ANALYTICAL CHEMISTRY

Shayla Kelley and Wei Zhou (PI)

Kennesaw State University

AC01: Quantitative analysis of kavain in various kava samples via GC-MS

Kava (*Piper methysticum*) is a perennial plant native to the South Pacific that has long been utilized for ceremonial and medicinal purposes. However, due to recent abuse of kava products for their anxiolytic and sedative properties, concerns of side effects such as severe liver problems, fatigue, and dizziness are on the rise. Kava products are freely available in the form of teas, capsules, and powders, and are found easily at many online and physical storefronts as it is not well-regulated in the US despite being a controlled substance in other countries. In this study, the psychoactive compounds found in kava (kavalactones) were extracted from various forms of kava (pill, powder, raw root, and tea) using methanol and analyzed via GC/MS. Though there are six major kavalactones, only kavain was quantified. Within each sample, <1% by mass of kavain was found, save for the powder, which contained ~3% by mass kavain. As research on the effects of kava continues, this data can later be used to help determine safe dosage levels for its various forms.

Elijah Langston and Royce Dansby-Sparks (PI)

University of North Georgia

AC02: Simultaneous Mass and Electrochemical Detection of Stress Hormone

Small single stranded artificial DNA sequences, known as aptamers, have recently shown promise as molecular recognition probes in biosensors. Current methods utilize either quartz crystal microbalance (QCM) to detect small mass changes or electrochemical oxidation of methylene blue for quantification. The objective of this research is to use an electrochemical QCM (eQCM) modified with custom designed ssDNA aptamers to selectively detect cortisol binding and subsequent removal from the biosensor through simultaneous mass change and electrochemical means. This preliminary work demonstrates the ability to functionalize gold electrodes with aptamers by thiol bond formation. The electrodes were further exposed to capture probe aptamers with the ability to bind to cortisol with high selectivity. The modified electrodes were characterized by electrochemical impedance spectroscopy (EIS) and cyclic voltammetry (CV) for conformation of binding and senor fabrication. After characterization, aptamer modified electrodes were exposed to methylene blue which binds to guanine nucleotides in the aptamers. The methylene blue is detected by differential pulse voltammetry (DPV) which forms the basis for electrochemical detection. Once fully developed this system should be easily adaptable for a variety of capture aptamers with known binding affinities to other analytes.

Erika Guzman-Cantellano and Lori Wilson (PI)

University of North Georgia

AC03: Advancing Water Quality Analysis for Residents of Lumpkin County, Georgia

Domesticated groundwater wells are a potential source of heavy metal contaminants, yet they are largely unregulated. Approximately 60% of Lumpkin County residents rely on private wells as their main water source. Our main goal is to screen private well water samples for bacteria, determine heavy metal concentrations using Total Reflection X-Ray Fluorescence (TXRF), and provide detailed homeowner reports with EPA primary and secondary standards at no cost. The TXRF machine generates an X-Ray beam that hits the sample disc exciting the electrons in the inner K and L shells. As a result, each element in the sample produces a set of characteristic fluorescent x-rays that is unique, allowing us to identify it. We evaluated the accuracy and precision of the TXRF analysis using a secondary standard water sample. Our findings revealed that our technique was accurate and precise for the elements Fe, Cu, Mn, and Zn. To improve our evaporation process, we tested a photo-molecular effect via a green LED light. We found that the LED light decreased the amount of time it took for evaporation to occur by approximately 30%. We concluded that this was due to an increase in temperature caused by the LED light. After re-evaluating our method, with temperature accounted for, we determined that the decrease in evaporation time using an LED light was minimal. In addition to measuring elemental composition, this project will also conduct bacterial screening using an enzyme-substrate test. Furthermore, bacterial screening using an enzyme-substrate test identified coliform presence in two water samples. In the future, we hope to uncover elemental contamination patterns in Lumpkin County wells and begin mapping groundwater concentrations based on bedrock type and location.

Angel Jaimes, Wei Zhou (PI), Olivia Laflamme and Shannon Hipp

Kennesaw State University

AC04: How Hot Are Spicy Peppers? Quantification of Capsaicin in Various Peppers using GC/MS

To compare the hotness level among different types of peppers, we are using GC/MS (Gas chromatography Mass Spectrometry) to quantify capsaicin in various spicy pepper samples. Dried peppers were purchased either from online or local stores, and they were further dried at ~80 °C for two hours before being destemmed and crushed into fine powders using a mortar and pestle. The powdered samples of different peppers were gently refluxed for 5 hours in ethanol at 78 °C. The solutions were then filtered (0.45 PTFE filter) and collected in a round bottom flask. The solutions were then rotovapped at 75 °C before they were re-dissolved in a mixture of dichloromethane and ethanol (25:1). A set of standard capsaicin solutions was prepared with a range of 80 ppm to 500 ppm. All solutions were analyzed using GC-MS (the Shimadzu GCMS-QP2010 Plus system. A calibration curve with excellent linearity ($R^2 = 0.990$) has been constructed, and capsaicin has been identified and quantified in different peppers. The ghost pepper yielded 0.0212 grams of capsaicin per gram of dried pepper while the jalapeño sample had 0.00132 grams of capsaicin per gram of pepper. Quantitative analysis and more comparisons among different peppers will be presented from this research.

Briana Andronicescu, Tanner Harkin and Joshua Driver (PI)

University of North Georgia

AC05: Qualitative and Quantitative Determination of Fluoride Ion Concentration Present in Name Brand Toothpaste Using ^{19}F-NMR

Fluoride is an element that is widely used in small concentrations for the maintenance of water and cavity prevention in Dentistry. However, an excess of fluoride is widely associated with various health problems, but the most significant one relating to toothpaste is fluorosis. Furthermore, to additionally benefit from toothpaste, a high enough concentration must be met to prevent decay from occurring. The research conveyed a qualitative and quantitative analysis of fluorine consisting compounds in two tubes of Crest toothpaste. The active ingredient in the Crest toothpaste brand is sodium fluoride with one bottle varying of 0.16% W/V fluoride ions and another 0.15% W/V fluoride ions. Three trials of the two toothpaste bottles were ran in a ^{19}F-NMR instrument with Ethyl-4,4,4-Fluoroacetoacetate as the internal standard.

Daygan Wasson, Isaac Agyekum (PI) and Alexander D. Smiarowski

University of North Georgia

AC06: Online Catalyst Free Gas-phase Esterification of Fatty Acids in Jorō Spider Web *Via* Gas Chromatography- Mass Spectrometry (GC-EIMS)

Fatty acids are essential lipid components that play crucial roles in membrane dynamics and metabolic processes. They are key analytes for assessing nutritional value and can significantly impact serum lipid levels. In the cosmetics industry, fatty acids serve diverse functions, including acting as emulsifiers and stabilizers.

For analyzing fatty acids in biological samples, gas chromatography coupled with electron impact ionization mass spectrometry (GC/EI-MS) is a widely used technique. Chemical derivatization, particularly converting fatty acids into fatty acid methyl esters (FAMEs), enhances detectability and improves peak shape in GC-MS analyses. Traditional methods for this derivatization typically involve acidic or basic catalysts, which can present challenges such as lengthy reaction times or the need for hazardous reagents. To address these challenges, there is growing interest in greener and more efficient esterification methods. An innovative on-line gas phase esterification technique has been successfully applied to qualitatively profile fatty acids in Jorō spider webs, showcasing its potential for analyzing complex biological samples while minimizing environmental impact.

Luke Caldwell, Adam Kiefer (PI), Caryn Seney, William B. Stewart, D. Christian Grizzle, Joaquin Urbina

Mercer University

AC07: Identification and quantification of Pb-containing pigments in outdoor fitness equipment

Compounds of lead (Pb), particularly lead (II) chromate ($PbCrO_4$), lead chromate molybdate sulfate (CI Pigment Red 104, PR104: $PbCrO_4 \bullet PbMoO_4 \bullet PbSO_4$), and lead sulfochromate (CI Pigment Yellow 34, PY34: $PbCrO_4 \bullet PbSO_4$) are frequently employed as additives in paint and coatings for their intense colors, anti-corrosive properties, and durability. Like all Pb compounds they are highly toxic, with exposure typically occurring through ingestion or inhalation of contaminated particulate matter originating from the degradation of the paint or coating. Although Pb intoxication originating from degraded paint can occur at any age; children and adolescents – particularly those living in Lower- and Middle-Income Countries (LMICs) – are at greater risk for exposure to Pb. While multiple publications highlight the Pb exposure risk presented by the coatings of playground equipment, individual pieces of Outdoor Fitness Equipment (OFE) are also frequently used by children and adolescents and must similarly be durable and withstand frequent use; as well as resistant to seasonal changes in weather, exposure to UV-radiation, and vandalism. Thus, it is possible that the coatings on OFE may also contain Pb-based pigments. Herein we report the determination of Pb in the exterior coatings of OFE located in an LMIC. *In situ* screening for Pb using the Lumetallix instant lead detection kit and portable X-Ray Fluorescence (pXRF) analysis identified multiple locations where OFE contained levels of Pb exceeding 40,000 ppm. Collected samples were dried, homogenized and re-analyzed under laboratory conditions employing pXRF analyzers and inductively-coupled plasma-optical emission spectroscopy, confirming high levels of Pb in the exterior coatings. Raman spectroscopy confirmed the speciation of Pb in the coatings to contain $PbCrO_4$ in the form of PR104 for the red-colored coating. The yellow coating similarly contained Pb as $PbCrO_4$, likely as PY34.

Fernando Garcia, Isaac Agyekum (PI), Patricia M. Todebush and Barnabas Otoo

University of North Georgia

AC08: Online Catalyst Free Gas-Phase Synthesis of Pyranones:
A Versatile Building Block for Bioactive Compounds

A novel gas-phase synthesis of 2H-Pyran-5-carboxylic acid, 4,6-dimethyl-2-oxo, ethyl ester, and 2H-Pyran-2,4(3H)-dione, 3-acetyl-6-methyl- was achieved in a GC inlet at 300°C without a catalyst, using methyl acetoacetate and ethyl acetoacetate as precursors. Pyran molecules and their derivatives are valuable precursors in the synthesis of various bioactive compounds, including pharmaceuticals, agrochemicals, and natural products. Their unique structure and functional groups make them essential building blocks for designing molecules with potential therapeutic applications. This gas-phase catalyst free method offers, for the first time, a rapid, efficient, and sustainable route to potentially access pyran intermediates in drug discovery, organic synthesis, and medicinal chemistry.

Addison Bowen and Elaine Bailey (PI)

Piedmont University

AC09: Is Honey Really the Bee's Knees?

Honeybees are known to be bioindicators of environmental pollution. Agricultural products, automobiles, and industrial byproducts are just some of the pollutants found in the environment. Many of these produce heavy metal contaminants that can infiltrate the honey produced by honeybees. Honey is known to contain trace amounts of heavy metals like zinc, manganese, and copper. Honey contaminated by heavy metals like, cadmium, lead and chromium could potentially cause some health issues for humans when consumed. The purpose of this research was to determine if there was a correlation between heavy metal content in honey and the area in which it was obtained. Honey was collected from three different locations (urban, agricultural, and rural) in Georgia, each representing different environmental conditions. The urban honey sample was collected from Atlanta, the agricultural sample was collected from a farm in Banks County and the rural sample was collected near a busy road in Habersham County. Each honey sample was warmed, then dissolved in 1% nitric acid. Constant volume standard addition was used to prepare five solutions of each of the honey types. The solutions were spiked with heavy metals lead, zinc, cadmium or chromium. Flame atomic absorption analysis was performed to obtain absorbance values for each of the solutions. A regression analysis was done to determine the best-fit line, and the concentrations of the metals were calculated. The results of this research found that concentrations of Zn ranged from 3.01-3.54 ppm, 4.70-7.11 ppm for Pb, 5.56-5.91 ppm for Cr and that none of the samples contained Cd. It was found that there was no significant difference between the honey locations in terms of total heavy metal content. All of the different honey types were determined to contain safe levels of heavy metals.

Carter Barnes and Catrena Lisse (PI)

Georgia College & State University

AC10: Spectrophotometric Determination of the Chelating Behavior of Metal Ions and EDTA Encapsulated in Sol-Gel Matrix

Ethylenediaminetetraacetic acid (EDTA) has numerous medicinal applications across a wide variety of fields, including veterinary medicine. Magnesium and calcium ions, in excess, can negatively affect the quality of life for many animals and can be destructive to certain medical devices due to mineralization. Using the chelating ability of EDTA, the complexation of metal cations with EDTA can result in decreased amounts of metals in the system. This project investigated EDTA encapsulated within a silica sol-gel matrix with a metal cation sensitive dye, pontachrome violet SW. When placed in a cation rich environment, ultraviolet/visible (UV/Vis) spectroscopy was used at 575 nm to determine the concentration levels of the target ions isolated by the EDTA sol-gel matrix. This presentation will highlight the experimental methodology and preliminary results of the study.

Alexandra Frusina, Isaac Agyekum (PI) and Fernando Garcia

University of North Georgia

AC11: Catalyst-Free Gas-Phase Aldol Condensation of Hexanal: A Sustainable Pathway to 2-Butyl-2-Octenal

Aldol condensation reactions are pivotal in organic synthesis, enabling the formation of C-C bonds with broad applications in fine chemicals and fuel precursors. Traditional liquid-phase aldol condensations often require catalysts and harsh reaction conditions, which can complicate scalability, affect product isolation, and increase environmental impact. In contrast, gas-phase, catalyst-free aldol condensations present a promising, sustainable alternative, potentially minimizing the need for solvents and reducing operational costs. This study explores the self-condensation of hexanal under catalyst-free gas-phase conditions, leading to the formation of 2-butyl-2-octenal. By investigating the reaction mechanisms and optimizing the reaction environment, we demonstrate the feasibility of this approach; highlighting its potential for more efficient and eco-friendly synthesis of α,β-unsaturated aldehydes.

Celeste Echols, Nadia Hanceri, Julia Oung, Edith Dominguezchavira, A 'Leah Frazier, Brandon Persaud, Aishwarya Ramoudit, Brett Whitson and Ajay Mallia (PI)

Georgia Gwinnett College

AC12: Chemicals in Tomatoes: Extraction, Purification, and Antioxidant Properties of Lycopene

Tomatoes are a great source of nutrient chemicals that have positive benefits for human health. They are rich in antioxidants, such as phytochemicals, vitamins, carotenoids and other nutrients. Tomatoes are abundantly rich in a carotenoid called lycopene, which gives it its color. This component will be extracted to analyze the properties that contribute to the value of tomatoes. A variety of tomatoes were harvested, store bought, and sundried. First, extractions were done with 'traditional' solvents such as acetone to remove the lycopene, and then purified using column chromatography. Secondly, a greener method using a CPS emulsion in the extraction step, followed by filtration, and rotary evaporation gave crude lycopene. A third method of extraction used 1,2-dichloroethane as a green solvent to extract lycopene. In the first method, 5.00 g of Sundried tomatoes yielded 40.0 mg of lycopene vs. 3.54 mg with the second (greener) method. These results were determined quantitatively using with UV-Visible spectroscopy, and TEAC Assay to assess the tomatoes' antioxidant properties. Results to confirm characterization were qualitatively analyzed via Thin Layer Chromatography and Infrared Spectroscopy. The third method, using 1,2-Dichloroethane, was determined to be the best extraction method for lycopene.

BIOCHEMISTRY

Sophia Barthel, Kyle Biegasiewicz (PI) and Elizabeth Gross

Emory University

BC01: Expression and Activity Analysis of a Mutant Vanadium Haloperoxidase Enzyme

As biocatalysts for chemical synthesis, enzymes provide an attractive alternative to traditional catalysts which typically require harsh conditions or produce excess waste. This study examines the process for expressing a vanadium haloperoxidase enzyme mutant which had previously been reported to show up to a 100-fold higher halogenating activity at alkaline pH compared to its wild- type counterpart. This workflow entailed designing genomic plasmids, transforming bacterial cells, sequencing for fidelity, optimizing expression, and finally purifying the protein via nickel affinity chromatography. Although the mutant enzyme was acquired in good yield, we found that the mutant surprisingly showed lower halogenation activity on our substrate of interest, resulting in a mono-chlorinated product as opposed to the di-chlorinated product obtained through the wild-type enzyme.

Xiaofang Ke, Jenny J. Yang (PI), Anita Dorabadi, Sophia Bamishaye, Francas Akinlotan, Jingjuan Qiao and Zongxiang Gui

Georgia State University

BC02: Optimized Purification and Characterization of ProCA32.collagen1: A Novel MRI Contrast Agent for Improved Clinical Diagnosis of Collagen Type I-Related Fibrosis

ProCA32.collagen1 is a novel protein-based MRI contrast agent specifically designed to target collagen type I, a key protein involved in liver fibrosis. Hepatic fibrosis, caused by excessive collagen deposition, can progress to cirrhosis if left untreated, making early detection crucial. Conventional MRI contrast agents often require high doses and pose safety concerns. ProCA32.collagen1 addresses these limitations by enhancing the sensitivity and specificity of fibrosis detection while maintaining a safer profile. The purification of ProCA32.collagen1 was optimized using ion-exchange chromatography and redox buffer systems, resulting in high-purity samples with superior imaging capabilities. Validation through SDS-PAGE, relaxivity analysis, and ELISA demonstrated the agent's high relaxivity and strong binding affinity to collagen type I. This innovative agent shows potential not only in liver diagnostics but also in the imaging of fibrosis-related conditions in other organs such as the lungs and heart, offering a promising tool for early disease intervention and improved patient outcomes.

Zaria Vulu, Michelle Gaines (PI), Grace Anderson and Ariel Furst

Spelman College

BC03: Biomaterial Reformulation of *Mycobacterium bovis* Bacillus Calmette-Guérin for Bladder Cancer Treatment

The immunotherapy BCG bladder cancer treatment is efficacious but paired with adverse effects that prohibit patients from completing treatment. The project aims to understand the release of polymer-encapsulated *Mycobacterium bovis* Bacillus Calmette-Guérin (BCG) coated in Metal-Phenolic Networks (MPNs) that protect microbes from external stressors for long-term sustained delivery. Understanding release rate/duration and cell survivability alludes to improvements in immunotherapy. A buffer release assay using a related bacterial strain was conducted over a four-week period to observe the impacts of phosphates and ions on the bacterial release post-encapsulation, and the results were then compared to a synthetic urine assay. *Mycobacterium smegmatis* was encapsulated in alginate and was released into various buffers. MOPS postponed release while phosphate and iron-rich buffers quickly released bacteria and lost viability over time. Quick bacterial release was most prevalent in the PC buffer, resulting in the lowest viability at the end of the assay (~10^2 CFU/mL). Furthermore, different MPN coatings were evaluated based on the viability of microbes under elevated temperature, mocking the environment of a bladder. The results from the buffer, MPN, and elevated temperature assays were analyzed using various microscopy techniques and allude to optimal conditions for BCG drug-loading immunotherapy.

Susanna Huang, Adegboyega Oyelere (PI), Ryan Kern and Uche Arunsi

Georgia Institute of Technology; Parker H. Petit Institute for Bioengineering and Bioscience

BC04: Synthesis and Cell-Line Activity of 3-Hydroxypyridine-2-thione (3-HPT)-Based Compounds for Prostate Cancer

Prostate cancer is one of the leading causes of cancer-related deaths in men. Histone Deacetylase 6 (HDAC6), a cytosolic protein involved in prostate cancer metastasis, has been established as a key protein target for prostate cancer treatment. It has been demonstrated by the Oyelere Lab that 3-hydroxypyridin-2-thione (3-HPT) is an HDAC6-targeting warhead with nanomolar IC_{50} values in HDAC6 enzyme assays. While inhibition of HDAC6 was successful in enzymatic assays, no inhibition activity was observed in cell-line assays, which was attributed to the polar nature of 3-HPT and its inability to pass through cell membranes. In this work, we seek to improve the pharmacokinetic properties of 3-HPT by introducing nonpolar characteristics to the compound through alkylation. 3-HPT derivatives with fluorinated alkyl groups were docked onto HDAC6 in the molecular docking software PyRx. The derivatives either had similar or stronger binding affinities to HDAC6 than that of the 3-HPT compound. Since these binding affinities were promising, two sets of 3-HPT-based compounds were synthesized and tested for biological activity against cancer cell lines. Here we report that the set of compounds with the unaltered 3-HPT moiety has demonstrated strong activity against cancer cell lines, which indicates that the addition of aliphatic groups onto the 3-HPT moiety does indeed increase the pharmacokinetic properties of 3-HPT compounds.

Charlotte Miller, Nicolle Chavez, Raquel L. Lieberman (PI) and Dustin Huard

Georgia Institute of Technology

BC05: Predicting Pathogenicity of Glaucoma-Related Myocilin OLF Variants

Mutations localized to the C-terminal olfactomedin (OLF) domain of the protein myocilin are linked to primary open-angle glaucoma, a leading cause of irreversible blindness worldwide. Glaucoma-associated myocilin variants tend to be less thermally stable than wild-type protein, and are prone to aggregation which leads to a toxic gain-of-function disease progression pathway. We have been working to biophysically characterize 9 new OLF variants, some of which are known in the general population. Several online databases such as AlphaFold, SIFT, and PolyPhen were applied to these mutations to predict their pathogenicity before conducting experiments. After recombinantly expressing and purifying the OLF mutants, we conducted size-exclusion chromatography (SEC) to assess the pathogenicity of the mutations based on their tendency to aggregate. As of now we are conducting differential scanning fluorimetry (DSF) experiments to determine their thermal stability parameters as well as their secondary and tertiary structural signatures for comparison with the wild-type protein. Our initial results indicate that 4 of the 9 mutations are likely pathogenic. In future experiments, we will attempt to crystallize those OLFs that are wild-type like to determine the impact of these mutations on protein structure at the atomic level.

Valentina Esho, Chris Rodgers (PI), Rowan Gargiullo, Jessica Mai and Cedric Bowe

Department of Neurosurgery, School of Medicine, Emory University

BC06: A comparison of Histological Techniques for Identifying Amyloid-Beta (Aβ) Plaques in a Mouse Model of Alzheimer's Disease

Alzheimer's disease has been demonstrated to impair cognition, memory, and language and cause dementia. Literature review yielded a "linear" theory: amyloid plaques (or the amyloid-beta (Aβ) peptides that make them up) are the direct cause of AD. However, this theory is controversial because it does not fully consider the complexity of the brain. For example, Aβ interacts with other components, causing inflammatory responses from microglia (cells that respond to neuronal damage). Another perspective places the cause on abnormal processing of APP (amyloid precursor protein) being cleaved at different places to create Aβ42. Studies suggest Aβ42 causes AD by instigating neuron damage—such as synapse loss, inflammation, and oxidative damage. So, lowering Aβ oligomers (chain of multiple molecules) could be a valuable medicinal approach. To stain for these Aβ42 plaques, fluorescence imaging can be used. Brain images of AD mice were taken with a variety of stains used, including methoxy (a fluorescent dye injected *in-vivo* that is well-used and well-researched) and CRANAD-28 (a different fluorescent dye that can be used *ex vivo*). Analysis determined that methoxy successfully stains for plaques and does not leak into other channels. CRANAD-28 and methoxy have significant overlap in what they stain, indicating CRANAD-28 likely also stains for plaques.

Li Xu, Ting Du, Jenny j. Yang (PI), Xiaofang Ke, Yushan Zhang and Anita Dorabadizare

Jenny J. Yang (PI)

Georgia State University

BC07: ELISA-Based Detection of Collagen-Specific MRI Contrast Agent for Enhanced Liver Fibrosis Imaging

Liver fibrosis, characterized by the excessive accumulation of collagen and extracellular matrix, is a common consequence of chronic liver diseases (CLD). Early detection is crucial for halting or potentially reversing fibrosis, which can significantly improve patient outcomes. This study emphasizes the importance of early diagnosis and the development of non-invasive detection methods for liver fibrosis and related conditions. While Magnetic Resonance Imaging (MRI) is a powerful tool for visualizing internal organs, its effectiveness is often limited by the current contrast agents available. To address this issue, researchers have developed hProCA32.collagen1, a protein-based contrast agent with high specificity for human collagen type I. This agent's strong affinity for collagen I enhances tissue targeting, allowing for improved imaging precision and reduced dosage.

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 if the proteins were the proteins we want, SDS-PAGE was used to visualize the results, Bradford assay was used to determine the concentration if the proteins and ELISA was used to determine the characteristics like binding affinity of the proteins.

Kayla Phillips, Jennifer Coronado Lerma and Jinkyung Park (PI)

Georgia Gwinnett College

BC08: The Anti-Obesity Effects of Cauliflower Mushroom Insights on Lipid Metabolism and Weight Management

The purpose of this study was to investigate the effects of *Sparassis crispa* (SC), also known as cauliflower mushroom, on adipogenesis and lipid metabolism in C57BL/6J ob/ob mice. After acclimation for one week, male mice were divided into four groups (n = 8) and administered treatments via gavage three times per week. The control group (HF) received a high-fat diet and distilled water, while the positive control group (SIB) was fed a high-fat diet and treated with sibutramine (5 mg/kg). Two experimental groups received SC extract at doses of 100 mg/kg (SC100) and 300 mg/kg (SC300).

Following the treatment period, blood and liver samples were analyzed for triglycerides, total cholesterol, glucose, and hepatic lipid content, as well as protein expression of CPT-1 and UCP2 in hepatocytes. Results showed that SC significantly reduced lipid accumulation in adipocytes in a dose-dependent manner and lowered serum triglycerides (TG) and total cholesterol (TC). Additionally, SC increased CPT-1 expression, indicating enhanced fatty acid oxidation in the liver, though UCP2 expression was not significantly affected.

The SC groups (SC100 and SC300) also significantly prevented weight gain by 62.1% and 64.2%, respectively, compared to the HF group ($P < 0.05$), while the SIB group prevented weight gain by 43.36% ($P < 0.05$). These findings suggest that SC may effectively inhibit adipogenesis and promote lipid oxidation, offering potential therapeutic applications for hyperlipidemia and obesity. Further research is necessary to identify the active components responsible for these effects.

Aurora Arjmand and Jill Penn (PI)

Georgia Gwinnett College

BC09: Can We Slow Down the Process of Aging?

This study is investigating the possibility of slowing down the process of aging by looking into the Hutchinson-Gilford Progeria Syndrome. Progeria is a genetic disorder that causes rapid aging in children due to a point mutation in exon 11. A nine nucleotide sequence in the wild type allele, CAG GTG GGC, differs from the consensus splice donor site by two nucleotides. The point mutation that causes Progeria results in the stretch of nine nucleotides differing from the consensus sequence by only one nucleotide, CAG GTG GGT. In patients with progeria this cryptic splice site is used more often than in wildtype and results in a shorter mRNA and eventually a toxic protein called progerin that distorts the structure of the nuclear membrane. Progerin is produced in large quantities in Progeria patients. In addition, smaller amounts of progerin protein can be found in unaffected individuals, with increased amounts found in older individuals. Here we have used bioinformatics software, to align the sequence of the nine nucleotides in a variety of placental mammals. Surprisingly, the stretch of nine nucleotides in exon 11 is highly conserved. However, we found 8 species of mammals that differ from the consensus splice donor site by three nucleotides. We predict that in this subset of mammals, the cryptic splice will not be used, or will be used less often, compared to species with the evolutionarily conserved sequence. We also predict that little to no progerin will be present in the nuclear membranes of these 8 species. Absence of progerin might protect the species from the effects of aging. Consistent with this prediction, the life span to age of maturity ratio was larger for the species that differed from the consensus splice donor sequence by 3 nucleotides compared to species with the conserved sequence.

Yasamin Mofrad, Kathryn Grant (PI), David Brewer, Kristina Ilina and Henary Maged (PI)

Georgia State University

BC10: Near-infrared Carbocyanine Dye for DNA Photocleavage via Mitochondrial Targeting with Triphenyl Phosphonium Groups

Photodynamic therapy (PDT) is an emerging cancer treatment that utilizes light-activated photosensitizers (PS) to generate reactive oxygen species (ROS), which induce targeted DNA damage. Near-infrared (NIR) light is particularly effective in PDT due to its ability to penetrate tissues deeply, facilitating efficient PS activation. Cyanine dyes, noted for their strong NIR absorption, show significant promise in PDT applications. This study examines a carbocyanine dye functionalized with triphenyl phosphonium groups to enhance mitochondrial delivery in cancer cells. Upon NIR irradiation, this dye facilitates apoptosis, potentially bypassing common cancer resistance mechanisms. The dye's spectroscopic and photochemical properties, as well as its DNA interactions, were analyzed. Results reveal notable DNA photocleavage upon NIR exposure, highlighting the dye's potential as a therapeutic agent in photodynamic applications.

Benjamin Kerbey, Malathy Shanmugam (PI), Remya Nair and An Vu Hong

Emory University School of Medicine - Department of Hematology and Medical Oncology

BC11: Inducing Ferroptosis In ETC Suppressed Multiple Myeloma

Venetoclax (Ven), a B-Cell Lymphoma 2 (BCL-2) inhibitor, has demonstrated notable efficacy in Multiple Myeloma (MM), particularly in patients with the t(11;14) translocation. Our lab has previously reported that diminished electron transport chain (ETC) function and reduced oxidative phosphorylation (OXPHOS), characteristic of t(11;14) MM, predict Ven sensitivity. Given that iron is a critical cofactor for maintaining ETC efficiency and mitochondrial enzyme activity, we investigated the effects of iron supplementation on MM cell growth and response to Ven. Strikingly, iron supplementation inhibited the proliferation of Ven-sensitive t(11;14) MM cells, while having no impact on resistant non-t(11;14) MM cells. Additionally, iron supplementation enhanced the cytotoxicity of Ven, allowing for increased efficacy at lower doses in t(11;14) MM. Yet, this combination had no effect on Ven-resistant non-t(11;14) MM. Mechanistic studies revealed that the iron-induced sensitization to Ven occurred through ferroptosis, an alternative form of cell death that is increasingly being recognized as a promising target in cancer therapy. Iron supplementation reduced the expression of the antioxidant protein GPX4, increased mitochondrial ROS levels, and triggered lipid peroxidation- all key hallmarks of ferroptosis. Furthermore, ferroptosis was confirmed as the driver of cell death, as treatment with the ferroptosis inhibitor ferrostatin significantly rescued cells from iron-induced death. This is the first study to demonstrate the sensitivity of Ven-sensitive t(11;14) MM to iron supplementation, offering a translationally relevant strategy for enhancing Ven efficacy in this subset of patients. Furthermore, our findings show the vulnerability of ETC-suppressed MM to ferroptosis, providing a promising avenue for future therapeutic exploration.

Yushan Zhang and Jenny J. Yang (PI)

Georgia State University

BC12: Optimized Purification of hProCA32.collagen1 for early diagnosis of CLDs (Chronic Liver Diseases)

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 a pivotal role. The fractions obtained from the SP column were dialyzed for effectively removing impurities evident on gel analysis.

The study conducted large-scale 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

Lu Chen, Jenny J. Yang (PI) and Enxi Zhang

Georgia State University

BC13: Mechanistic Study of the Calcium-Sensing Receptor (CaSR) in Cancer Progression and Therapeutic Potential

Calcium-sensing receptors (CaSRs) are critical G-protein coupled receptors involved in calcium homeostasis and have been linked to cancer progression; especially in cancers like prostate, breast, and colon, where CaSR expression is high in metastatic tissues. This study examines CaSR's role in cancer cell invasion and growth, highlighting its potential as a therapeutic target. Using a 2.1 Å resolution crystal structure, we identified key binding sites, providing insights into functional assays. In prostate cancer cell lines C4-2B-TaxR and CwR22Rv1, CaSR expression was significantly elevated compared to normal HEK293 cells, suggesting a link between CaSR and cancer cell invasiveness and drug resistance. Further, we investigated TNCA, a novel CaSR agonist, which enhances receptor activation in response to Ca^{2+} and Mg^{2+}, showing a tenfold higher efficacy than existing agonists like AMG416. This research supports the therapeutic potential of CaSR modulation in cancer treatment.

CHEMISTRY EDUCATION

Isaiah Paris, LaTonia Taliaferro-Smith, Simbarashe Nkomo (PI) and Austin Scharf (PI)

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CE01: Introduction to Green Chemistry: Bioreduction of (R)-Carvone and Chalcones Catalyzed by Baker's Yeast (BY) in Aqueous Mono- and Bi-Phasic Systems for Oxford's CHEM 203 L

The integration of green chemistry principles into undergraduate curricula is crucial for preparing future chemists. This study presents the development and implementation of a laboratory experiment utilizing Baker's Yeast (BY) as a biocatalyst for the asymmetric reduction of (4R)-(−)-carvone to (1R,4R)-dihydrocarvone in Oxford College of Emory University's CHEM 203L. Baker's Yeast is a widely used biocatalyst in green chemistry due to its high selectivity and mild reaction conditions. While previous studies have explored BY-mediated reductions of α,β-unsaturated carbonyl compounds, the selective production of (1R,4R)-dihydrocarvone from (4R)-(−)-carvone remains an area of interest. This study builds on existing literature which showcases the efficacy of the bioreduction of the α,β-unsaturated systems found in carvone and chalcone derivatives and seeks to optimize the biocatalytic reduction of carvone reaction for undergraduate laboratory experience. The curriculum design focuses on optimizing reaction conditions while introducing students to key concepts in biocatalysis, stereochemistry, and sustainable chemistry. The experimental protocol was systematically refined to balance educational objectives with practical constraints of an undergraduate laboratory setting. Students investigate the effects of BY and substrate concentrations, temperature, pH, and additives on the biotransformation. Optimal conditions (3.0 g BY, 2 mL substrate, pH 6.5, 40 °C, monophasic system) were identified, yielding 70-74% conversion and 92-99% diastereoisomeric excess of (1R,4R)-dihydrocarvone. The curriculum incorporates hands-on experience with Infrared Spectroscopy (IR), Gas Chromatography with Mass Spectrometry (GC-MS), and ^{1}H Nuclear Magnetic Resonance (NMR) for product analysis and purification, reinforcing spectroscopic interpretation skills and purification techniques. This multi-week experiment allows students to engage with green chemistry principles, experimental design, and advanced analytical techniques. Assessment of student learning outcomes demonstrates improved understanding of biocatalysis, stereochemistry, and sustainable reaction processes. The experiment's scalability and adaptability make it suitable for various undergraduate levels, from introductory organic chemistry to advanced biochemistry courses. This curriculum design not only contributes to the growing body of green chemistry education literature but also provides a model for incorporating industrially relevant, sustainable processes into undergraduate laboratories. Future work will focus on expanding this approach to other terpene derivatives and exploring potential interdisciplinary connections.

Eziada Ezinwa-Ezuma, Emmanuel Buabeng (PI), Sydney Taylor, Cierra Hickson, Ajahni Rodriguez and Gray Stamper

Georgia State University

CE02: Exploring Factors Influencing Student Enrollment Disparities in STEM Courses During the COVID-19 Pandemic

The COVID-19 pandemic has induced transformative shifts in the landscape of higher education, particularly impacting student enrollment patterns within the Science, Technology, Engineering, and Mathematics (STEM) fields. This research aims to investigate the factors that contribute to the differential enrollment rates observed across sessions of the same STEM course. The study specifically examines variables such as professor ratings, teaching styles, grading methods, class meeting durations, and other relevant aspects that have emerged as pivotal influencers during the pandemic era.

Observing a discernible trend of enrollment imbalances across multiple sessions of a single STEM course, this research seeks to understand what drive students to prefer one session over another. Notably, certain sessions witness a surge in enrollment accompanied by extensive waitlists, while others experience lower student interest, sometimes leading to the unfortunate closure of sessions. Through a comprehensive qualitative and quantitative analysis of the aforementioned factors, we aim to elucidate the mechanisms behind these enrollment disparities and provide insights that can inform administrative decisions and educational practices.

COMPUTATIONAL CHEMISTRY

Teresa Ariza, Yakini Brandy (PI), Linda Ho, Ivey Portis, Irma Ramirez-Rodrigues, Insherah Qazi, Danni Nguyen and Zaina Chagani

Agnes Scott College

CC01: The Development and Testing of Docking Parameters in COX-1 and 2 Enzymes

Cyclooxygenase-2 (COX-2) is responsible for catalyzing the conversion of Arachidonic Acid to prostaglandins that induce pain and inflammation in the body, while Cyclooxygenase-1 (COX-1) produces prostaglandins that maintain homeostatic functions in the body. Since both enzymes share similar structures, traditional Non-steroid Anti-inflammatory Drugs (NSAIDs) like aspirin do not effectively inhibit COX-2 without negatively affecting COX-1. Therefore, selective COX-2 inhibitor NSAIDs are desirable, but most of them are cardiotoxic. Hence, there is a need to find effective selective COX-2 inhibitors with fewer side effects. Maestro was used to develop docking parameters to prepare for future *in silico* studies of both the COX-1 and COX-2 enzymes. Our models have successfully discriminated between the known active and inactive COX-1 and 2 selective ligands found in the DUD-E database. The parameters have comparable AUC values of 0.75 and 0.77 in COX-1 and 2, respectively, while the COX-2 model exhibited a hit rate of 94% in the first 50 molecules.

Nicholas Wong, Dharmeshkumar Patel (PI), Daniel Hua, Daniel Pun, Andrew Wang and Raymond Schinazi

Emory University

CC02: Computational Approach to Predict Neuraminidase 1 Drug Resistance to Oseltamivir and Zanamivir

Influenza is an infectious virus responsible for numerous pandemics from the 20th century and the 21st century. Its virology is dependent on the mechanism the NA enzyme which facilitates the release of the virus from infected cells. Although drugs such as zanamivir and oseltamivir have been developed to inhibit NA through direct interactions with the active site, there are accounts of drug resistance towards either or both drugs in NA. Most drug resistance mutations in NA emerged through the N1 neuraminidase subtype because of single nucleotide substitution and such mutations were responsible for the 2009 H1N1 pandemic. Modern experimental and clinical approaches to study drug resistance are laborious and time costly. So, computational predictions would help to design better drugs which are not impacted by those mutations. As such due to the prevalence of drug resistant mutations in N1, we validated our in-house computational method to predict such resistance and dual resistance mutations in N1 for oseltamivir and zanamivir. The binding sites from 3-D structures of N1 complexed with either oseltamivir, zanamivir or sialic acid were selected for the prediction each residue within the binding pocket was mutated initially through residue scanning and Prime MM-GBSA calculations. MM-GBSA calculations with decreased affinity to oseltamivir and retained or enhanced affinity to sialic acid were studied to see if these mutations were a result of single nucleotide polymorphism. We successfully predicted four clinically reported to drug resistance mutations in oseltamivir and 2 that exhibited dual resistance characteristics to zanamivir. 33 additional mutations were also predicted to correspond to drug resistance in oseltamivir and 24 in zanamivir.

Matthew Rohan, Joshua Kretchmer (PI), Yi-Siang Wang, James Zhong Manis and Thomas Orlando

Georgia Institute of Technology

CC03: Modeling Intermolecular Coulomb Decay with Non-Hermitian Real-Time Time-Dependent Density Functional Theory

In this work, we investigate the capability of using real-time time-dependent density functional theory (RT-TDDFT) in conjunction with a complex absorbing potential (CAP) to simulate the Intermolecular Coulombic Decay (ICD) processes following the ionization of an inner-valence electron. We examine the ICD dynamics in a series of noncovalent bonded dimer systems, including hydrogen-bonded and purely Van der Waals (VdW)-bonded systems. In comparison to previous work, we show that RT-TDDFT simulations with a CAP correctly capture the ICD phenomenon in systems exhibiting a stronger binding energy. The calculated time scales for ICD of the studied systems are in the range of 5−50 fs, in agreement with previous studies. However, there is a breakdown in the accuracy of the methodology for the pure VdW-bonded systems. Overall, the presented RT-TDDFT/CAP methodology provides a powerful tool for differentiating between competing electronic relaxation pathways following inner-valence or core ionization without necessitating any *a priori* assumptions.

Evan Myers, Raphael Ribeiro (PI) and Gustavo Aroeira

Department of Chemistry, Emory University

CC04: Spectral Measures of Quantum Chaos and Wavefunction Delocalization in Photonic Wires

Achieving efficient energy transport is a central challenge in developing photonic devices. Polaritons formed by cavity-mediated strong light-matter interactions have gained significant attention for unique physical properties and applications to enhance energy transport in photonic technology. Here, we employed a theoretical model of a nanoscale quantum wire that confines photons to two dimensions and hosts molecules represented as dipoles. Important parameters in this model are the static disorder, which measures the spread of excitation energies in the molecular ensemble, and detuning, which is the difference between the average molecular excitation and the minimum photon energy. We study how these parameters affect quantum chaos and wavefunction delocalization in our photonic wire model, which are known to enhance energy transport. To characterize the quantum chaos in our model, we probe the level spacing ratio (<r>) of the eigenstates of weakly and moderately coupled polaritonic states. Moderate static disorder gives <r> values consistent with those expected for a chaotic system and energy relaxation properties. Positive (negative) detuning led to <r> values consistent with a system displaying quantum chaos under higher (lower) disorder, indicating robust delocalization. In every considered case, suppressed energy transport and a lack of chaotic dynamics were observed at high disorder. Insights gained from this work may prove useful in amplifying energy transport in novel photonic devices.

Brandon Persaud and Neville Forlemu (PI)

Georgia Gwinnett College

CC05: Computational Investigation of the Interactions of Quinoline Derivatives with NS3 Dengue Fever Protein

Dengue fever remains a critical public health concern due to its global prevalence (2.5 billion people) and potential for severe outbreaks. This research investigates the potential of modified chloroquine derivatives as potential therapeutic agents for Dengue fever focusing on the Dengue virus's Non-Structural Protein 3 (NS3). This crucial enzyme plays a vital role with its helicase and protease functions. A 3D model of its tetrameric structure (UniProt ID: 7VMV_F) was obtained from Protein Data Bank. *In silico* ligand modification of chloroquine and existing synthesized derivatives using SwissDock molecular suites software was used to explore their interactions with NS3 protein. A molecule's effectiveness was determined by lowest Attracting Cavities values, which has a linear relationship to adsorption energy. The lower adsorption energy increases the thermodynamic favorability of sterically hindering the helicase and protease function of NS3. The energetically favorable molecules were found to be Isoquine, Amodiaquine, and Chloroquine.

Michelle Yusupov, Neville Forlemu (PI) and Jaydy Hernandez

Georgia Gwinnett College

CC06: Exploring 4-Aminoquinolines as Antiviral Agents for Molecular Docking

The effectiveness of current COVID-19 antiviral therapies and vaccines continues to be impacted by mutations that result in changes in viral DNA and protein structures. In this study, quinoline-4-amines are modeled as viable drug candidates by fine-tuning to increase binding affinity. The binding affinity of 42 derivatives of quinoline-4-amines and eight COVID-19 receptors were estimated through molecular docking using the Molecular Operating Environment software. The three-dimensional structures of the COVID-19 receptors used were downloaded from the protein databank and include Main-protease (Mpro with PDB ID-1P9S), Transmembrane Serine Protease (TMPRSS2 with PDB ID-7MEQ), and Janus Kinase 2 (JAK 2 PDB ID-8BA4). These receptors are critical in processing viral polyproteins into functional components and facilitating viral attachment to host cells. The 4-aminoquinoline derivatives are grouped into six categories based on a balance between hydrophobicity and polarity dependent on the position and number of aryl groups on the quinoline framework, heterocyclic nitrogen, and oxygen ring structures. Final docking calculations were performed using over 35,000 solution structures generated from conformational space calculations of 42 quinoline-4-amines derivatives at a pH of 7.

Preliminary analysis of the data indicates that the affinity between all the ligands and their solution conformation with the protein receptors are strong and range from –5 kcal/mole to –9 kcal/mol. All the favorable conformational complexes are stabilized by a mix of hydrogen bonding and hydrophobic aromatic interactions. The strongest affinities are observed with the coronavirus spike glycoprotein (PDB ID-6VXX) and C-terminal tail of SARS-CoV-2 Orf6 complex (PDB ID-7VPH). The critical amino acid residues and contacts were examined as well as methods to improve binding affinities of the quinoline-4-amine ligands.

Ethan Waybright, McKenzie Campbell (PI) and Shannon Yost

Anderson University

CC07: A Proposed Synthetic Ligand for the Treatment of Diabetes Insipidus

Central diabetes insipidus is a condition characterized by inadequate production of the hormone vasopressin, resulting in polydipsia and polyuria. The current treatment for this condition is a synthetic analog of vasopressin known as DDVAP or desmopressin. This medication, while a potent treatment, exhibits a poor binding probability for the Vasopressin 2 Receptor (V2R). This, as well as its poor gastrointestinal absorption, means a larger dose at more regular intervals is required to be effective. Thus, a more efficient treatment is needed to better treat patients suffering with polyuria and polydipsia without increasing the cost of synthesis.

The Swiss Institute for Bioinformatics provides a suite of bioinformatic programs as free online resources that are not only reliable tools, but also are user friendly, requiring minimal experience to use. By capitalizing on these tools, a novel treatment has been constructed computationally that exhibits the potential to outperform DDVAP in combating the effects of diabetes insipidus.

INORGANIC CHEMISTRY

Trinity Brooks and Ryan Meier (PI)

University of North Georgia

IC01: Effects of Surrounding Gas on Triboluminescence Complexes

Triboluminescence (TL) is the phenomenon where light is emitted when a substance is ground, crushed, or struck. This mechanism is not well understood and is still a topic of active research today. A variety of substances and compounds were studied to determine the effects of gases on TL such as $[Cu(NCS)(py)_2(PPh_3)]$, sucrose, and wintergreen mints. Substances were studied in a glove bag under different gaseous conditions (sulfur hexafluoride, helium, and argon) to observe changes in color and intensity of TL. Attempts were made with other triboluminescent compounds such as $[Mn(Ph_3PO)_2Br_2]$ and $[EuD_4TEA]$. These new findings provide insights to how different factors have an effect on TL and provide a deeper understanding to the phenomenon.

ORGANIC CHEMISTRY

Nyasha Musoni and Frank McDonald (PI)

Emory University

OC01: Development of Enantioselective Hantzsch Ester Synthesis for Drug Repurposing Applications

Nicardipine, a commercially available drug used to treat hypertension as a racemate, also inhibits the EED biochemical pathway, impacting chemotherapy drug resistance in cancer cell lines. Having an extensive pharmaceutical profile for treating hypertension, nicardipine's potential uses for prostate cancer are of interest, especially in the context of drug repurposing. Previous enantiomeric resolution work has revealed a relationship between nicardipine enantiomers and the two pathways: the R-enantiomer favoring anti-hypertension and the S-enantiomer favoring anti-chemoresistance. We hypothesize that the chirality of the groups attached to the third carbon of the central ring core may impact nicardipine's sensitivity to the chemotherapy resistance pathway and minimize sensitivity to the anti-hypertension pathway. Thus, the synthesis of novel chiral nicardipine analogs applicable to an increased scope is the focus of this work. To find an optimized procedure for enantioselective synthesis of nicardipine analogs with different chirality at this carbon, work was done in two steps: 1) optimizing the synthesis and purification of the ligand and reagents necessary for the reaction and 2) using N,N'-dioxide-metal complexes in an enantioselective Hantzsch Synthesis seen in the literature for dihydropyridine products similar to nicardipine. Nuclear magnetic resonance (NMR) shows the successful and reliable synthesis of the desired chiral ligand, oxobutanoate reagent, and aminocrotonate reagent in relatively high yield. Though a general procedure for synthesizing this family of ligands can be found in the literature, none prior existed for the specific chiral ligand used here. It was found that the dialkylation of this ligand synthesis results in a faster second alkylation than previously anticipated. Control experiments of the Hantzsch Synthesis without the ligand and without catalyst show the successful synthesis of the intended dihydropyridine product, providing a reference for comparison for future enantioenriched products. With the first goal complete, work on the enantioselective Hantzsch Synthesis of more nicardipine analogs sensitive to the anti-chemoresistance pathway is possible and in progress.

Kathomias Turnage and Ajay Mallia (PI)

Georgia Gwinnett College

OC02: Comparison of Spectroscopic, Thermal, and Gelation Properties of Anthraquinonylalkanamides

Anthraquinonylalkanamides with varying alkyl chain lengths (n = 12, 14, 16, and 18) were synthesized and characterized. Anthraquinonylalkanamide in dichloromethane exhibits absorption and emission maxima centered at 415 nm and 526 nm, respectively. The properties of their gels in varying polarity of liquids, including critical gelator concentrations, periods of stability, and gel melting temperatures, as well as the thermodynamic and spectroscopic properties of the anthraquinonylalkanamides, will be presented.

Sebastian Cruz and Maged Henary (PI)

Georgia State University

OC03: Synthesis of Squaraine Dyes for Potential Targeting and Imaging of Mitochondria

Biological sensors that absorb and reflect light within the NIR region are increasingly being recognized for their *in vivo* optical clarity, as NIR wavelengths exceed the absorption limits of most biomolecules. This results in a higher signal-to-background noise ratio (SNR) due to less light scattering and autofluorescence from biological molecules. Various compound classes, including the squaraine dye, have been developed and enhanced to maximize NIR properties. Squaraine fluorophores have demonstrated high fluorescent quantum yields, strong absorbance bands, and significant molar absorptivity. By functionalizing these compounds with a moiety targeting mitochondria, we can selectively stain mitochondrial cells to monitor their activity. Mitochondria, critical in apoptosis, are key targets in cancer cell imaging. The inner mitochondrial matrix (IMM) exhibits a unique, highly negative membrane potential distinct from other organelles. To effectively target the mitochondria, a highly charged catanionic dye with adequate lipophilicity is required for accumulation and uptake into the matrix. Incorporating a triphenylphosphine moiety allows the dye to mimic the behavior of the cationic DTTP molecule, targeting and binding to the mitochondrial matrix and integrating into the inner membrane. Herein, we report the synthesis and optical properties of a novel set of squaraine dyes functionalized with triphenylphosphine, aimed at enhancing mitochondrial targeting and imaging.

Renee Perez, Maged Henary (PI) and Guliz Ersoy

Georgia State University

OC04: New Hemicyanines as Potential Optoacoustic Agents

Recent advancements in biomedical imaging have underscored the potential of new contrast agents that offer high specificity and sensitivity. Optoacoustic imaging is particularly notable for its ability to penetrate deeper into tissues and reduce scattering compared to traditional techniques like MRI, CT, PET, and fluorescence imaging. Unlike fluorescence imaging, which relies on light emitted from excited molecules, optoacoustic imaging employs ultrasound waves generated during molecular relaxation, providing superior imaging depth. This study centers on the synthesis of a sulfur-substituted hemicyanine derivative via a retro Knoevenagel reaction, characterized using ^{1}H NMR and UV-Vis spectroscopy. The replacement of oxygen with sulfur may significantly enhance the photothermal efficiency of hemicyanines and optimize the optoacoustic signal.

Whitney Wallace, Sahithi Doddaka and Margaret Meadows (PI)

Mercer University

OC05: Progress Toward the Synthesis of a Color-Changing Molecular Sensor for Phthalate Esters

Phthalate esters are endocrine disrupting chemicals (EDCs), which are often used as plasticizers with both home and medical applications. Recent data show an association between phthalate esters and hypothyroidism, a deficiency in thyroid hormones, with broad neurological, cardiovascular, and developmental implications. Our research addresses this by developing a color-changing molecular sensor for detecting phthalates in aqueous solutions. Previous research has reported a sensor for carboxylate dianions, including phthalates, with moderate success. However, their synthetic approach uses harsh reagents and limits the sensor's potential applications. Using more accessible and safer techniques, we are exploring two synthetic routes to our target molecular sensor. Following the synthesis of our target, we plan to use it for the detection of hydrolyzed phthalate esters in aqueous solutions. This research can help develop reliable, safe sensors for a wide range of environmental and biological applications.

PHYSICAL CHEMISTRY

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Spelman College[1], University of Massachusetts Amherst[2],

PC01: Advancing Hair-Typing with Mechanical Analysis

The diversity of hair textures has necessitated characterization using hair typing systems, such as the Andre Walker system that differentiates straight, wavy, curly, and coily hair with numbers 1-4, respectively, and secondary characteristics such as thickness with letters a-c. These systems fall short in that they lack the quantitative characterization of hair needed to optimize hair treatment. This study aims to bridge that gap by investigating the tensile strength and elasticity of 12 human hair samples across four hair textures (straight, wavy, curly, and coily), focusing on the effects of different conditioner treatments. A texture analyzer was used to collect stress-strain data, and the mechanical properties of elastic modulus and ultimate tensile strength were evaluated. Hair samples were washed with a 1% sodium dodecyl sulfate solution and treated with six conditioners in two categories - oil-soluble (cyclomethicone and stearyl alcohol; prepared with coconut oil) and water-soluble (glycerine, d-panthenol, hyaluronic acid, and aloe vera; prepared with DI water). Preliminary results demonstrate that conditioner treatments had a net positive effect on elastic modulus, particularly for curly and coily textures - suggesting treatment integration into the hair fiber composite. The effects on tensile strength were less conclusive, with mixed results across textures. Future research incorporating microscopy is proposed to further investigate porosity and treatment penetration. This study highlights the need for a more data-driven hair-typing system focused on mechanical properties, offering valuable insights into hair care optimization.