T. Gandhi
Title: Alternate Synthesis of Phthalate Chemical Sensors

Phthalate esters are endocrine disrupting chemicals (EDCs) which are often used as plasticizers with both home and medical applications. Specifically, recent data shows an association between phthalate esters and hypothyroidism, a deficiency in thyroid hormones with broad neurological, cardiovascular, and developmental implications. Sancenón *et al.* developed a method for the colorimetric sensing of carboxylate dianions including phthalates with moderate success. However, their synthetic approach involved volatile perchlorates, reducing the sensor's applications. We are currently examining several alternative syntheses using more accessible chemistry. Following synthesis of our target sensor, we plan to use it for the detections of hydrolyzed phthalate esters in aqueous solutions.

ORGANIC CHEMISTRY (OC 6)

Presenter: Marissa “Rose” Wagley
PIs: Wathsala Medawala and Ronald Okoth (Georgia College and State University)
Title: Two-Step Synthesis of a Novel Phthalein-Based pH Indicator

Conventional phthalein dyes are used as pH indicators due to their distinct color change in solutions of different pHs. For example, a solution of phenolphthalein in water turns from colorless to pink as the pH of the solution is increased from acidic to basic. Here, we propose a two-step synthesis of a novel phthalein based pH indicator from commercially available materials that utilizes reactions commonly encountered in undergraduate organic chemistry courses. In step 1, the pure product of 1-phenyl-2,3-naphthalenedicarboxylic anhydride was obtained and verified through the use of melting point and NMR analysis. After step 2 was completed a product that contained acid base indicator properties was obtained however the end product was not pure due to the inability to remove phenol from the end product. In the future, toluene will be used as the solvent and phenol will only be used as the reactant. Once the pure indicator product is obtained, the synthesis will be incorporated into the organic chemistry and quantitative analysis laboratory curriculum at Georgia College with the aim of enhancing student learning outcomes through a student-centered hands-on pedagogy.