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Poster 1 (Biochemistry): A salivary hormonal study on individuals of African ancestry living in different socioeconomic environments, in order to understand etiology of prostate cancer

Presenter: Brittany Jones

PI: Wathsala Medawala

Co-authors: Rachael Cundey, Megan Andrews, Dr. Ernie Kaninjing, Dr. Chavonda Mills and Dr. Solomon Rotimi

Institution: Georgia College and State University

This study aims to better understand the etiology of prostate cancer in men of African ancestry. While incidence and mortality of prostate cancer have decreased in the US in recent decades, men of African descent are disproportionately affected. This work examines hormone levels in saliva samples and demographic data of men in different socioeconomic environments to better understand their possible link to prostate cancer onset and progression. Using ELISA kits specific to either testosterone, cortisol, or dehydroepiandrosterone (DHEA), hormone levels were determined for each individual's saliva using standards and low- and high-quality control samples for validation. The saliva samples collected from individuals living in African countries (n=21) had a mean testosterone concentration of 93.43 pg/mL with a standard deviation of 35.924 pg/mL, a mean cortisol concentration of 0.120 mg/dL with a standard deviation of 0.078 mg/dL, and a mean DHEA concentration of 79.169 pg/mL with a standard deviation of 60.098 pg/mL. The saliva samples collected from individuals with African ancestry in the United States (n=92) had a mean testosterone concentration of 94.680 pg/mL with a standard deviation of 35.218 pg/mL, a mean cortisol concentration of 0.136 mg/dL with a standard deviation of 0.101 mg/dL, and a mean DHEA concentration of 57.263 pg/mL with a standard deviation of 52.033 pg/mL. The study will help understand how hormone levels change in different environments, and further research and studies will assist in linking the data to the onset of prostate cancer.

Poster 2 (Biochemistry): *Proteolysis of the Ribosome*

Presenter: Jennifer Seoyoung Kim
PI: Loren Dean Williams
Co-authors: Kavita R. Matange
Institution: Georgia Institute of Technology

The *E. coli* 70S ribosome is composed of a large 50S subunit (LSU) and a small 30S subunit (SSU). The LSU contains the active site which forms peptide bonds and the SSU decodes mRNA, together forming the translation system which synthesizes all proteins a cell needs. The ribosome can be interpreted as a molecular fossil that provides a record of the biochemical processes that led the evolution of life today. At the core of the ribosome are universal ribosomal proteins that are conserved across all three domains of life. Previous experiments using protease Trypsin to digest the *E. coli* ribosome in the presence of ions has demonstrated that as the amount of Mg^{2+} increases, there is a decrease in the digestion of ribosomal protein (rProtein) L2, a 30 kDa rProtein located in the LSU. One explanation for the Mg^{2+} dependency of L2 is its ability to form Mg^{2+} mediated interactions with rRNA which stabilizes the structure of the ribosome. Here we digested *E. coli* ribosome using a variety of proteases including Proteinase K, Elastase, and Chymotrypsin. Digestion using Proteinase K displays a clear digestion product of L2 of about 28 kDa. Similarly to Trypsin, Chymotrypsin also demonstrated preliminary results of a relationship between the concentration of Mg^{2+} ions and the extent of digestion of L2. Overall, these results suggest that proteases exhibit different behaviors and results from one another in digesting the ribosome. Ultimately our goal is to minimize the ribosome by using a protease cocktail to digest parts of the ribosome to obtain structural and functional information that could provide insight into the history and development of biology on Earth.

Poster 3 (Biochemistry): ***Miconazole Nitrate: Utilization of Topical Antifungals for Seborrhœic Dermatitis and its Stimulatory Effects on Hair Growth***

Presenter: Imanii Kolailat
PI: Michelle Gaines
Institution: Spelman College

Malassezia is a fungus that normally lives on the scalp and has been proven to result in oxidative damage. This yeastlike fungus is the primary cause of dandruff, which affects over half of the global adult population. Similar to Candida overgrowth during yeast infections, dandruff is caused by the overgrowth of skin cells with Malassezia fungi. Miconazole Nitrate is the antifungal active ingredient found in Candida antifungal suppositories (Monistat®) that removes fungus within cells. Malassezia removal has also been observed to combat dandruff, when Miconazole Nitrate creams are applied to the scalp. The most attractive reason to apply Miconazole Nitrate products to the scalp is to induce hair growth. However, there are major concerns with using Miconazole Nitrate as a long-term hair growth reagent, including neurological complications such as ear ringing and headaches and additional hair loss. This research project focuses on determining an appropriate dosage of Miconazole Nitrate that can still induce hair growth but minimize the disconcerting side effects. To answer this research question, a methodical review of the literature was conducted from SciFinder and PubMed. After narrowing the search terms, a handful of articles were compiled and used as evidence to support the project objective.

Poster 4 (Biochemistry): ***Identifying Antibiotic Resistant Bacteria from Raman Spectra via Neural Network Analysis***

Presenter: Alice Lundgren
PI: Marcus Cicerone
Co-authors: Jessica Zahn and Arno Germond
Institution: Georgia Institute of Technology

Raman spectroscopy, aided by machine learning techniques, can provide label-free discrimination between highly similar biological species. Here we compare two classification models, an Artificial Neural Network (ANN) and a Support Vector Machine (SVM) for discriminating between Raman spectra of eleven bacterial mutants of *Escherichia coli* MDS42. We also extract strain-specific (and function-specific) spectral features emphasized by the models. We find that, for the present dataset, both models discriminate with similarly high accuracy, sensitivity, and specificity a 1:2 ratio of input features to training samples per class. There are, however, some notable differences which we discuss in terms of specific spectral features emphasized by each model and of generic model properties.

Poster 5 (Medicinal Chemistry): Sildenafil Analogs as PDE5 Inhibitors Localized in the GI Tract

Presenter: Colin Miller, Jr.
PI: Dr. Iryna Lebedyeva
Co-author: Dominique Lyons
Institution: Augusta University

Sildenafil is a drug commonly used for the treatment of erectile dysfunction. It has been known to have many beneficial effects, such as its aid in helping to prevent heart failure. Many of these effects occur due to Sildenafil working as a PDE5 inhibitor. PDE5 is an enzyme that facilitates the control of blood flow and cell signaling. By inhibiting the PDE5 enzyme, muscles and blood vessels tend to relax, increasing blood flow. Recently, it has been discovered that drugs known as phosphodiesterase-5 inhibitors (PDE5i) can prevent colorectal cancer in animals, and recent evidence suggests that these drugs will also be effective in humans. A problem with repurposing contemporary PDE5i such as Sildenafil for colon cancer prevention is the drug's side-effects and drug-drug interactions. In this project we created novel PDE5i drugs that eliminates these unwanted effects by keeping the drugs in the colon, where they can work their magic, minimizing or completely avoiding leakage into the bloodstream. This project is exploring Sildenafil alongside other PDE5 inhibitors designed to remain in the Gi tract. By modifying the structure of Sildenafil, we have created novel drug candidates that are expected to be localize in the colon while keeping their beneficial effects of being a PDE5 inhibitors. As a result, the onset of colon cancer in humans can be prevented.

Poster 6 (Biochemistry): *Isobarbaloin (Aloin B) Inhibits the Enzymatic Activity of Papain like Protease (PLpro) but not 3-Chymotrypsin like Protease (3CLpro) of SARS-CoV-2 in vitro*

Presenter: Devin Shane Lewis

PI: Vicky Mody

Co-authors: Joanna Ho, Savannah Wills, Srujana Rayalam and Shashidharamurthy Taval

Institution: Philadelphia College of Osteopathic Medicine

The most common host entry point of human adapted coronaviruses (CoV) including the recent pandemic SARS-CoV-2 is through the initial colonization is in the nostril and mouth region which is responsible for spread of the infection. Most recent studies suggest that the commercially available oral and nasal rinse are effective in inhibiting the viral replication. However, the anti-viral mechanism of the active ingredients present in the oral rinses have not been individually studied. Several studies have suggested that the viral proteases play a major role during the viral replication therefore serve as better drug targets. PLpro and 3CLpro are proteases that are essential for replication of the emerging infectious CoV including SARS-CoV-2. Therefore, in the present study we have investigated the enzymatic inhibitory activity of active ingredients of commonly used oral rinses against SARS-CoV-2 PLpro and 3CLpro enzymes. We have performed the in vitro enzymatic assay in presence of aloinB, chlorhexidine, ecalyptol, hexetidine, menthol, triclosan, methyl salicylate, sodium fluoride and providoneiodide to investigate their inhibitory activity against two important proteases of SARS-CoV-2. Importantly, we observed that only aloinB effectively inhibits the PLpro but not the 3CLpro. Structural analysis of aloinB interaction with PLpro revealed that, aloinB forms Hydrogen bond with Tyr268 of PLpro, which is critical for its enzymatic activity. Taken together, these studies suggest that aloinB, a phenolic small molecular weight compound present in Aloe vera plant inhibits the enzymatic activity of PLpro of SARS-CoV-2 suggesting the potential beneficial effect in reducing the spread of SARS-CoV-2 virus. However, these studies need to be validated in pre-clinical and clinical studies.

Poster 7 (Environmental): Rapid Evaluation of Sustainable Barrier Layer Film Performance Using Polarized Optical Microscopy

Presenter: Callie Goins
PI: Eric Shen
Institution: Georgia Institute of Technology

Cellulose nanocrystals (CNCs) and chitin nanofibers (ChNFs) are two biologically sourced materials that can be used to create biodegradable and sustainable oxygen and moisture barrier materials comparable to widely available barrier layers like PET. ChNF-CNC films are prepared by collaborators by spraying coatings of these two materials onto cellulose acetate (CA). Previous work has demonstrated a link between the oxygen permeability, and therefore performance as a barrier layer, and the microstructure of cellulose based barrier layers, but this has not yet been demonstrated for ChNF-CNC blends. While work with CA-ChNF-CNC layers has proved that the films are successful as barrier materials, a central goal of the current project is to be able to compare the microstructure of CA-ChNF-CNC films to their individual oxygen permeabilities in order to optimize these barrier properties. This will be done by examining polarized optical microscopy photographs of films in order to determine order parameter. From this, we demonstrate how polarized optical microscopy is a simple and straightforward technique for evaluating order parameter and investigate the relationship between order parameter and oxygen permeability for a series of ChNF-CNC films coated under various conditions.

To further demonstrate the effectiveness of these barrier layers, we encapsulate electrochromic polymers (ECPs), materials which undergo user-controlled on-demand color change and have been targeted for applications in printed displays, but are very sensitive to a combination of oxygen and sunlight. We compare the performance of the ChNF-CNC barrier layers to PET, which is widely used industrially, by tracking the loss in absorbance of each of two polymers: P[DOT-(C₈H₁₇)₂] and P[DOT-(OEtHx)₂]. This will be done by looking at the loss of absorbance in each polymer as the ECP films are irradiated under PET as a function of time. A central finding of this is that while P[DOT-(OEtHx)₂] is essentially fully degraded after 252 hours of irradiation, P[DOT-(C₈H₁₇)₂] does not significantly degrade even after long amounts of irradiation. These results are consistent with previous tests using ChNF-CNC films as barriers, demonstrating that these films perform comparably to PET.

Poster 8 (Environmental): Greening The Copper Cycle

Presenter: Byron Fisher
PI: Cynthia Woodbridge
Co-author: Tracy Conrad
Institution: Georgia Gwinnett College

Through modification of the procedure, the overall E-factor of the Copper Cycle lab will be reduced. Using the original lab as the reference point, steps were added/removed, and the percent recovery of copper yielded with those changes were compared to the original lab. The modifications include heating the solution with the CuO precipitate for 5 minutes and letting it cool for another 5 minutes; the use of a Buchner funnel after heating the CuO solution; cutting up the aluminum foil before adding to the CuCl₂ solution; and storing the recovered copper for future reuse. Through these adjustments, we hope to reduce the high E-factor of the Copper Cycle lab and reduce overall costs associated with the lab.

Poster 9 (Environmental): Recycling of Iron Oxide for Photoelectrochemical Cells

Presenter: Danielle Mckay
PI: Linda de la Garza
Institution: Valdosta State University

Iron(III) oxide, Fe₂O₃, an abundant and stable semiconductor found in rust, has become increasingly studied over the years in photoelectrochemical cells because of its ability to convert energy in the visible electromagnetic spectrum and split water to produce hydrogen gas. Nanoparticulate solutions of Fe₂O₃ were prepared using the hydrolysis reaction of iron(III) ions from both lab grade and recycled rust materials. Absorbance measurements were then taken using the UV/Vis-NIR Spectrophotometer. Solutions were concentrated and applied onto conductive indium tin oxide (ITO) slides using a dip coating method. To increase the photocurrent production and improve the fast recombination rates of Fe₂O₃, the nanoparticulate films were further modified with small molecules such as dopamine and 3,4-dihydroxyphenylacetic acid. The films were lastly characterized and compared using spectroscopic and electrochemical techniques. For both dopamine and dopac modified films, the current is higher than for unmodified Fe₂O₃ films between 350 and 500 nm. The IPCE% increases about 4 times upon molecule modification from 0.50% to almost 2.0% at 400 nm.

Poster 10 (Science Education): Student Learning Experiences During and After an Online Chemistry Course

Presenter: Leah Davenport
PI: Dr. Kathryn Kloepper
Co-author: Kaylee Barger
Institution: Mercer University

All students experience remote learning differently. This difference in experience is largely based on a student's own learning and study strategies, their attitudes towards science, and how their professors contribute to their remote learning. This work builds on a previous study that investigated student learning values in an online chemistry course for non-majors across four years, the pre-COVID-19 cohorts of 2017, 2018, and 2019, and the post-COVID-19 remote instruction cohort of 2020. Here we extend the study to a 2021 cohort to investigate (1) similarities and differences in learning strategies and (2) similarities and differences in student values for faculty support. Surveys were coded using thematic analysis and compared across five years of students. We also report on future plans for investigating long-term persistence of science attitudes and application of learning.

Poster 11 (Inorganic): Corrosion Prevention on Aluminum Alloy

Presenter: Andrea Brenner
PI: Bharat Baruah
Institution: Kennesaw State University

Aluminum alloy (Al-alloy) is a widely used metal in construction, aerospace, aviation, and other necessary fields due to its lightweight and tweakable properties. However, corrosion is inevitable on metals and alloys, and that causes millions of dollars of revenue loss every year. Therefore, we propose to research the fabrication of a coating to prevent corrosion on Al-alloy. This study uses an iron-based metal-organic framework (MOF) and polyurethane (PU) based composite coating to prevent corrosion on the Al-alloy. The makeup of the composite material is changed by varying the percentage of MOF. In addition, a binder, curcumin, is used to enhance the homogenization between MOF and PU. We characterize the coating by FTIR, XRD, UV-visible-DRS, and SEM. The corrosion prevention properties of the coating are assessed using electrical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP).

Poster 12 (Inorganic): Crystal Engineering in Gel

Presenter: Nathan O'Neill
PI: Peter Rosado
Co-author: Joseph White
Institution: Georgia College & State University

It is common knowledge that the growth of crystals is usually done through the dissolving of a solute in a supersaturated solution and allowing said solution to cool. There is an inherent necessity to grow larger and more characterizable crystals for processes such as X-ray diffraction and other physical characterization techniques. The field of crystal engineering has seen a boom as of late in pharmaceuticals[1] and material science[2]. Thus, the aim of this project is to utilize the well-known gel technique to calcium maleate crystals, to pin-point adequate and consistent crystal growing techniques to apply to other systems. By growing these crystals inside of a gel, the crystals are given a three-dimensional space to grow in without any walls for support. This process was attempted in several ways with various results. Such as a salt solution injected into the center of the still forming gel, added on top of a still forming gel and mixed, as well as placing the solution on top of a formed gel and allowing small amounts of solution to diffuse throughout the gel. Generally, the crystals grown in gel become cubical in shape and significantly more resilient than their non-gel counterparts depending on the point within the gel that the crystal formed with the crystal sizes increasing the further they have traveled into the gel. The density of the gel and the method with which the salt solution was introduced had a considerable impact on the crystals formed resulting in crystals between 3 and 5 mm in length. Here are discussed the attempts to control growth of crystals through silica gel media.

References:

1. Z. Gao; S. Rohani; J. Gong; J. Wang. *Recent Developments in the Crystallization Process: Toward the Pharmaceutical Industry. Engineering*. Vol. 3. 2017. pp. 343-353.
2. D.G. Patel; J.B. Benedict. *Crystals in Materials Science*. IntechOpen [online]. 2012.

Poster 13 (Inorganic): Surfactants Contribution to Tress Damage of Human Hair

Presenter: Orlasha Phillips-Pickens
PI: Dr. Michelle Gaines
Institution: Spelman College

Human hair can become damaged in many ways thus affecting its properties, and surfactants are one of those ways. In this research, I aimed to conduct a Critically Appraised Topic (CAT) and use the PICO method. It is hypothesized that by understanding the surface chemistry of hair strands, their interaction with different surfactants will determine the mechanism in which the surfactants contribute to the damage of the hair fiber. The fiber's charge, density, and shape could all contribute to the way that surfactants such as hair gels and components in shampoos affect the strand. To determine the possible interactions, the properties of surfactants were first studied to understand their general nature. The surface properties of hair were then researched to compare to the found properties of surfactants. Surfactants are amphoteric and cationic surfactants influence the deposition of cationic polymers onto keratin surfaces due to their large molecular weight. The buildup of keratin in the fiber seems to build its strength. This research consisted of conducting a systematic review into the demethylation of keratin protein residues in the hair and the role that surfactants contribute to that. The primary search engines used were SciFinder and PubMed.

Poster 14 (Analytical): Analysis of different types of alcohol using gas chromatography

Presenter: Ann Cormier
PI: Dr. Anne Gaquere-Parker
Co-author: Abigail Watson
Institution: University of West Georgia

A series of primary homologous alcohols, starting from 1 carbon to 11 carbon atoms, was chosen to be analyzed by gas chromatography at different temperatures ranging from 50 °C to 200 °C. Retention times were collected to establish a relationship between the retention times and the molecular mass of the alcohols at different temperatures. Results show an inversely proportional relationship between the molecular mass and the retention time with a correlation coefficient of 0.972.

Poster 15 (Organic): Diversifying the Toolkit: Peptide Macrocyclization through Cobalt-catalyzed Carboamination

Presenter: Sophia Xu
PI: Simon B. Blakey
Co-author: Christopher D. Poff
Institution: Emory University

Direct interactions between proteins are important in regulating biological systems, have disease implications, and have become a focus in drug discovery. However, these protein-protein interactions (PPIs) are often viewed as challenging or even “undruggable” targets. Due to their potential of modulating PPIs, macrocyclic peptides are recognized as a promising class of bioactive molecules for therapeutics, with other pharmacological advantages including high binding affinity, metabolic stability and target selectivity compared to acyclic counterparts. Therefore, it is highly desirable to develop chemical methods for the synthesis of peptide macrocycles. Recently, transitional metal-catalyzed C-H activation has shown to aid in macrocyclization of peptides, especially those not accessible to traditional methods including enzymatic resolution. Although most of the current approaches involve palladium or copper as catalysts, attention has been brought to other metals as the field diversifies. Herein, we propose a cobalt-catalyzed carboamination process to achieve an intramolecular macrocyclization of linear peptides. With preliminary success on an intermolecular model system, the current emphasis is on linear peptide synthesis to test macrocyclization.

Poster 16 (Organic): Synthetic Efforts Towards CD437-Azaborine Analogs

Presenter: Brittney Haney
PI: William Wuest
Co-author: Cassandra Schrank
Institution: Emory University

A specific retinoid against methicillin-resistant *Staphylococcus aureus* (MRSA), known as CD437, has piqued our interest and led to the development of a range of analogs, some of which have demonstrated significant activity against gram-positive pathogens in past research. Our best performing compound, analog 2, has also shown a high affinity for retinoid-binding proteins with a concentration-dependent relationship and a low solubility in serum. These factors force us to question the therapeutic viability of these compounds but have also brought us to the consideration of isosteric substitutions within the scaffold of the molecule to circumvent these issues. We proposed a new class of analogs incorporating an azaborine substitution in place of the naphthalene moiety. Azaborines have a nitrogen-boron bond in place of a carbon-carbon double bond which alters the electronics of the parent scaffold and has been explored successfully in cancer research. Using this information, our desired analogs integrating the desired isometric substitution were synthesized and their antimicrobial activity was measured and documented.

***Poster 17 (Organic): Directed Monomer Incorporation in Radical Copolymers
Using Cyclic Xanthate Radical Ring-Opening Polymerization***

Presenter: Liam Ordner
PI: Will Gutekunst
Co-author: Ronald Smith
Institution: Georgia Institute of Technology

Radical ring-opening polymerization (rROP) can be used to introduce labile ester groups into the backbone of otherwise rigid radical polymers, improving their chemical reactivity and degradability. However, this technique has been characterized as having poor reactivity with less activated monomer species such as acrylates and styrene. The Gutekunst group conceptualized the use of a cyclic thiocarbonyl monomer platform to overcome the common issues seen with typical rRO monomers and facilitate targeted degradation. While a proof-of-concept 7-membered ring thionolactone (7RTL) has been successful for this project, new monomers must be synthesized and studied to achieve different incorporation profiles with acrylate species, facilitate reactivity with styrene, and advance mechanistic understanding of this new monomer class. A new, analogous 6-membered ring cyclic xanthate (6RCX) monomer has been identified that copolymerizes readily with dimethyl acrylamide, but incorporates in a gradient fashion, rather than a perfectly random one. Under the right conditions, this monomer has also been shown to homopolymerize readily into a high molecular weight, regioregular polymer. Both the co- and homopolymerizations of the 6RCX are explored, along with the syntheses of alternately-substituted derivatives of this monomer.

Poster 18 (Organic): Engineered Myoglobin Biocatalysts in Deep Eutectic Solvents Under Aerobic Conditions

Presenter: Karla Solis
PI: Gopeekrishnan Sreenilayam
Co-author: Kevin Eppes
Institution: Valdosta State University

Deep Eutectic Solvents (DES) are a new generation of sustainable solvents prepared by mixing two or more individual components. DESs have many desirable physicochemical properties compared to traditional organic co-solvents used in biocatalysis such as negligible vapor pressure, high thermal stability, non-flammability, conductivity, easy recycling, biodegradability, and little to no toxicity. Moreover, these solvents can be easily synthesized from cheap, commercially available, and naturally occurring renewable materials. Biocatalysis (using enzymes and proteins as catalysts) is increasingly used in organic synthesis due to its excellent chemo-, regio- and stereo- selectivity, environmental sustainability, milder reaction conditions, improved productivity, simplified work-streams and greater economical saving potential. Aqueous/organic co-solvent-based biocatalytic reactions suffer from disadvantages such as lack of substrate scope and substrate solubility, catalyst stability, catalyst recycling, decreased reaction kinetics, high toxicity, low sustainability index, etc. One way to overcome these limitations is to perform biocatalytic reactions in an aqueous/DES solvent mix or in a pure DES solvent system. The objectives of this project are to synthesize a set of 10-15 DESs and study the stability of engineered heme biocatalysts (purified enzyme) in these DES using UV-Vis spectroscopy to identify the best catalyst-DES combinations. Subsequently, the activity of the biocatalyst will be evaluated in the above-mentioned DES solvent system to establish the optimal reaction conditions. Our initial results showed that DES solvents outperforming traditional aqueous/organic co-solvents, especially under aerobic reaction conditions.

Poster 19 (Organic): Tunable Properties of Metal-Cages

Presenter: Taylor Talley
PI: Jeremiah Johnson
Co-authors: Matthew Pearson and Michelle Gaines (Spelman College)
Institution: Massachusetts Institute of Technology

Metal-organic cages (MOCs) are discrete coordination cages composed of metal ions which are connected by organic ligands. The modularity and inherent porosity of MOCs make them attractive materials for applications in gas storage and separation, though they often suffer from a lack of processability. We, therefore, sought to develop a hybrid polymer-MOC (polyMOC) material with accessible permanent porosity that could enable more favorable mechanical properties. We utilized a Radical Addition-Fragmentation Transfer (RAFT) polymerization due to its ability to control the molecular weight and dispersity of chains and allow the synthesis of block copolymers and polymers with more complex architectures. We developed a procedure using the RAFT polymer ligand, free isophthalic acid, and $\text{Cu}(\text{NO}_3)_2 \cdot 2.5\text{H}_2\text{O}$ to form novel polymer- $\text{Cu}_{24}(\text{m-BDC})_{24}$ cage hybrids. Using a series of ratios of free ligand to polymer-bound ligand we determined the crystallinity of the material could be tuned, based on PXRD. ^1H NMR of digested materials and IR spectroscopy further confirmed the successful incorporation of the polymer ligand in the material and that polymer incorporation varied by the initial stoichiometric ratios. This research lays a foundation for the development of bulk copper and rhodium polyMOC materials, including the addition of multiple polymer blocks for processable polyMOC materials.

**Poster 20 (Organic): Synthesis, Characterization, and Cytotoxic Activity
of Asymmetric N,N'-bis-substituted 1,2,3-Triazolium Salts**

Presenter: Dominic Fico
PI: Kerri Taylor
Institution: Columbus State University

Cancer therapeutics often compromise the immune system of patients, making microbial infections one of the most common complications during treatment. Thus, researchers are motivated to develop medicines that serve a dual purpose: combating both cancer and opportunistic infections for the immunocompromised. Medications housing the imidazole moiety, like clotrimazole (antifungal) and dacarbazine (anti-cancer), are currently being used therapeutically as anti-tumor and antimicrobial agents. But researchers have noted issues when attempting to unify both types of anti-proliferative activities into one compound; most iterations of imidazole-based drugs are relatively insoluble in aqueous. Triazole, though only differing by one nitrogen atom, arguably has a greater dipole moment compared to imidazole. Furthermore, the transformation of triazole heterocycles into a salt form has made the organic building block a superior pharmacophore system by virtue of its potentially greater solubility. This multidisciplinary project focuses on the synthesis, characterization, and biological activity of asymmetric N,N'-bis-substituted 1,2,3-triazolium salts to further elucidate which lipophilic and/or hydrophilic substituents exhibit optimized cytotoxicity against breast and prostate cancer cell lines (MDA-MB-468 and PC-3, respectively) and 6 ESKAPE pathogens: *Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Enterobacter* species.

**Poster 21 (Organic): Facile Synthesis of Arylpropionic Acids:
Carboxylation of Arylacetylenes via the Grignard Reaction**

Presenter: Ashley Cronan
PI: Ronald Okoth
Co-author: Erison Cronan
Institution: Georgia College and State University

Phenylpropionic acid is an acetylenic compound derived from propynoic acid that has a phenyl group in place of the acetylenic hydrogen. Phenylpropionic acid was successfully synthesized via direct carboxylation of arylacetylenic Grignard reagent with carbon dioxide followed by acidic workup using aqueous hydrochloric acid. The arylacetylenic Grignard reagent was obtained through an acid-base reaction between phenylacetylene and ethylmagnesium bromide, which are both commercially available. The phenylpropionic acid obtained was characterized using NMR spectroscopy and melting points. Even though the synthesis attempted produced relatively pure phenylpropionic acid, the percent yields recorded were quite low. However, attempts are currently underway to improve the percent yield of the reaction.

Poster 22 (Organic): Catalytic Living Ring-Opening Metathesis Polymerization (ROMP)

Presenter: Ekuia Beneman
PI: Dr. Jeremiah Johnson
Co-author: Dr. Michelle Gaines (Spelman College)
Institution: Massachusetts Institute of Technology

The ability to deliver drugs for cancer treatment with improved efficacy and decreased toxicity is vital to treating new diseases and enhancing the utility of developed drugs. Specifically, the Johnson group has shown that bottlebrush polymer architecture pro-drugs are an effective platform for drug delivery because of their synthetic modularity through Ring-Opening Metathesis Polymerization (ROMP). ROMP enables the synthesis of bottlebrush polymers while achieving near quantitative conversion. However, ROMP requires stoichiometric use of a ruthenium catalyst which results in relatively high levels of metal in the final products. This residual metal content of the bottlebrush drug delivery materials made through ROMP prevents their use in a wider variety of applications where higher or more frequent doses of material are required. Catalytic living ROMP has been proposed as a method to make these types of polymers using 100-1000x less catalyst and lower metal loadings using a chain transfer agent (CTA). In our research, we validated, synthesized and tested derivatives of previously used chain transfer agents using a palladium cross coupling reaction. We used these synthesized CTA's to conduct catalytic living ROMP with methyl-oxa-methyl-norbornene-imide (MOMNI) and its *endo* isomer as monomers. We found that CTA-5 was the most efficient in initiating new chains with both monomers. This research advances minimal metal usage when creating bottlebrush polymers which aids in the suggested multifaceted usage of bottlebrush polymers.

Poster 24 (Organic): The Application of Polymeric Hydrogels on Curly Human Hair Fibers to Induce Hydration

Presenter: Taylor Beverly
PI: Michelle Gaines
Institution: Spelman College

A large percentage of the world's population has hair that is characterized as either wavy, coily, curly, or a mixture. Those with these varied curl patterns often struggle with maintaining proper hydration, which tends to lack nutrients or feel brittle and dry. Maintaining hydrated hair plays a major role in hair hygiene and management. Hydrogels are network polymers that have been swollen in water, and these materials are often used in personal care products to help maintain hydration of the skin across the body. This research investigates the hydration behavior and surface chemistry of curly hair fibers after applying hydrogels to the hair fiber surface. This project begins by employing a methodical literature search in SciFinder and PubMed, to gain a global perspective of the existing literature on hair hydration for hair of all types. The list of articles was narrowed by applying several appropriate search terms, and these articles were used as evidence to explain hydration in coily and curly hair. Future experiments will involve designing experiments to measure hydration in hair samples of varying curl types or different length scales. The information highlighted in the compiled subset of articles will help with experimental design. This research was supported by the Spelman NSF LSAMP Award.

Poster 25 (Organic): Synthesis, Characterization, and Photophysical Studies of 2-(3,5-Dimethoxybenzylidene)Indan-1-one

Presenter: Madeline Faass
Co-PIs: Ajay Mallia and Joseph Sloop
Institution: Georgia Gwinnett College

The present study describes the synthesis, characterization, photoisomerization, and photophysical studies of (E)-2-(3,5-dimethoxybenzylidene)indan-1-one (E-DMBI). E-DMBI was prepared by the reaction between 1-indanone and 3,5-dimethoxybenzaldehyde. The synthesized compounds were characterized using thermal (melting point, DSC) and spectroscopy studies (IR, NMR, UV, fluorescence) and the characterization details will be presented. Photoisomerization, kinetics studies, and rate constants of E-DMBI to Z-DMBI were studied using UV spectroscopy in various polarity liquids will be discussed.

Poster 26 (Organic): Synthesis, characterization, and fluorescence properties of acridinyl and quinolinyl derivatives of aminobenzenesulfonamides

Presenter: Klaudia Figueroa
Co-PIs: Ajay Mallia and Neville Forlemu
Institution: Georgia Gwinnett College

In the present study acridinyl and quinolinyl-linked aminobenzenesulfonamides have been synthesized and characterized. Synthesis of N-(acridin-9-yl)-4-aminobenzenesulfonamide, and 4-amino-N-(quinolin-5-yl)benzenesulfonamide were carried out by the reaction between 4-acetamidobenzenesulfonyl chloride with 9-aminoacridine and quinolin-5-amine respectively. Final compounds were obtained after the deprotection of the acetyl group. Characterization details including spectroscopic studies of the synthesized compounds will be presented. Excitation and emission properties of the synthesized sulfonamides and the temperature dependence will be presented.

Poster 27 (Medicinal Chemistry): Synthesis of Analogs of PDE5 Inhibitor Tadalafil

Presenter: Hailey Ramos
PI: Iryna Lebedyeva
Co-author: Mackenzie Williams
Institution: Augusta University

Tadalafil is a commonly used drug that can treat erectile dysfunction as well as high blood pressure. This drug is successful in its ability to inhibit the enzyme called PDE5. PDE5 is an enzyme that facilitates blood flow and cell signaling. By inhibiting PDE5 enzyme with a drug such as tadalafil, blood vessels and muscles undergo relaxation, which results in an increase of blood flow throughout the body. It was discovered that drugs known as phosphodiesterase-5 inhibitors (PDE5i) can possibly prevent colorectal cancer in mice, and recent studies have suggested that this can also be effective in humans. However, an issue arises when PDE5 inhibitor is used as a drug for colon cancer prevention as it was found to rapidly leave the colon and enter the bloodstream. In this project, we work on eliminating these effects by creating a novel analog of tadalafil that will remain localized in the GI tract with minimize leakage to the bloodstream. The structure of tadalafil will be modified by adjusting its molecular weight and polarity, in which a novel drug candidate will be created. The new compound will be localized in the colon while still being an effective PDE5 inhibitor. As a result, the onset of colon cancer can be prevented.

Poster 28 (Physical): Synthesis, gelation, and spectroscopic studies of 4-hydroxy-1-anthraquinonylalkanamide based low molecular mass gelators

Presenter: Bao Dang
PI: Ajay Mallia
Institution: Georgia Gwinnett College

The present study discusses the synthesis and gelation studies of 4-hydroxyanthraquinonylalkanamides (alkyl chain lengths C₁₂, C₁₄, and C₁₆) as low molecular mass gelators. Gelation studies of synthesized compounds have been examined in varying polarity liquids. Correlations between the molecular structures of the anthraquinonylalkanamide gelators and the properties of their gels, and gel-sol transition temperatures, thermodynamic and spectroscopic properties will be presented.

Poster 29 (Physical): Self-assembly, gelation, mechanical and thermal properties of molecular gels based on alkanolic acids and ammonium alkanooates as low molecular mass gelators

Presenter: Joel Suazo
PI: Ajay Mallia
Co-authors: Brian Matei and Farisha Sultan
Institution: Georgia Gwinnett College

Self-assembly and gelation studies of alkanolic acids (carbon chain length = 12, 14, 16, 18, and 20) and the ammonium salts will be presented. Thermal properties of the gels were determined using differential scanning calorimetric studies, and the gel melting temperatures. Rheology studies show that storage modulus (G') of a 5 wt % ammonium alkanooate in toluene increases on increasing the alkyl chain length of the ammonium alkanooate. Correlations between the molecular structures of the ammonium alkanooate gels, including gel-sol transition temperatures, thermodynamic properties will be presented.

Poster 30 (Physical): Use of Electrostatic Tuning Maps to Visualize Molecular Basicity

Presenter: James Gay
PI: Samer Gozem
Institution: Georgia State University

In a previous project, we developed a protocol to construct electrostatic spectral tuning maps (ESTMs) to represent how nearby charges affect the excitation energies of flavin. ESTMs are constructed by moving a charge around a molecule and mapping the changes in excitation energy. The maps provide a helpful visual guide and may be used in applications to protein engineering, interpreting the spectra of chromophores, and providing a starting point for further quantum mechanic/molecular mechanic studies. One project recently built upon this concept by replacing the charges with water molecules to generate "hydrogen-bonding maps" showing where stable hydrogen bonds can be formed with a chosen molecule. The resulting structures were then used to predict how various hydrogen-bonding interactions affect a molecule's vibrational frequencies. In this project, we explore the extension of ESTM protocol to basicity. The resulting maps can be used either in an educational setting to teach students about molecular properties and trends or as an intuitive research tool, particularly in the case of students that are new to computational chemistry.

Poster 31 (Physical): Infrared and Raman Vibrational Spectra of $H_5O_2^+$ and its Deuterated Analogs

Presenter: Oluwaseun Omodemi
PI: Martina Kaledin
Co-authors: Ivonne Meares, Gabriella Garofalo
Institution: Kennesaw State University

This work describes infrared (IR) and Raman vibrational spectra of $H_5O_2^+$ protonated water dimer using the computational chemistry method, the normal mode analysis (NMA) at the density functional theory with B3LYP functional and MP2 perturbation theory to the second order. We have used Dunning's basis sets aug-cc-pVXZ (X=D,T) and Pople's basis set 6-311++G(d,p). $H_5O_2^+$ stationary points have been optimized using the Gaussian 16 program. The $H_5O_2^+$ Zundel complex serves as a benchmark system to implement molecular polarizability surface in the analytical form. The analytical potential energy (PES) and dipole moment (DMS) surfaces are available in the literature. Bowman's research group provided PES and DMS surfaces at the CCSD(T)/aug-cc-pVTZ and MP2/aug-cc-pVTZ levels of theory, respectively. This work investigates IR and Raman intensities for $H_5O_2^+$ and its deuterated analogs, $D_5O_2^+$, $D_4HO_2^+$, and $H_4DO_2^+$.

Proton transfer frequencies estimated at the MP2/aug-cc-pVTZ frequencies for $H_5O_2^+$, $D_5O_2^+$, $D_4HO_2^+$ and $H_4DO_2^+$ are 911.3 cm^{-1} , 660.2 cm^{-1} , 831.2 cm^{-1} and 719.6 cm^{-1} , respectively. We located stationary points on the potential energy surface at the B3LYP/6-311++G(d,p) level of theory. These stationary points will serve as an initial guess to locate the stationary points on the analytical potential energy surface. Imaginary frequencies of the transition states shown on Figure 1 are $204.7i\text{ cm}^{-1}$ (C_s -TS), $493.8i\text{ cm}^{-1}$ (C_s -HH), $176.1i\text{ cm}^{-1}$ (C_{2h} -trans), and $210.6i\text{ cm}^{-1}$ (C_{2v} -cis). Proton motion in $H_5O_2^+$ yield high IR activities, while OH-stretch vibrations show strong Raman activities. The Raman intensities were found at 3745.0 cm^{-1} and 3822.0 cm^{-1} for $H_5O_2^+$. Currently we are running the molecular dynamics simulations to obtain IR and Raman spectra and this normal mode analysis study will provide the baseline information to assess the anharmonic effects in the vibrational spectra.

Poster 32 (Physical): Ab initio study of the proton transfer motion in $H_5O_2^+$ and its methylated derivatives

Presenter: Sarah Sprouse
PI: Martina Kaledin
Co-author: Destyni Herbert and Branden Freeman
Institution: Kennesaw State University

This work studies the structure, vibrational spectra, and hydrogen bond strength of proton shared complexes $[A\cdots H^+\cdots B]$, where A and B are dimethyl ether $(CH_3)_2O$; methanol, CH_3OH , and water, H_2O . We study the effect of larger molecular scaffolds $(CH_3)_2O\cdots H^+\cdots O(CH_3)_2$, $(CH_3)_2O\cdots H^+\cdots OH(CH_3)$, $(CH_3)HO\cdots H^+\cdots OH(CH_3)$, and $(CH_3)_2O\cdots H^+\cdots OH_2$ on structural properties, molecular vibrations, and energetics of the hydrogen-bonded complexes comparing to the Zundel ion, $H_5O_2^+$. Understanding proton transfer in the hydrogen-bonded network is essential to explain the charge transport mechanism across cell membranes. Computer simulations of these model systems can provide insights into the proton transfer and proton migration dynamics in solution. $[A\cdots H^+\cdots B]$ ions are of particular interest because they are stable, and the proton is trapped in the three-dimensional potential energy well. The minimum geometries and vibrational frequencies have been obtained at the B3LYP/aug-cc-pVDZ and MP2/aug-cc-pVDZ levels of theory, respectively. The shape of the interaction potential depends on the atomic groups attached to the proton. Vibrational spectra characterizing proton transfer motion are diffuse, and the proton transfer vibrational motion span from 700 to 2600 cm^{-1} . The hydrogen bond strength is in the range of 25 to 40 kcal/mol, and it depends on the symmetry of the molecular complex.

Poster 33 (Physical): Multi-scale modeling of Deoxyribonucleic acid (DNA) methylation and a computational study of orbital interaction, band gap and binding energies associated with the process

Presenter: Brandon Persaud
PI: Rosi Gunasinghe
Institution: University of North Georgia

DNA encodes genetic instructions relevant to the development and functioning of living organisms and viruses. One of the primary regulators of gene transcription is DNA methylation. DNA methylation occurs at specific sites in DNA, referred to as genetic hot spots or CpG islands. However, aberrant DNA methylation patterns such as hypermethylation and hypomethylation have been recognized in variety of human malignancies. As a result, the process has become one of the most thoroughly investigated epigenetic modifications in mammals. Experimental evidence shows cancer-specific differential DNA-methylated regions correspond to the loss of sharply defined methylation boundaries at CpG islands. Developing effective cancer therapeutic requires a proper understanding of gene silencing and gene expression associated with methylation and demethylation. However, the relevance of methylation or demethylation to cancer is far from being well explained. Interactions between nucleic acids and graphene were studied as an approach to study the interaction between proteins and methylated DNA. Nucleic acids have shown a planar orientation on graphene due to the influence of π - π interactions. Dispersion-corrected density-functional calculations demonstrate that nucleotide base-oriented conformations transfer more charge than phosphate-oriented conformations. The constructed double-strand DNA sequences contain only Cytosine and Guanine in the double-strands for simplicity. Constructed CpG islands are the localities where methyl groups attach to cytosine. The constructed structures vary from an unmethylated DNA (0% or hypomethylated), to 10% methylated DNA, and to 20-100% (hypermethylated) DNAs. Study shows that the increasing methyl concentration decreases the binding energy with an increase of the average distance between the strands. Consequently, normal regulation of gene can be disrupted. Energy gap between filled and empty orbital in the methylated double strand DNA increases with increasing concentration of methyl group in the DNA. Results indicate that abnormal DNA methylation is affecting the electronic structure of the DNA and hence effecting the proper bio-functioning of vertebrates.

Poster 34 (Computational): The Isomerization of H_2XY to $HXYH$ ($X, Y = O, S, Se$)

Presenter: Addison Bralick
PI: Henry Schaefer
Co-author: Boyi Zhang
Institution: University of Georgia

Oxywater (H_2OO) is an intermediate in the oxidation of hydrogen peroxide ($HOOH$), and along with its relatives H_2SS and H_2SeSe , plays an important role in atmospheric and biochemical processes. In this research, we study the isomerization of H_2XY species to $HXYH$ ($X, Y = O, S, Se$) using highly rigorous ab initio methods. Geometries and harmonic frequencies were obtained using both a scalar relativistic X2C-1e-CCSD(T) approach and non-relativistic CCSD(T) using an effective core potential on Se. The two methods are compared for their ability to capture relativistic effects. A focal point approach was used to extrapolate electronic energies at CCSD(T)/aug-cc-pVTZ geometries to a CCSDT(Q)/CBS level of theory. The isomerization reactions of H_2XX to $HXXH$ have barriers of 6.6, 20.6, and 14.1 kcal/mol and exothermicities of 45.8, 27.2, and 28.3 kcal/mol for $X = O, S,$ and Se , respectively. The isomerization reactions of H_2OS and H_2SO to $HOSH$ have barriers of 15.4 and 44.2 kcal/mol and exothermicities of 36.2 and 17.7 kcal/mol. The isomerization reactions of H_2OSe and H_2SeO to $HOSeH$ have barriers of 10.1 and 36.2 kcal/mol and exothermicities of 33.5 and 31.7 kcal/mol. The isomerization reactions of H_2SSe and H_2SeS to $HSSeH$ have barriers of 16.2 and 18.1 kcal/mol and exothermicities of 23.3 and 32.1 kcal/mol. Periodic trends in geometries and isomerization barriers are established and analyzed.

Poster 35 (Organic): Exploring Alternative Heterocycles for NIR Squaraine Dyes

Presenter: Shahir Sarasiya
PI: Dr. Maged Henary
Co-author: Ken Aratame
Institution: Georgia State University

Squaraine dyes utilizing indole heterocycles have been the subject of intense modification and study. Considerable work has been done, but results have, thus far, fallen short of the wavelength < 700 nm. Efforts have largely focused on modifying the heterocycles by adding different substituents such as ester and quaternary nitrogen. While these modifications can improve biological effects, improvements in λ_{max} are approaching a limit. Instead, the implementation of various heterocycles such as quinoline and 2,3-dihydro- 1H -perimidines can yield strong improvement in the dye optical properties. These aromatic groups further extend the π -electron conjugated system, producing λ_{max} values beyond 800 nm. Herein, we are reporting the synthesis and characterization of these redshift dyes.