Herty Medalist Undergraduate Research Symposium

September 20, 2019

Georgia Gwinnett College, Lawrenceville, GA

1 SACNAS, Advancing Chicanos/Hispanics & Native Americans in Science at Georgia Gwinnett College

Leslie Orduno, Cindy Herrera, Joel Gabriel, Daniel Herrera and Omar Villanueva
Georgia Gwinnett College, ovillanueva@ggc.edu

A SACNAS Chapter has been established at Georgia Gwinnett College for the purpose of fostering the success of our large population of Hispanic students at this institution. SACNAS (the Society for Advancement of Chicanos/Hispanics and Native Americans in Science) is an inclusive (national) organization that for the past 45 years has been dedicated to fostering the success of Chicano/Hispanic and Native American scientists, from college students to professionals, in attaining advanced degrees, careers, and positions of leadership in STEM. This presentation will showcase the goals and initiatives of the GGC SACNAS Chapter and will highlight the recent activities this we have carried out on campus to promote STEM to our large Hispanic population of students.

2 Start your journey here: Georgia Gwinnett College chemistry outreach

Madeline Faass, Katie Coscia, Esperanza Lopez, Robert Varner and Russell Sumling
Georgia Gwinnett College, grudd@ggc.edu

Our nearly seven year chemistry club continues with its success here at Georgia Gwinnett College. NCW on campus events include: mole day guacamole and chips, program in a box, and student led chemistry demonstrations such as, exploding pumpkins, screaming gummy bears, elephant toothpaste, green extraction of orange oil and lots more. NCW off-campus at Fernbank science center in Atlanta, celebrated out of this world chemistry, making edible water bottles with an assortment of liquid cores. Other on campus events include a celebration of Halloween with a food day of dragons' breath and liquid nitrogen ice cream, and helping out during GGC's open house. Continued success with our GGC S3 "Super Saturday Series" combining chemistry with technology, with emphasis on the chemistry of space.

3 Peer Supplemental Instruction (PSI) in Introductory Chemistry Courses

Carmen Roland, Purva Lotwala and Daniel Herrera
Georgia Gwinnett College, plotwala@ggc.edu

In the fall of 2015 Georgia Gwinnett College (GGC) started offering Peer Supplemental Instruction (PSI) for introductory chemistry (CHEM 1211K and CHEM 1212K). In the fall of 2018 it was expanded to include Organic Chemistry I (CHEM 2212K). PSI is based on the Supplemental Instruction (SI) model developed in early 1970's at the University of Missouri, Kansas City. PSI sessions offer a place to go for extra help where students can work with their fellow peers in groups to solve problems related to course material. The sessions are facilitated student leaders who have already taken the classes and been successful. PSI sessions are the place to gain a deeper understanding of the material being covered in the course. The sessions are group-based learning; meaning students help each other learn. Lab classes at GGC are capped at 24 students which means there are a large number of sections being taught by many different instructors. This has required the model at GGC be modified from the traditional SI model. One of the focuses of the PSI program is to work on STEM skills in addition to the chemistry content. Students are given the opportunity to develop more than just chemistry skills, such as scientific communication, study strategies, and psychological skills. Data collected at GGC attests to the success of the program. Data collected in the fall of 2017 demonstrates that students who regularly attend PSI sessions show a statistically significant improvement in course grades

4 Preliminary Results for the Development and Assessment of an Outreach Program

Chloe Durden
Mercer University, chloe.l.durden@live.mercer.edu

The art of brewing great beer is a talent many recognize but the science behind it is often disregarded. This research examines best practices for outreach curriculum development and assessment. Our curriculum will help connect the interest of the public to the science of brewing through a series of informational sessions using a variety of presentation modes, including oral communication, visuals, and hands-on activities. Using this approach should make the outreach events interesting and informative. Upon completion of the outreach event, participants will be asked to complete a survey designed to assess the scientific impact of the program. The feedback collected may help show the most effective teaching style, how much information was retained, and the level of interest in future real-world chemistry outreach programs.

5 Analysis of General Chemistry Student Samples for Concentration of Copper in a Percent Composition Laboratory Experiment

Emily Storck & C. Ohrenberg
University of North Georgia, enstor2639@ung.edu

General chemistry students at the University of North Georgia perform an experiment in which copper is precipitated from copper (II) chloride dihydrate solutions, through the addition of magnesium turnings, in order to calculate the percent composition of copper in the compound. Students allow the reaction to continue until it is apparent, based on the color of solution, that all of the copper was precipitated from solution. When the solution is colorless, students assume no more copper is left in solution. Afterwards, excess magnesium is reacted with hydrochloric acid and the solution is filtered to separate the copper. From previous studies on this experiment, it has been shown that a colorless solution is not necessarily indicative of full precipitation. In this study, a Spectronic 20 was utilized to determine the concentration of copper (II) chloride left in student filtrates after the removal of copper. Samples were collected from multiple lab sections. The amount of magnesium added by the students varied across different lab sections. A calibration curve was used to calculate the concentration of copper remaining in the filtrates from the measured absorbance values. The average concentration of copper left in the student solutions was .00687 M.

6 Lawrenceville Science Tavern

Cheyenne Letson
Georgia Gwinnett College, cletson1@ggc.edu

Major scientific concerns are growing in the general population with topics such as climate control, vaccination risks, and wildlife conservation gaining recent popularity. Scientists and the community have become divided, with scientists publishing in peer-reviewed scholarly articles, and the community receiving their news through various print and television sources and social media. The Lawrenceville Science Tavern is aimed to help “bridge” the divide between the community and scientists, in order to bring the research-backed information on popular topics to the community. The events are held at a venue in the community that is easily accessible and provides a relaxed atmosphere. Various scientists prepare their research to be presented in a concise and basic level. Anyone in the community, regardless of background and education, can attend and understand the material being discussed. The goal of Lawrenceville Science Tavern is to create an area for the community and local scientists to interconnect and share information and perspectives.

7 Students' Perceptions of Specifications Grading

Jenai' DaCosta
Georgia Gwinnett College, jdacosta@ggc.edu

This project evaluated student perceptions of specification grading using one-on-one interviews. Interview questions included topics such as expectations of specification grading, differences between specifications and traditional grading methods, expectations of amount of time studying, and advantages and disadvantages of specifications and traditional grading methods. Session participants will be provided with information from the student’s perception regarding specification grading methodology. This type of information will assist participants in decision making regarding use of this type of assessment methodology as well as an understanding of advantages and disadvantages based on what students experience.

8 The Chemistry of Biology

Martin Penaherrera, Cindy Herrera, Brian West and Samantha Baxley
Georgia Gwinnett College, mpenaherrera@ggc.edu

In an increasingly competitive world, STEM skills are especially important to secure successful careers in the scientific field. Students need to be able to solve problems and connect and relate different STEM concepts. Based on interconnectivity of scientific disciplines, biology leaders of the Peer Supplemental Instruction (PSI) program developed interactive lesson plans and strategies to help students understand and learn about some core topics from Principles of Biology I (BIOL 1107K), Principles of Biology II (BIOL 1108K), and Cell Biology (BIOL 3400K), and their connection with chemistry concepts. The activities were developed to understand the relationship between Biology and Chemistry and focused on the chemical and biological properties of water molecules, and the types of bonds and functional groups involved in the synthesis of macromolecules. The results of this endeavor, that is the extent to which students are engaged in learning the chemistry of biology, will be presented. This exercise will allow us to create additional dynamic activities that can link the two disciplines in a more fluid way. In conclusion, students are given the tools for their improvement in STEM skills by engaging in activities that emphasize the importance of knowing basic material from both subjects in order to build a more holistic knowledge about science. These activities are based on the premise that our learning in these courses includes understanding the chemical processes involved in biological life.

9 A Salivary Hormonal Study on Individuals of African Ancestry Living in Different Socio-Economic Environments in Order to Understand Etiology of Prostate Cancer

Megan Andrews, Wathsala Medawala, Ernie Kaninjing, Chavonda Mills, Solomon Rotomi and Wathsala Medawala
Georgia College, megan.andrews@bobcats.gcsu.edu

Prostate cancer ranks high among some of the most serious public health problems that significantly impact the lives of men globally. Established risk factors for this disease include age, family history and African ancestry. While incidence and mortality of prostate cancer has decreased in the US in recent decades, men of African descent are disproportionately affected. To better understand the etiology of prostate cancer among men of African ancestry, this study examined hormonal differences among men of African descent living in different socio-economic environments by using their saliva samples to study their hormone levels. Using ELISA kits specific to either testosterone or cortisol, 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 and standard deviation of 35.924 pg/mL while the mean cortisol concentration was 0.120 mg/dL and the standard deviation was 0.078 mg/dL. The saliva samples collected from individuals with African ancestry in the United States (n=84) had a mean testosterone concentration of 94.680 pg/mL with a standard deviation of 35.218 mg/dL while the mean cortisol concentration was found to be 0.136 mg/dL with a standard deviation of 0.101 mg/dL. This poster will explain data collected for both hormones for males living in African countries and the United States, and will discuss whether these hormone levels can be used to determine individuals at risk for prostate cancer. Any observed effects from socio-economic differences will also be discussed.

10 The Creation of 3D Printed Specialized Lab Instruments for Students With Autism Spectrum Disorder (ASD)

Ira Moore and Damario Cooper
Morehouse College, ira.moore@morehouse.edu

Improper job placement and support of people dealing with autism spectrum disorder (ASD) has been the cause of high unemployment rates leaving ASD individuals dependent on others for their daily living needs. One area that these individuals have shown aptitude in is STEAAM (science, technology, engineering, arts, agriculture, and mathematics) but without a specialized system in place that is consistent, even this opportunity for growth and independence is denied to them. With the creation of specialized lab instruments that are applicable to the way they retain information then employment could be available to these individuals in labs and STEAAM related positions.In order to create this system current lab instruments must be modified so that they can be used consistently by students on the spectrum. Blender 3-D modeling software allows for the easy creation of these specialized instruments.

11 Research and Development of 3D Printed Quantitative Chemical Containers for Autism Spectrum Disorder

Damario Cooper and Ira Moore
Morehouse College, damariocooper6@gmail.com

There is an ever growing need to address those affected by Autism Spectrum Disorder, and the applications they have to the workforce. According to the Center for Disease Control (CDC), "1 in 59 children in the United States has been identified with an Autism Spectrum Disorder (ASD)." This statistic has been rising with time; however, the unemployment rate of those with autism is astronomically high compared to that of the national average. 85 percent of those with ASD and college degrees are unemployed. Many of these individuals have the mental capacity to acquire the skills needed for a variety of industries, but they lack the desired social skills. Providing accommodations for those with ASD in the workforce would greatly boost the American economy. This would also provide a source of confidence and financial stability in autistic people.

In order to strengthen this initiative, a methodology to design and 3D print Quantitative Chemical Containers (QCCs) will be established. QCCs will be lab equipment recreated using digital modelling software. The design will be optimized to be used for people diagnosed with Autism Spectrum Disorder. Specifications and numerous tests will be administered to ensure the precision of these tools in comparison to standard glassware. 3D printing was chosen as a means of prototyping and producing a final product. The filament used in the design process will be more durable than glassware in the anticipation of dropping. Through the use of specific customized equipment, QCCs will allow those displaced by the workforce to become active participants.

12 The State of Research on the Effect of Interpersonal/Intrapersonal Biases on Maternal Health of Black Mothers: A Rising Issue

Makaila Jackson
Spelman College - Authority Health, mjacks58@scmail.spelman.edu

It is reported that approximately 700 pregnancy-related deaths occur annually. African-American women remain as the population who suffers the most from complications and death during their pregnancy. Experts often report that being poor and uneducated are the reasons black mothers are more susceptible to complications and death. Yet many black women who are financially stable and educated are experiencing maternal complications and death. Through a literature review, meta-analysis from state health departments, PRAMS from all participating states, and articles from PubMed databases from 1994 to 2019 and it is suggested that racial biases may affect maternal outcomes of minority mothers dating back to early years. Research reveals that women who have experienced racism early in their lives are subject to having more complications during their pregnancy. There is a need for the opportunity to report in real-time any concerns minority mothers may have throughout their pregnancy and after to ensure they are healthy as well as if they feel their physician may have preconceived notation towards them, to ensure proper training and review of patterns in physician behavior. Data analysis has suggested that policies be placed in hospitals to ensure training on interpersonal and intrapersonal biases in healthcare.

13 Measuring Fear Potentiation by Assessing Stress, Anxiety, and Depression Levels in Morehouse College Students

Alexis Schenck
Morehouse College, aschenck@scmail.spelman.edu

Fear potentiation is defined as a mental and physical reaction to a startling, but harmless, stimulus. Out of the 16 % of African Americans in the United States, 6.8 million people are affected by some type of mental illness which increases fear potentiation. This research assessed how stress, anxiety, and depression play a part in affecting fear potentiation in two different communities of people. Descriptive statistics were conducted using Google surveys by collecting the answers of the stress, anxiety, and depression survey; which were sent out to Morehouse students via email/social media/Group Me's. Results show that compared to predominantly Caucasian students, students that attend Morehouse College have a higher fear potentiation by 64%. We believe this to have a direct correlation to the different demographics and different events that can occur in the two different communities. Future research will quantitatively measure the startle reflex of fear potentiation in college students of the AUC, and how it is compared to other communities within the Atlanta Metro area.

14 The Impact of Age and Falls Risk on Static Balance Among African American Women

Cherise Miller
Spelman College, cmille26@scmail.spelman.edu

Age and weight are two factors that are generally proportional to balance. Age is directly proportional to balance while weight is indirectly proportional to balance. This means that while age increases, balance increases, and while weight increases, your balance decreases. Control factors of balance include vision, vestibular systems and perception. Other factors such as medications and injury are also factors. Poor balance can have many different sources. Using the Korebalance machine, static balance was tested among college-aged African American women. Our hypothesis stated that age and weight would greatly affect falls risk and static balance. Static balance is the ability to stay in a steady motion, ultimately testing balance in the human body. A falls risk assessment revealing facts about the participant was used to test the hypothesis. Data from the Korebalance machine was also used to supplement data. The sample size was N = 22. Results indicated that over 45% of participants had a static Q score of >10000. This is a high falls risk for static balance given the age of our population.

15 Will a Mobile Application Increase the Screening Rate for Sexually Transmitted Infections/HIV in African American Males?

Madeleine Buckner-McCurdy
Morehouse College, mbuckne3@scmail.spelman.edu

Telehealth offers a new platform to promote health literacy, and assess/reduce risk regarding one's sexual health. Mobile phone applications can be tailored to a specific audience to provide treatment, prevention, and care. The main objectives to this study are to evaluate different phone applications that promote health literacy, preventative, and diagnostic care as it relates to human immunodeficiency (HIV) and sexually transmitted-infections (STI); and examine if African American men are more likely to get screened for a STI if a mobile application was tailored to them.

We searched the Apple iTunes and Android Google Play stores for HIV/STI related applications. Each application was assessed off of user ratings, functionality, price, device accessibility, and if it was tailored to a specific audience. It was also graded on STI/HIV prevention and care; condom promotion, HIV/STI testing information, STI/HIV health literacy. An online survey was also distributed amongst Morehouse College students to (a) collect information regarding demographics and assess potential risky sexual behaviors and (b) evaluate the likelihood of Morehouse College students who would use an application that caters to men's sexual health. 20 phone applications were evaluated. Seven (35%) applications fit all of the criteria of promoting health literacy, price affordability, accessibility on IOS and Android devices, and were well reviewed. 11 (55%) applications included special features like commodity orders for contraceptive delivery. Of the 20 apps reviewed, they were not tailored to a specific audience; rather they stated that they did not discriminate gender identity, race, or sexual orientation. 67 participants were recruited and 64 completed the survey (target population was college-aged 18-24).

It was concluded that Most HIV/STI related applications are not successful in gaining user attention or positive reviews. App developers and public health professionals should work together to make a compressive app that includes elements of evidence-based interventions for signs and symptoms. Morehouse College students get screened the recommended rate from the Center for Disease Control (CDC).

16 Detecting Endocrine Disrupting Compounds: Development of a Differential Sensing Array for Use in Aqueous Media

Travis C. Meeks
Mercer University, Travis.colter.meeks@live.mercer.edu

Endocrine Disrupting Compounds (EDCs), such as bisphenol A (BPA), have been shown to have negative effects on aquatic wildlife, such as fish and amphibians, female maturation and male reproductive systems, and have been implicated in an increased risk of cancer. Detection methods for EDCs do exist, but are typically highly specific for a given EDC and often require extensive sample preparation and instrumentation. Our research works to address this issue with the construction of a differential sensing array using β-cyclodextrin-based indicator displacement assays that respond to EDCs via patterned colorimetric changes. We have screened and chosen several promising indicators for their changes in absorbance and fluorescence with and without host. We have tested our indicator displacement assay against a selection of EDCs and are currently working to construct our sensing array for use against unknown samples. We plan to employ our array on real-world EDC sources, starting with the detection of BPA from thermal paper and moving toward testing unknowns from real-world aqueous samples.

17 Total Phosphorus Monitoring in Georgia's Lake Lanier Watershed

Mary Dennis
University of North Georgia, MEDENN6059@ung.edu

When excess nutrients such as nitrogen or phosphorous enter waterways, they can cause harmful algal blooms. The algal blooms are harmful because of the toxins they produce, which affect fish, shellfish, and in turn affect people, birds, and water mammals. Excess nutrients enter the water through various means, including wastewater from sewage treatment facilities, storm-water that carries nutrients and pollutants from cities and towns, and run off and soil erosion from agricultural areas that use fertilizers. It is therefore important to monitor the amount of nutrients in water sources to ensure an excess of one or more nutrients will not cause damage to the ecosystems contained within the water. This study focuses on the precision, limits of detection, and accuracy of the total phosphorus analysis performed by the University of North Georgia Water Lab which has maintained a continuous baseline water quality-monitoring program of the Lake Lanier Watershed since 1987 for The Upper Chattahoochee Basin Group (and its predecessors). Method performance criteria used for validation process were investigated on standard phosphorus samples: concentration linearity domain (by calibration curve), limit of detection (LOD), limit of quantitation (LOQ), precision and accuracy. Our results demonstrate the method is accurate and precise over the concentration range of 0.032 to 1 ppm P. The validated method was further applied to total phosphorus determination of water samples from Georgia's Lake Lanier Watershed.

18 PAHs Content in Air Samples

Katia del Risco Hernandes
Georgia Gwinnett College, kdelrisco@ggc.edu

Polycyclic aromatic hydrocarbons (PAHs) have shown mutagenic properties in bacterial and mammalian assays, and are classified by the International Agency for Research on Cancer (IARC) as probable human carcinogens. Combined with their tendency to bio accumulate, PAHs pose risks to both environmental organisms and humans. Sources of gas-phase and particulate PAHs include incomplete combustion processes such as vehicle (diesel) emissions, residential activity and industrial heating. Seasonal sampling of atmospheric PAHs was performed using passive air samplers (PAS) at four sites in the Atlanta metropolitan region, including an urban, a road side, a suburban, and a rural site. These sampling sites were co-located with Georgia Environmental Protection Division air quality sampling equipment for future analysis. Replicate samples were taken at each site over several season periods. Preliminary results from this analysis will be presented.

19 Comparing the Efficacy of Commercial Water Filters with Homemade Filters using Atomic Emission Spectroscopy

Andrea Green, Erica Browne, Leonce Diffo, and Sheniesa Walton
Georgia State University Perimeter College, agreen67@student.gsu.edu

Since the Flint, Michigan water crisis, clean drinking water and water filtration at home have been on the minds of many. In this poster results will be presented that describe the effectiveness of several different water filters. The filters studied were commercial water pitcher filters and homemade filters. The homemade filters were made using gravel, sand, charcoal and organic material. The organic materials tested were apple, apple peel, banana peel, fresh and dried cilantro, rice and lentils. The filters were tested by filtering water that contained Cd, Cr, Cu, Fe, Pb and Zn through the filters. The metal content of the water was measured before and after filtration using atomic emission spectroscopy.

20 Comparing the Efficacy of Commercial Water Filters with Homemade Filters using Atomic Emission Spectroscopy

Erica Browne, Leonce Diffo, Andrea Green and Sheniesa Whitton
Georgia State University Perimeter College, ebrowne4@student.gsu.edu

Since the Flint, Michigan water crisis, clean drinking water and water filtration at home have been on the minds of many. In this poster results will be presented that describe the effectiveness of several different water filters. The filters studied were commercial water pitcher filters and homemade filters. The homemade filters were made using gravel, sand, charcoal and organic material. The organic materials tested were apple, apple peel, banana peel, fresh and dried cilantro, rice and lentils. The filters were tested by filtering water that contained Cd, Cr, Cu, Fe, Pb and Zn through the filters. The metal content of the water was measured before and after filtration using atomic emission spectroscopy.

21 Gene Flow across the Eastern Continental Divide

Erin Menezes
Georgia Gwinnett College, e_menezes@live.com

Gene flow describes the transfer of genetic material between populations. The evolution of populations and the process of speciation depend on gene flow between populations. If part of a population is geographically separated from the rest, due to lack of gene flow, the genetic material in the two populations would slowly start to diverge from each other, potentially creating new species in the future. The Eastern Continental Divide in Georgia divides the flow of water, so that part of it flows east into the Atlantic Ocean, and part of it flows west into the Gulf of Mexico. Because these two waters never meet, it is hypothesized that there will be genetic differences between *Semotilus atromaculatus* (creek chub) from the east side and from the west side of the divide. To test our hypothesis, fish were caught in local streams on both sides of the divide. Because DNA is the molecule of choice for phylogenetic analysis of populations and species (differences in the DNA's evolution can impact the outcome of phylogenetic analysis), it was extracted from the fish. The Cytochrome C oxidase subunit 1 (CO1) gene was amplified by Polymerase Chain Reaction (PCR), sequenced, and analyzed phylogenetically. The data showed that the Eastern Continental Divide prevented gene flow in two separate species, *Semotilus atromaculatus* and *Nocomis leptocephalus*. Although *N. leptocephalus* was mistakenly collected due to misidentifications, the data revealed that there might be two subspecies of *N. leptocephalus* fish living sympatrically in the waters west of the divide.

22 Investigating Ice Nucleating Particles and Microgels in the Wave Flume Mesocosm

Josephine Rudd, Rebecca Simpson, Kathryn Moore, Russell Perkins and Paul DeMott
Colorado State University, rudd.josephinem@gmail.com

Ice nucleating particles (INPs) trigger the freezing of cloud droplets which impacts cloud behavior and thus precipitation patterns. This project aims to quantify the number of INPs and their pattern over time in a wave flume mesocosm to gain insight into the complex relationship between the oceans, INPs, and the atmosphere. Previous studies confirm the existence of INPs upon wave-breaking, in which the INPs are then transferred to the atmosphere. The ocean is a source of INPs, where polysaccharide marine microgels are thought to concentrate INPs into clustered microenvironments. Here, we show that breaking up these clusters can be achieved through use of the chelating agent EDTA. The samples collected from a laboratory wave flume include bulk, sea surface microlayer (SSML), and sea spray aerosol (SSA) samples. It was determined that EDTA added to bulk seawater had almost a five-fold increase upon the number of low-temperature active INPs. Additionally, INP levels and trends change based on the biology of the mesocosm, with warm-temperature populations forming and then disappearing over the course of a few days. These findings have important implications for marine cloud coverage and precipitation in current climate models affected by marine INPs, such as those which overestimate cloud coverage over the Southern Ocean. Future work includes testing INP levels after acidification to determine if many INPs are proteins adversely affected by changes in pH.

23 Nuclear and Mitochondrial DNA Variation Across the Eastern Continental Divide

Rehal Bollavaram
Georgia Gwinnett College, rehal_md@yahoo.com

The molecule deoxyribonucleic acid (DNA) is the molecule of inheritance for all living organisms. Variation in the structure (sequence) of this molecule has been used to investigate everything from the heritance of disease to the development of species. Our research has taken advantage of molecular techniques that allow the relatively cost-effective sequencing of DNA to analyze fish species in Gwinnett County. Gwinnett County is bisected by the southeastern continental divide that separates water flowing to the Gulf of Mexico and water flowing to the Atlantic Ocean. Given this geographical feature, Gwinnett County is an ideal area to test many different hypotheses regarding DNA variation among aquatic organisms across a continental divide. Select fish species in the genera *Semotilus*, *Nocomis*, and *Lepomis* were sampled for DNA analysis of variation within species. Previous analyses had shown distinction in DNA variation across the divide when it came to the *Nocomis* species, an indication of restricted migration between fish populations. Our supplementary results generally support previous results, but find that some species are not restricted by the continental divide, and there may be a previously unrecognized speciation event in the genus *Nocomis*.

24 Field Sparrow: Genetic Variability and Migratory Patterns

Hana Alhuneidi, Maribel Fernandez, Mia Malloy and Jill Penn
Georgia Gwinnett College, halhuneidi@ggc.edu

The Field Sparrow, also known scientifically as *Spizella pusilla*, is a small, warm-toned bird with a pink bill that resides in the eastern regions of North America. Unfortunately, due to the increase of the suburbs, populations of this sparrow have declined from the inability to nest in these areas. Therefore, the process of banding each individual bird, will allow researchers to keep track and analyze the population, breeding locations, and migration patterns to promote the increase in population, which can support the environment for the future. Field Sparrow populations have stayed more consistent in the prairies, and they can typically be found in the shrubs of certain areas. Interestingly enough, they exhibit an unusual behavior for birds in which they nest near the ground. Furthermore, migration plays an important part in the breeding and population. It is common to find the Field Sparrow migrating to the north to breed. They are also considered a partial migrant, in which they occasionally move south in the winter, depending on environmental conditions, rather than remaining near their breeding grounds year-round. Considering, that Field Sparrows are facultative and not obligate migrants, they can generally be found in Georgia year-round. However, it is unclear whether or not an individual Field Sparrow can be found in Georgia year-round, or if there are multiple populations that live in Georgia part of the year for breeding or optimal weather conditions. Genetic sequencing of the mitochondrial gene cytochrome c oxidase subunit 1 was performed to further understand the migration and breeding patterns. DNA sequence data was analyzed using Mega 7 software to determine consensus and rare haplotypes. The consensus or haplotype 1, which is the sequence that occurs the most, was CCAT. The majority of the Field Sparrows had the consensus sequence, suggesting that many of these birds are related. Additionally, birds with the consensus sequence were found in different geographical areas such as Virginia, North Carolina, Canada, and multiple regions in Georgia. This suggests a strong indication that Field Sparrows migrate between regions in the north and south due to breeding season or escaping cold weather conditions. In total there were 4 haplotypes found from 27 birds including the consensus haplotype. A phylogenetic tree was also constructed to appropriately group the haplotypes. This showed a strong relation between 3 birds found in Dacula, GA and one bird from Quebec, Canada. This rare haplotype shared between Georgia and Quebec Field Sparrow is consistent with the hypothesis that some winter Field Sparrows from Georgia migrate to Canada to breed. More research is necessary to determine if this applies to all winter Field Sparrows.

25 Water Quality Chemical and Microbial Analysis of Select Water Resources in Gwinnett County, GA

Jehan Sheikh, Thomas Gluick and Rashad Simmons
Georgia Gwinnett College, jehan.sheikh1950d@gmail.com

According to the EPA, both phosphorous and nitrogen are vital nutrients for plants and animals in aquatic environments. However, the disruption of phosphorus and nitrogen cycles due to manmade activities may lead to excessive levels of nitrate and phosphorus in water and eutrophication. Therefore, this project focuses on the safety and quality analysis of water samples from Shoal Creek at upstream and downstream sites of the Lawrenceville City Lake, and two locations along the Yellow River. In this project, the total nitrate and phosphate concentrations were determined via colorimetric assays. Nitrate concentrations ranged from 0.08 ppm to 15.78 ppm, and the phosphate concentrations were negligible in the low ppb. Non-purgeable organic carbon (NPOC) and total nitrogen concentrations in the water samples were measured using a Shimadzu TOC-L TOC analyzer. NPOC concentrations ranged from 1.12 ppm to 4.21 ppm, and the total nitrogen concentrations ranged from 0.21 ppm to 2.15 ppm. Additionally, investigated nitrate concentrations in the water samples via High-Performance Liquid Chromatography (HPLC). For the microbial analysis, the Most Probable Number (MPN) assay was performed to determine concentrations of viable microorganisms, most notably E. Coli.

26 Molecular Docking of the Interactions of Fluorinated Heterocyclic Sulfonamides with Human and *Plasmodium* DHFR

Miki Nguyen
Georgia Gwinnett College, nforlemu@ggc.edu

About half of the world's population lives in areas at high risk for malaria. This deadly scourge that results in 650,000 fatalities annually mainly targets children, pregnant women, and populations in tropical regions of the world. The folate pathway enzyme Dihydrofolate reductase-thymidylate synthase (DHFR-TS) is critical for producing key cellular components (amino acids and nucleic acids) required for the survival of the parasite *Plasmodium falciparum*, the causative agent of malaria. This, therefore, makes DHFR-TS a potential target receptor for antimalarial activity and the development of novel therapies. A number of antimalarial drug combinations have become ineffective due to parasitic resistance, as a result of point mutations of *Plasmodium* enzyme DHFR. In this study, we have used molecular docking, to calculate the binding energy of interactions between DHFR variants and heterocyclic sulfonamides. The affinities are benchmarked with common antimalarial drugs like artesunate, pyrimethamine, and chloroquine. The three-dimensional structures of human DHFR, wild type, double mutant, and quadruple mutant DHFR were acquired from the Protein Data Bank and the monomer structure was obtained using PyMOL. The monomer units of the DHFR variants were docked with seven heterocyclic sulfonamides and current antimalarial drugs using UCSF Chimera and Autodock Vina. Three sulfonamides showed greater interaction affinity with pfDHFR compared to current antimalarial drugs (chloroquine, pentamidine, pyrimethamine, and artesunate). Sulfonamide 7 selected against human DHFR the best out of the three with a binding energy of -8.4 kcal/mol with human DHFR compared to -9.7 kcal/mol and -10.1 kcal/mol. Sulfonamides 5-7 had 3 hydrogen bond donors compared to sulfonamides 1-4 which had 2 hydrogen bond donors. The sulfonamides in this study are comparable to current antimalarial drugs as potential ligands for new antimalarial drugs.

27 Predicting Micellization Behavior of Carboxylate Surfactants from Molecular Simulation

Mingning Zhu and Xiaokun Zhang
Emory University, mingning.zhu@emory.edu

Surfactants are amphiphilic compounds that form aggregates such as micelles in aqueous solution at concentrations above a critical micellar concentration (CMC). However, the structural disorder, polydispersity, and sensitivity to conditions of surfactants present challenges to the unambiguous determination of micelle properties through experiments alone. Molecular dynamics (MD) simulation has thus become a powerful tool to gain insights on the self-assembly of surfactants. This study aimed to use MD simulations to predict the self-assembly behavior of long-chain carboxylate surfactants, octanoates, with Na^+, K^+, and TMA (tetramethylammonium) counterions. As the fitted thermodynamic data are sensitive to the definitions of clusters, this study explored more accurate definitions of octanoate clusters with both alkali and organic cations. We input statistics from small systems and generated equilibrium constants of octanoate micellization through a global fitting procedure called the PEACH method. The resulting free energy statistics were used to predict critical micelle concentration (CMC), micelle size, and the degree of counterion binding versus concentration for bulk solutions. Our results showed that the trends in CMC with varying counterion are all consistent with experimental data. The generated free energy profiles can also be rationalized by a phenomenological four-parameter model. Work is in progress to analyze enthalpy changes associated with micellization and counterion binding for comparison with experimental calorimetry data.

28 The Effect of Solvation on the Oxidation of Trimethylamine

Marquell Cole
Morehouse College, Marquell.cole@morehouse.edu

A computational study of the solvation effects on the mechanism of the oxidation of trimethylamine with hydrogen peroxide is presented. The mechanism was studied in terms of reaction force, chemical potential, and reaction electronic flux (REF). The REF has been proven useful in tracking the formation of chemical bonds throughout the reaction's mechanisms. In this study, the mechanism is investigated by considering a reaction between trimethylamine and hydrogen peroxide. Density functional theory is used (at the B3LYP/6-31+G* level) to determine the reaction energy profile, while solvation effects are taken into account using a COnductor-like Screening MOdel (COSMO). The REF analysis shows a more favorable N-O bond formation in solvent than in the gas-phase.

29 Preparation of Biodiesel using a DES

Izza Tirmizi
Georgia Gwinnett College, izaat0704@gmail.com

To minimize the use of volatile organic solvents, a Deep Eutectic Solvent (DES) consisting of choline chloride and glycerol was introduced as the co-solvent in the trans-esterification reaction of vegetable oils to biodiesel catalyzed by sodium hydroxide. The DES used is an inexpensive, non-toxic, and biodegradable alternative when compared to the volatile and often toxic organic solvents. Through the evaluation of different oils and their effects as well as the repetition of the reaction to optimize results, biodiesel was eventually achieved. IR and NMR results indicate that a DES can be used as substitutes for the toxic and volatile organic solvents in the trans-esterification reaction of biodiesel.

30 Utilizing Modular Redox-active Ligands to Promote Aerobic Oxidations at Cobalt(II) and Copper(II) Metal Centers

Erika Diosdado, Omar Villanueva and Cora E. MacBeth
Georgia Gwinnett College & Emory University, ediosdado@ggc.edu

The selective functionalization of inert C-H bonds from petroleum feedstocks into value-added C-C bonds through the use of earth-abundant first-row transition metal catalysts remains an important research goal in synthetic organic chemistry. Converting C-H bonds to C-C bonds via transition metal catalysts that can utilize molecular oxygen as the terminal oxidant has received significant attention as this is a greener, yet more challenging approach to C-H functionalization. The central hypothesis of this research is that modular redox-active ligand scaffolds presented herein can be used to create reactive monomeric cobalt(II) and copper(II) complexes capable of promoting catalytic aerobic oxidation reactions. This research will present the reactivity of Co(II) and Cu(II) complexes, containing either an aminophenylaminate or an aminophenylurea redox-active ligand platform. We hypothesized that these systems could be utilized to construct C-C bonds from phenolic C-H bonds. To test our hypothesis, the aerobic oxidative coupling of 2,4-di-tert-butyl phenol was chosen as the model reaction. Methods used in this research include the use of cyclic voltammetry, NMR and UV-visible absorption spectroscopies, and reaction optimization for exploring optimal catalyst performance. This research has resulted in the preparation of cobalt(II) and copper(II) systems that are highly effective for aerobic oxidation reactions. Results obtained from this work will constitute a landmark innovation with the potential to impact the field of oxidation catalysis broadly.

31 Separation Chemistry and Crystallographic Investigation of Orthogonal Catalysis of a Conjugated Polymer by an Enzyme

Hunter Spivey
Kennesaw State University, hspivey3@students.kennesaw.edu

Hen egg white lysozyme's (HEWL) natural role is as a peptidoglycan hydrolase, however this enzyme has been observed to mediate a polymerization of 2-ethynylpyridine, which is the first example of hydrolase-meditated formation of a conjugated polymer. This project will guide green chemistry in the use of biological catalysts in polymer formation as opposed to metal catalysts which produce harsh organic wastes. The polymer product displays unique optical properties upon completion of the reaction. The aim of this project is to identify the structure of HEWL reaction products with 2-ethynylpyridine. This was done using three techniques, a size exclusion column to separate the products from the crude reaction; co-crystallization of the products with unreacted protein and X-ray diffraction of the co-crystalized products; then finally, NMR of the purified products. Prospects of additional analytical analysis will also be discussed such as LCMS, IR and CD spectroscopy. Assignment of polymer structure has been challenging. A crystal complex of HEWL and an competitive inhibiter to the 2EP reaction has been obtained. Further electron density models and spectral analysis of products will also be presented.

32 Polycarbonate Electrolytes for Solid-state Li-ion Batteries

Ammber Hoang, Shuai Xu, Huan Wang and Dr. Xiaodong Hou
Georgia Gwinnett College and University of North Dakota, ahoang1@ggc.edu

Currently, the dominant electrolyte in modern commercial Li-ion batteries (LIBs) is a liquid solution of lithium hexafluorophosphate (LiPF6) dissolved in a mixture of cyclic and linear organic carbonates (e.g. ethylene carbonate, ethyl methylcarbonate), which are extremely flammable and highly sensitive to trace moisture. This combination raises significant concerns related to safety and the cycling life at elevated temperatures. To address these issues, the goal of our research project was to develop and evaluate the efficiency of polycarbonate-based electrolytes for solid-state LIBS. A solid-state battery with a solid electrolyte would greatly improve upon Li-ion batteries and would be the ultimate solution to the safety issue. For our design, a solid polymer membrane was cut into discs, which were assembled into two types of coin cells, then analyzed using a battery testing system (BTS) and electrochemical impedance spectroscopy (EIS). Results indicated that the ionic conductivity of the membrane increased at elevated temperatures and exhibited stable charging/discharging plateaus. The charge/discharge specific capacities over cycle times were stable, but not optimal. In its present state, the novel solid-state electrolyte did not perform as well as the commercial liquid electrolyte LIBs, a limitation that we anticipate will be resolved with continued development.

33 Synthesis of a Novel Octadentate Bis(amidine): A Topological Approach to Twisted Molecular Copper Strings

Naza Okafor and Janet Arras
Kennesaw State University, cokafo13@students.kennesaw.edu

Multinuclear Group 11 clusters, specifically those that incorporate copper as the first choice of a cheap precursor coinage metal, have attracted considerable interest within in the past decade, since they facilitate closed-shell metal $M^{I}\cdots M^{I}$ ($d^{10}\cdots d^{10}$) interactions (M = Cu, Ag, Au). The fascinating luminescence properties of these multinuclear complex assemblies lead to applications as powerful building blocks for molecular/organic light-emitting devices/diodes (OLEDs). Polydentate ligands that are capable of accommodating defined linear arrangements of Cu(I) ions are of particular interest in this regard, as they can also serve as molecular wires in nanoelectronics. Our concept features a series of new polydentate bis(amidine) ligands LH_2 with a sterically protected flexible backbone. It has recently been demonstrated that LH_2 undergoes with mesitylcopper, a powerful synthon for a variety of unusual Cu(I) frameworks, a clean conversion into two simultaneously crystallizing Cu(I) complexes $[L_{12}Cu_4]$ and $[L_{14}Cu_8]$ that show blue (λ_{max} = 460 nm; $[L_{12}Cu_4]$) or green (λ_{max} = 495 nm; $[L_{14}Cu_8]$) light emissions in excellent quantum yields. We are now focusing on the exploration of novel bis(amidines) that provide additional terminal donor sites, with regard to the formation of new unusual cuprous metal clusters. We envision a molecular string with array of up to eight Cu^{+} ions to break the current world record of six.

34 Portable and Remotely Monitored Ultra-Violet Spectrophotometry

Ashkar Awal
Georgia Gwinnett College, stangira@ggc.edu

Ultra-Violet (UV) spectrophotometers are very useful, large, and immobile scientific equipment that are commonly installed and used in a laboratory setting. They have limited use if samples from remote regions are to be analyzed. In such cases, samples need to be collected, perhaps from hazardous and hard to reach environments and then be brought back to the lab for testing, risking contamination and loss as they are tested.

In this project, we present a working proof-of-concept a portable UV detector. It can be installed and used to detect, store, and transmit UV radiation data in the range 240 nm to 370 nm from remote environments which may not accessible by large equipment or human beings. Notably, our prototype takes a traditionally indoor laboratory chemistry photo-spectrometer and lends it applicable to an outdoor environment. The UV sensor employed in our detector is based on physical chemistry principles of semi-conductors. It has the advantages of short response times, high responsivity (typically 0.14 A/W) and very low dark current (max. 1 nA). We also present systematically collected data and discuss the characteristics of the UV detector along with its possible uses in chemistry.

35 Optimization of the Synthesis of N-[2-(5-hydroxy-1H-indol-3-yl)ethyl]-2-oxopiperidine-3-carboxamide (HIOC), a Potential Neuroprotectant

Taylor Dover
Emory University - Department of Chemistry, tldover@emory.edu

N-[2-(5-hydroxy-1H-indol-3-yl)ethyl]-2-oxopiperidine-3-carboxamide (HIOC) exhibits protective activity against retinal damage in animal models, and thus has considerable therapeutic potential. This poster will describe improvements in the synthesis of HIOC, including assessing the configurational stability of the chiral center in HIOC and in synthetic precursors.

36 Proton Transfer in Supercooled Aqueous Solutions

Mayowa Sonola, Sam Wright and Frank Reece
University of West Georgia, msonola1@my.westga.edu

Supercooled liquids are intimately connected to developing new materials. These are metastable liquids, in which they have been cooled below the melting point, but not below the glass transition temperature (T_g). In this study, the structure of supercooled aqueous solutions in the temperature regime near the glass transition is probed using photo-induced proton transfer. These solutions contain 2-nitrobenzaldehyde (NB) and bromocresol green (BCG). When excited with 355 nm light, NB undergoes a photochemical reaction that results in a rapid release of a hydrogen ion (proton). A fraction of these hydrogen ions migrate until they protonate a BCG molecule. BCG prior to protonation absorbs 622 nm light. When protonated, BCG absorbs 450 nm light. Following laser excitation, we measured the growing absorption at 450 nm resulting from protonation of BCG. The time courses measured display sigmoidal behavior, and have been fitted to a functional form described by the Weibull equation for a cumulative distribution function:

$$I(t) = A(1 - e^{(-kt)^d})$$

The change in absorption intensity, is defined by A, k, and d (A is the final absorption intensity, k is the rate that absorption increases and d is the statistical shape parameter). We relate these parameters to the structural heterogeneity of these supercooled solutions.

37 Development of Asymmetric Redox-Active Ligand-Scaffolds for C-H Bond Activation

Eric Juarez and Dan Liu
Emory University, eric.juarez@emory.edu

First row transition metal mediated C-H functionalization has been shown to be an effective synthetic strategy for the formation of C-C, C-O and C-N bonds with low cost. However, due to the one-electron reactive nature of these metals, this type of chemistry is challenging. The MacBeth group has successfully incorporated redox-active ligands with first row transition metals for catalyzing multi-electron chemistry processes such as C-H oxygenations and aminations. Nevertheless, an issue that our group has encountered with this chemistry is that our catalysts did not show good enantioselectivity. In order to improve our catalysts' selectivity, a series of asymmetric redox-active ligand scaffolds will be designed and synthesized in this presentation. Those ligands will be fully characterized and then metallated with transition metals such as cobalt and nickel.

38 A Calorimetric Study of the Exchange of Chloride-Nitrate on Hematite Nanoparticles

Natasha Clarke, Mollient Oganga Cooper, Dr. Elina Stroeva, Dr. Hind A. Al-Abadleh and Dr. Nadine Kabengi
Georgia State University, nclarke5@student.gsu.edu

Many chemical and biological reactions in soils are impacted by the presence of natural organic matter (NOM) such as citric or oxalic ions, that often enhances the bioavailability of nutrient and overall soil fertility. In soils, NOM is strongly correlated with the Al and Fe-oxides content of soils. Therefore, it is important to study the surface interactions of organic molecules with Fe-oxides, particularly at various pH conditions that might control whether organic ions are retained in solid or released to nearby aquatic systems. The presence of NOM in soils affects the following accumulation and redistribution of chloride and nitrate ions which are in most common species of fertilizers. It is also known that the hematite surface charge is pH-dependent and develops different number of active sites of different nature.

To that end, this research aims to study the interaction of alternative pair of chloride/nitrate ions exchanging on hematite nanoparticles at pH 7 and concentrations 1, 10, 100, and 1000 mM of chloride/nitrate in cycles before and after oxalate-ion interaction with a hematite surface. These experiments were conducted using method of flow microcalorimetry as it allows for real time and *in situ* examination of the exchange and adsorption processes. Experimental results manifested gradual reduction in heat of oxalate adsorption with decreasing of ionic strength of chloride/nitrate solutions with exception for 100 mM solution. Future research will be conducted.

39 Synthesis and Crystal Structure Analysis of Indenochalcones Using Green Chemistry

Elvia Encarnacion-Thomas, Joseph Sloop and Ajay Mallia
Georgia Gwinnett College, eencarnacionthom@ggc.edu

In this project, the preparation of a series of chalcones analogs synthesized via a base-promoted Claisen-Schmidt reaction and different alkyl chain lengths using solventless processes is under investigation. Due to its biological properties, 1-indanone was used as a potential pharmacophore in these experiments. A new chalcone, (E)-2-(3,5-Dimethoxybenzylidene)-1-indanone, was prepared *via* a solventless process. The molecular structure was confirmed through X-ray Crystallography and characterized with ^{1}H and ^{13}C NMR. Reaction conditions (sonication *vs*. hot sand bath) were studied for yield optimization, the latter providing the highest yield. Product yield in four trials were 15 %, 31%, 31 %, and 56%. Additionally, an isomerization through UV radiation over the course of 96 hours is under investigation with the purpose of obtaining the Z-chalcone isomer.

40 Accessing Novel Metal Organic Frameworks Using Reticular Chemistry

Emily Shrewsbury
University of North Georgia, edshre7434@ung.edu

Zeolitic imidazolate Frameworks (ZIF's) are a subfamily of porous MOFs mimicking the 145° angle in zeolite minerals that are prepared using reticular chemistry to form materials that aid in gas separation, drug delivery, and catalysis. The purpose of this research is to study the steric and structural directing effects of unexplored disubstituted and trisubstituted linkers such as 4,5-diphenyl imidazole, 2,4,5-trimethyl imidazole and 2,4,5-triethyl imidazole on the formation of zeolitic imidazolate frameworks. These chosen linkers add hydrophobic dynamics to the framework at the 2-, 4- and 5- positions in the form of two phenyl rings (disubstituted) or three carbon chain groups (trisubstituted). Currently, experimentation with altering concentrations, reaction times, and temperature fluctuations of the furnace are being done using the 4,5-diphenyl imidazole. The reaction was observed to have formed large white urchin-like structures that coagulated together. When the product was observed under an optical microscope, the material had long thin hair-like features. Different metal salts containing cobalt and iron have also been investigated with the 4,5-diphenyl imidazole to study the potential linker to metal coordination patterns. Additional trials, including addition of a variety of strong bases to the reaction mixture to aid in deprotonation of the trisubstituted imidazole linkers and structural identification of the obtained solid/crystalline products are underway.

41 The Chemistry of Glazes

Emily Robison, Tamera Taylor, Cecilia Redding and Dave Collins
University of West Georgia, erobiso1@my.westga.edu

Chemistry of Art has shown that chemical understanding of pigments, dyes, binders, and alloys, only to cite a few, is essential to understanding how and when artworks have been created and how to best care for them on a long-term scale. The field of ceramics, also, is rich in chemistry and many chemical reactions take place during the firing process, making the study of ceramics an exciting topic for a chemistry project. In this presentation, we will explain the different chemical components found in a ceramic piece, describe the firing process and use glazes as a teaching tool for a chemistry of art class for non-science majors. Data collected from over 40 samples of clay and glazes of various compositions have been analyzed, leading to a fruitful discussion on the chemistry of ceramics.

42 Observation of Rotational Dynamics of Gold Nanoparticles using Cytochrome C as a Model protein

Khalif Joseph and Kuangcai Chen
Georgia Gwinnett College, kjoseph1@ggc.edu

Gold nanoparticles (AuNPs) are becoming increasingly important in the study of biological systems at the microcellular level. Their usefulness comes from their anisotropic properties and how they interact with light. The phenomenon known as localized surface plasmon resonance (LSPR) is the oscillation of surface electrons in noble metals such as gold and silver under electromagnetic irradiation. This property is used to study the rotational dynamics of AuNPs and homodimers.

In this research project, AuNPs were studied using a Nikon ECLIPSE 80i microscope with dark field microscopy and differential interference contrast (DIC) microscopy capabilities. Results of this study revealed that the rotation of immobilized AuNPs on a glass surface corresponded to fluctuations in light scattering intensities under DIC microscopy. Dark field microscopy was used to obtain spectral information on the AuNPs and homodimers. The mean wavelength of single AuNP was found to be 541 nm. The interparticle separation of homodimers before and after Staurosporine (STS) treatment was reported to be 11 nm and 6 nm respectively. The corresponding rotational relaxation time before and after STS treatment was found to be 0.95 ± 0.83 s and 1.36 ± 0.82 s. This study illustrated how the anisotropic properties of AuNPs is correlated to rotational information.

43 Synthesis and Comparative Characterization of Cellulose-Base and Acrylamide-Base Hydrogels for Nutrients Recycle

Abigail Budu, Stefan Muamba, Madison Preston and Sahba Khorsandzadeh
Georgia Gwinnett College, abudu@ggc.edu

Valuable nutrients such as nitrogen, phosphorus and potassium from various sources are discharged to water bodies, causing water pollution and a net loss of the nutrients. There is increasing interest in the unit processes for source separation and treatment for nutrient recycling and reduction of load to water treatment. Derived from natural or synthetic polymers to create a network of polymers, hydrogels have been approved risk free and efficient for nutrients recycling due to their unique characteristics including an ability for high water retention as well as the capability for the adsorption/desorption of various chemical compounds, making hydrogels a good option for the recovery of nutrients from aqueous solutions. This study aims at providing systematic comparison of physicochemical characteristics between cellulose-base and acrylamide-base hydrogels and advanced synthesis utilizing liquid nitrogen. The performance of hydrogels was tested for swelling, adsorption/desorption, and the equilibrium partitioning and kinetics study are being conducted. In the performance studies, the cellulose-base hydrogels showed a much higher swelling ratio and adsorption capacity than the acrylamide counterpart while acrylamide hydrogels showed a greater mechanical strength over time in aqueous solutions. A new synthesis of cellulose-based hydrogel employing liquid nitrogen dramatically reduced the reaction time with the performance commensurate to that by a previous method with freezing-thawing cycles. This new method of cellulose synthesis is in attempt to reduce impurities in the cellulose hydrogels that are caused from unreacted monomers. With a focus on developing the optimal synthesis condition, the structure of the hydrogels has been identified using IR spectroscopy, and various drying methods adopting air convection and dehydration using organic solvents were tested. The adsorption/desorption behavior was evaluated using urea solution as well, and finally, the parameters were correlated to the properties of the hydrogels. Future studies include isotherm studies to provide information on mechanisms of nutrients adsorption/desorption, development of a prototype of adsorption columns, and free-radical polymerization of hybrid hydrogels containing carboxymethyl cellulose and acrylamide.

44 Carbon Dioxide Adsorption on a Stilbene-based Manganese Metal-Organic Framework

Talia Ferguson, Saki Golafale and Dr. Conrad Ingram
Clark Atlanta University, talia.ferguson@students.cau.edu

A metal-organic framework (MOF) was synthesized by combining manganese (II) nitrate tetrahydrate with two organic ligands, 2,2'-bipyridine and 2,2'-dinitro-4,4'-stilbenedicarboxylic acid at 200°C for 48 hours. This material was characterized using FTIR, TGA and non-ambient X-ray diffraction analyses with the later indicating a very stable structure up to 200 °C, and upon slow cooling from 250 °C to 25 °C the structure was restored. This was followed by degassing the MOF at various temperatures (25 °C, 50 °C, 100 °C, 120 °C and 180 °C) under vacuum and CO_2 adsorption at 256 K after each degas temperature. The CO_2 adsorption capacity was highest at the degassing temperature of 180 °C. Further analyses and results showed that at 256 K, 273 K and 298 K, the CO_2 adsorption capacities were 1.52 mmol/g, 1.55 mmol/g and 0.77 mmol/g, respectively. The experimental isotherms were fitted using a modified Langmuir-Freundlich isotherm model. The thermodynamic parameters calculated showed that at 256 K and 273 K the adsorption process was spontaneous, while at 298 K it was non-spontaneous. With these results, this MOF can be of great interest based on its intriguing thermal stability and its capacity to adsorb CO_2.

45 Preparation and Studies and Thermal Properties of Choline Chloride Based Deep Eutectic Solvents and Molecular Gels Based on Ammonium Alkanoates

Joel Suazo
Georgia Gwinnett College, joelsuazo3@gmail.com

Present study describes the preparation, spectroscopy and thermal properties of deep eutectic solvents and gelation properties of ammonium alkanoates as low molecular mass gelator. Binary and ternary mixtures with various concentrations of naturally occurring amino acids (L-phenyl alanine, L-glutamic acid, L-tyrosine, L-aspartic acid, glycine), choline chloride and glycerol were prepared. Thermal properties of the mixtures were determined differential scanning calorimetry and melting point analysis. 1:3 and 1:2 binary mixtures of L-glutamic acid/choline chloride were observed to liquid at room temperature in the examined mixtures. The binary mixtures were also characterized using IR and NMR spectroscopic techniques. Preparation and gelation studies of ammonium alkanoates (carbon chain length n = 12, 14, 16 and 18) will be presented.

46 Synthesis, Characterization and Gelation Studies of N-(phenylalkyl)octadecanamides as Low Molecular-Mass Gelators

Jennifer Kim
Georgia Gwinnett College, jenniferjkim01@gmail.com

A new class of low molecular-mass gelators (LMGs), based on N-(phenylalkyl)octadecanamides (alkyl chain length n = 0, 1, 2, 3 and 4) and the properties of their gels have been investigated using structural, spectroscopic and rheological techniques. Gels were prepared using solvents of differing polarity for each LMG and critical gelator concentration (CGC) and gel melting temperatures and gel stabilities were noted. A direct relationship between the length of the alkyl chain and solvents effectively gelled was observed. Furthermore, N-(phenyloctadecanamide and N-benzyloctadecanamide exhibit gelation property in water and organic liquids (ambidextrous gelators). Comparison and correlation of the molecular structures of these gelators and the properties of their gels using critical gelator concentrations and gel melting temperatures will be presented. Some of the molecular gels have been found to be thixotropic and recover a large part of their viscoelasticity being destroyed by excessive strain shearing. Optical micrographs of the gels show that the self-assembled fibrillar networks consist of spherulitic objects.

47 Synthesis, Characterization and Gelation Properties of N-(acridin-9-yl)alkanamides-based Low Molecular Mass Gelators

Sokhna Ndiaye
Georgia Gwinnett College, sndiaye@ggc.edu

N-(acridin-9-yl)alkanamides with dodecyl (9A12) and tetradecyl (9A14) carbon chain have been synthesized using lauryl chloride and myristoyl chloride. All synthesized compounds were characterized using spectroscopic analysis. Preliminary gelation studies show that 5 wt % 9A12 and 9A14 gelate organic liquids (silicone oil, safflower oil and DMSO) and water. Systematic analysis of gelation properties various polarity liquids and correlations with structure of gelators will be also discussed.

48 Preparation, Thermal Properties and Gelation Studies of 3β-cholesteryl N-(9-acridinyl) carbamate as Low Molecular Mass Gelator and Aggregation Studies with DNA

Jordi Lainez, Tyler Sawyer, Neville Forlemu and Thomas Gluick
Georgia Gwinnett College, jlainez1@ggc.edu

Acridine based compounds have been known to exhibit many biological functions. In the present study 3β-cholesteryl N-(9-acridinyl) carbamate (CAC) was prepared by the reaction between 9-aminoacrdine and cholesteryl chloroformate as potential low molecular mass gelator (LMG). 5 and 10 wt % preparations of CAC have been shown to gelate DMSO, *tert*-butanol mesitylene and safflower oil. Correlations between self-assembly and gelation properties of CAC in various liquids and thermal properties will be presented. Computational studies of complexation with DNA shows that CAC binds DNA strongly compared to pyridinyl cholesteryl carbamate or 9-aminoacridine.

49 Preparation, self-assembly and gelation studies of N-(4-hydroxyphenyl)alkanamides as low molecular mass gelators

Clarissa Landaverde, Sandra Farre
Georgia Gwinnett College, clandaverde@ggc.edu

Three derivatives of N-(4-hydroxyphenyl)alkanamides with varying alkyl chain length (n = 12, 14 and 18) have been synthesized and characterized using IR and NMR techniques. Gelation studies of N-(4-hydroxyphenyl)alkanamides were investigated in various polarity liquids. The gels formed were studied based on its physical appearance, solubility, gel formation time and melting point. It has been observed that both carbon chain length and the organic solvent altered gelation properties. Polarizing optical micrographic studies of 5 wt % silicone oil gel of N-(4-hydroxyphenyl)alkanamides exhibit spherulitic textures.

50 Fluorescent Sensing of Nitroaromatic Compounds Utilizing Anthracene Based Metal-Organic Frameworks

Paris Grady, Saki Golafele
Clark Atlana University, paris.grady@students.cau.edu

Metal organic frameworks (MOFs) are crystalline solids made from organic ligands and metal cations. These MOFs can be utilized in many applications such as sensing nitro-aromatic compounds. The synthesis of MOFs using lanthanide metals have been an interest for chemical sensing due to their optical properties. Several 9,10-anthracene dicarboxylate (ADC^{2-}) lanthanide-based MOFs were previously synthesized. These MOFs contain the metals ions, terbium and dysprosium, and are currently being evaluated for nitro-aromatic compound sensing. Preliminary studies conducted on the terbium and dysprosium MOFs show broad peaks in the fluorescence spectrum similar to the H2ADC ligand and an absence of characteristic fluorescent peaks for the metal ions, this signifying that the fluorescence is ligand based. The range for the emission test was 390 nm - 600 nm. The lanthanide MOFs suspended in ethanol, show emission maximum at wavelength 445 nm. Adding small aliquots of nitro-aromatic compounds, dissolved in ethanol, to a stable suspension of the terbium and dysprosium MOFs show significant reduction in fluorescence intensity thereby signifying quenching of the MOFs fluorescence. In conclusion, lanthanide MOFs with the H2ADC ligand can be a possible tool for detecting nitro-aromatic compounds. Further details on the fluorescence behavior with and without the presence of nitroaromatic compounds will be presented.

51 Synthesis and Gelation Studies of Anthraquinonylalkanamides as Low Molecular Mass (5%) Gelators

Erica Lee, Dr. Ajay Mallia and Tamilore Dairo
Georgia Gwinnett College, elee21@ggc.edu

The purpose of this study is to synthesize and to gelate anthraquinonylalkanamides. Aminoanthraquinone is known to exhibit anti-cancer effects, and adding alkyl chains to aminoanthraquinone is expected to improve its pharmaceutically beneficial effect and deliverability. 1-aminoanthraquinone (AAQ) was reacted with lauroyl chloride (AAQ-12) and stearoyl chloride (AAQ-18); 1,4-diaminoanthraquinone (DAAQ) was reacted with lauroyl chloride (DAAQ-12). Thermal and gelation properties for the products were studied. AAQ-12 gelated in silicone oil, *tert*-butanol and safflower oil; and DAAQ-12 gelated in silicone oil, *tert*-butanol, ethanol, isopropanol, cyclohexane, diethyl ether, and 1-butanol. AAQ-18 gelated in silicone oil, safflower oil, ethanol, isopropanol, DMSO, and 1-butanol. The only solvent that gelated all three product was silicone oil.

In future experiments, reactions for AAQ with myristoyl chloride; DAAQ with myristoyl chloride, DAAQ and stearoyl chloride will be conducted. DNA interactions with the six different anthraquinonylalkanamides will be also examined to compare their anti-cancer effect.

52 Deformability Analysis of Ultra Soft Microgel Particles on Flat Surfaces

Ericka Westbrook and Gabrielle Brim
Spelman College, ewestbro@scmail.spelman.edu

Microgels, soft hydrogel particles, are of interest for applying in the development of new biological, chemical and technologies, including promoting bacterial adhesion inhibition and organic coatings. The objective of this research project is to analyze the interfacial properties between poly *n*-isopropylacrylamide (NIPAM) polymer microgel particles on flat surfaces. NIPAM microgel particles were synthesized with varying molar densities of N,N′-methylenebisacrylamide (BIS) crosslinking agent, ranging between 0 - 2%, which caused the particles to display a range of stiffnesses. It is expected that the microgels containing 0% BIS should be the most deformable a flat surface, because they do not contain any additional concentration of BIS crosslinking agent. However the microgels containing 2% BIS are expected to be less deformable, by displaying a change in diameter and height, compared to the 0% BIS particles. This hypothesis was verified by measuring the diameter of the particles and height of the micron-sized particles, using light microscopy and atomic force microscopy (AFM). Experimental results confirmed our hypothesis was correct such that the diameter of the 0% BIS microgels were larger and flatter than the 2% BIS microgel particles. From these results, the material properties of the microgel particles will help in future applications involving microgels.

53 Lignin-coated Cellulose Nanocrystals in Polylactide Acid: Thermal Analysis and Microscopy

Ivey Frazier and Asya Tucker
Clark Atlanta University, ifrazier@scmail.spelman.edu

Throughout this research we have investigated the thermal properties of PLA based nanocomposites. Poly(lactide acid) (PLA) is a bio-based, biocompatible, thermoplastic and is being extensively researched for its potential uses in the various fields such as, dental and biomedical fields. The aim of this research was to enhance the thermal properties of these nanocomposites by covalently bonding lignin coated cellulose nanocrystals (L-CNCs) to the PLA chains using a radical initiator, Dicumyl peroxide, which is also known as, DCP. Our samples were prepared by chemically incorporating lignin coated cellulose nanocrystals into polylactide acid by high torque melt mixing, while utilizing DCP. Using the melt mixing technique, we were able to evenly distribute and disperse the fillers (L-CNCs) into our standard PLA. We used two different methods to process two covalently bound filler/polymer composites: PLA/DCP/LCNCs and PLA/LCNCs/DCP. Differential scanning calorimetry, thermal gravimetric analysis, and microscopy were carried out on composites with these two methods of composite processing at constant L-CNC loading. The cold crystallization enthalpy melt peak enthalpy, glass transition temperature, and degradation temperature was determined for each composite by using TA Universal Analysis. Significant results include a decrease in glass transition temperature for the PLA/DCP/LCNCs, and there was an increase in degradation temperature for samples in which the LCNCs were chemically bound into the PLA. Overall, the results indicate the physical and chemical modifications changed the rate of crystallization yet retained the thermal stability of each composite. This work was funded by National Science Foundation GA-AL LSAMP Grant HRD-1305041.

54 Adsorption and Reaction of the Chemical Agent Simulant Dimethyl Chlorophosphate (DMCP) with Zirconium Hydroxide

Julian Mory
Kennesaw State University, julianmory@gmail.com

The development of technologies that can be used to protect against chemical warfare agents is becoming critically important, given the relative ease of production and deployment of these weapons. Zirconium hydroxide, a polymorphic zirconia material, has recently been shown to be one of the fastest-acting solids for decomposing VX, an extremely toxic and very fast-acting chemical warfare agent. The present study builds upon our earlier work examining the adsorption and decomposition of dimethyl methylphosphonate (DMMP) on zirconium hydroxide and extending that work to an examination of the adsorption and decomposition of dimethyl chlorophosphate (DMCP) with the same substrate. DMMP does not have a phosphorus-halogen (P-X) bond whereas DMCP does, suggesting that DMCP may prove to be a better simulant for the surface reactions of nerve agents that contain a phosphorus-fluoride bond.

Our investigation was carried out using two different methods: 1) Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) to examine the surface reactions between DMMP and the solid; and 2) a flow reactor system that monitored gas phase reaction products produced by the surface reaction. The poster presents the comparison of the surface species formed upon the adsorption and reaction of DMCP with $Zr(OH)_4$ as well as the amounts and identities of the products formed, and compares those to the products formed with DMMP. Our results will also be compared to similar studies carried out at Edgewood Chemical and Biological Center with real chemical agents.

55 Preventing Cathode Dissolution by Homogeneous Sol-Gel Coating Method on Manganese Dioxide Nanofibers to Extend Battery Performance

Zeljka Zec and Milan Haddad
Kennesaw State University, zzec@students.kennesaw.edu

The cathode dissolution is a known occurrence for manganese dioxide (MnO_2) based cathode materials in both aqueous and non-aqueous batteries. Upon battery discharge, reduced Mn^{3+} species disproportionate ($2\ Mn^{3+} \rightarrow\ Mn^{4+}\ +\ Mn^{2+}$) and Mn^{2+} dissolves into the electrolyte causing the loss of active material, making the problem evitable. MnO_2 serves as an ideal cathode due to its availability and affordability. Nevertheless, the electrochemical performance is limited during battery cycling due to the dissolution of the cathode. In this project, a homogeneous sol-gel SiO_2 coatings with various thicknesses (0.5 - 5 nm) on α-MnO_2 nanorods are coated by insoluble oxide layers and characterized to ideally suppress and/or migrate the dissolution. The sol-gel SiO_2 coating is achieved by hydrolysis-condensation of TEOS (tetraethyl orthosilicate) under mild reflux conditions. In-depth characterization of SiO_2 coated α-MnO_2 are done by XRD, BET, XPS, EDX and SEM/TEM to analyze the surface of the silica coated α-MnO_2 cathodes, which will further be studied in zinc batteries. The cathode dissolution is investigated by determining the Mn^{2+} content in the electrolyte by electrochemistry process and characterization of the used electrodes. This ultimate solution will help utilize dissolution in aqueous-batteries and thus extend battery performance as well as overall life of batteries.

56 Investigating the Mechanisms of Aniridic Cataract

Katie Coscia, Samuel G. Novo, Mahbubul H. Shihan, Yan Wang, Paige Faasuamalie and Melinda K. Duncan
University of Delaware, kcoscia@ggc.edu

Aniridia is a congenital disorder of the eye whose hallmarks are the absence or malformation of the iris and underdevelopment of the fovea and optic nerve. These structural deformities are associated with many complications such as photophobia and decreased quality of vision early in life, as well as an increased predisposition to the premature onset of vision-threatening diseases such as glaucoma, keratopathy, and cataracts. Patients with aniridia will often require a lifetime of ophthalmological care, including many costly, invasive surgical procedures which carry their own set of risks and complications.

Aniridia is caused by heterozygous inheritance of a mutation of the PAX6 gene, one of the key regulatory transcription factors crucial for the proper formation and maintenance of the tissues of the eye. This haploinsufficiency of the PAX6 gene is implicated in the failure of the eye to maintain clarity of the lens and the premature development of cataracts in aniridic patients. In order to explore the molecular mechanisms behind cataract development, several fibrotic markers with altered levels of transcription were identified via mRNA sequencing of wild type and Pax6 mutant lens epithelial cells. Immunohistochemical staining was performed to investigate the role that four of these notable indicators of potential fibrosis play in the manifestation of the aniridic phenotype. There was a noticeable upregulation in the expression of α-smooth muscle actin protein and fibronectin in the lens cells that did correlate with the upregulation shown in the RNAseq data. In contrast, while collagen I mRNA levels are also upregulated by RNAseq, no discernible changes in its protein expression level was detected. Further, while the mRNA levels of extracellular matrix protein 1 are upregulated, the levels of this protein appear to have decreased in the lens capsule and increased in the lens cells. Such discordant results suggest that the protein levels of ECM1 and Collagen I may be controlled via post-transcriptional mechanisms such as translational control. Overall, these results suggest that the Pax6 heterozygous lens is sensitized to undergo fibrosis, which may explain the propensity of the aniridic lens to develop early onset cataract.

57 Characterization of the *Thermus thermophilus* Transcription Factor TTHA1719 by Use of the Combinatorial Method REPSA

Camille Atlan, Emily Clay and Michael Van Dyke
Kennesaw State University, catlan@students.kennesaw.edu

The hyperthermophile and halotolerant *Thermus thermophilus* is a Gram-negative aerobic bacterium capable of growing at temperatures ranging from 50°C to 82°C and surviving a wide range of salt concentrations. Transition metal ions are essential for all living organisms but are very toxic in excess concentrations. The expression of bacterial transporters is transcriptionally regulated to maintain cellular metal-ion concentrations. The model organism *T. thermophilus* HB8 contains 2,245 genes, with over 70 having recognized homology to known bacteria transcriptional regulators. Gene TTHA1719 from *T. thermophilus* HB8 is identified as an ortholog of the copper sensing transcriptional repressor (CsoR), a transcriptional regulator which regulates the expression of the copper-ion transporter gene. To better understand the biological roles of TTHA1719, we determined the binding specificity of this putative transcription factor, mapped its consensus sequence to the *T. thermophilus* HB8 genome, and identified those genes/operons potentially regulated by it. For this purpose, we devised a combinatorial method, Restriction Endonuclease Protection Selection and Amplification (REPSA), to identify consensus ligand binding sequences in DNA libraries. Our study provides a proof-of-concept for the application of REPSA for the identification of preferred DNA-binding sites for orphan transcriptional regulators and first step towards their full characterization.

58 Use of Zinc-Specific DNAzymes on Nucleic Acid Functionalized Nanocapsules for Sensing Applications

Brooke Tate and Shraddha Sawant
University of Connecticut, betate8361@ung.edu

Nucleic acid functionalized nanocapsules (NANs) are self-assembled micelles fortified with various crosslinkers and have been observed to be endocytosed. The NANs are crosslinked with either an ester crosslinker or a peptide crosslinker to be broken down by enzymes only within the cell, allowing the particles to be used for targeting intracellular functions. The design of the particle allows it to carry a hydrophobic load in its core, which would be released upon enzymatic cleavage of the crosslinker. The NANs can be functionalized with thiolated DNA by UV-assisted thiolyne chemistry. These strands can be functionalized with zinc specific DNAzymes, which in turn can be hybridized with a substrate strand containing a fluorophore and quencher for sensing applications. Fluorescent kinetics studies upon the particle show functioning of the attached DNAzyme strands, the functioning of particle degradation in the presence of enzymes and its stability on the particle surface. Polymerase chain reaction studies confirm attachment of the DNAzyme to the particle surface and help eliminate suspicions of the fluorescence of the kinetics studies being from free DNAzyme in solution.

59 Use of Ultrasmall Superparamagnetic Iron Oxide Nanoparticles (USPIO) to deliver Naringenin onto adipocytes

Nithin Naren, Mariam Drammeh and Ajay Singh
Department of Pharmaceutical Sciences - PCOM, nithin.naren1950d@gmail.com

According to the CDC, obesity is one of the main risk factor for cardiovascular disease and type-2-diabetes. Biologically active phytochemicals such as Naringenin (NG) have shown potential for promoting benefits again type-2-diabetes and obesity. Infact, NG has already showed to decrease adipose tissue mass, however, their bioavailability has remained controversial. Hence there is a need to develop targeted therapy, which will increase the concentration of NG in the adipose tissue. Currently, nanoparticles are used for drug delivery where conventional therapies have proven to be less effective. Among various types of nanoparticles, USPIO have found considerable attention in drug delivery as they are easy to synthesize, inert, and are biocompatible. However, to use them for drug delivery system, the USPIO need to be surface functionalized by ligands such as 3-aminotripropyl ethoxysilane (3-APTES-NH2). The use of 3-APTES provides an amine ($–NH_2$) functional group on the surface of USPIO. Once amine functionalized, the USPIO-NH2 will be conjugated to a NG via dicarboxylic tetraethylene glycol (TEG) linker (HOOC-TEG-COOH) to yield USPIO-TEG-NG. However, to increase the specificity of the nanoparticles to the white adipose tissue (WAT), a WAT specific peptide, P3 (CKGGRAKDC) will be conjugated onto USPIO-TEG-NG to yield a final product USPIO-TEG-NG-P3. The P3 peptide has been reported to bind specifically to WAT vasculature through the membrane protein prohibitin, hence the presence of P3 onto the nanoparticle will increase the specificity and selectivity of the nanoparticle to the adipose tissue. USPIO was synthesized using Fe(II) and Fe(III) chloride in presence of NaOH. USPIO obtained was later aminated in the presence of 3-aminotripropyl ethoxysilane (3-APTES-NH2). The presence of amine functional groups on the surface of nanoparticles was confirmed via FTIR and quantified using ninhydrin Assay. The ninhydrin assay revealed the presence of 4.5μM of amine groups per mg of the USPIO. TEM analysis showed that the USPIO and USPIO-NH2, particles were all spherical in shape with the average particle size of 20 and 25, respectively. Once developed, the bioavailability of USPIO-PEG-NG-P3 will be evaluated both *in vitro* and *in vivo*.

60 Synthesis of glycosyl triazole sulfonamides as potential inhibitor for CA-IX and CA-XII

Tuyen Tran and Emmanuel Buabeng
Georgia State University, tran2579@gmail.com

Carbonic anhydrases (CA) are a group of enzymes that are responsible for acid-base balance and homeostasis by converting carbon dioxide (CO_2) and water (H_2O) into bicarbonate anions (HCO_3^-) and proton (H^+). However, carbonic anhydrase IX and XII are found to be cancer-associated enzyme due to their overexpression in cancer tumor. Both carbonic anhydrase IX and XII induced hypoxia and acidosis which are critical conditions for survival, metabolic performance, and proliferation of cancer cells. In this piece of work, sugar based sulfonamide derivatives have been synthesized via click chemistry to serve as competitive inhibitor for carbon dioxide and also to determine the rotatable effect on the activity of these inhibitors. Elucidations of the structures were confirmed by Nuclear Magnetic Resonance spectroscopy (NMR). Further analysis on the properties and affinity of the compounds when interacting with CA-IX and CA-XII is needed to study the function of these compounds and provide future guidance for the development of antitumor agents.

61 Innovative Gadolinium-Based MRI Contrast Agent with Chemokine Receptor 4 Binding Affinity, hProCA32.CXCR4, for Early Detection of Liver Metastasis

Jen Kong
Georgia State University, dkong2@student.gsu.edu

Magnetic resonance imaging (MRI) is widely used in clinical practice for the non-radiation, high resolution and no depth limitation properties. Contrast agents are utilized by MRI to improve the sensitivity; however, the current contrast agents for clinical usage are not capable of detecting early stages of cancer and liver metastasis due to the low relaxivity, high toxicity, and lack of targeting capability. Liver metastases are observed in variety of cancers including uveal melanoma, breast, and colon cancer. Early detection and staging of liver metastases can be extremely beneficial for diagnosis and treatment stratification. CXCR4-CXCL12 axis is playing an important role in the organ-specific cancer metastases and CXCR4 is a potential biomarker for imaging liver metastases of cancers. We report the development of several CXCR4 contrast agent variants with the goal to optimize their biomarker targeting capabilities. Their expression and purification have been achieved through bacterial expression and chromatographic techniques. The modification of targeting does not reduce its metal binding property while maintaining high relaxivity. They exhibit high r1 and r2 values, which are 8-10 folds higher than current clinical contrast agents. Further development of hProCA32.CXCR4 is expected to have translational potential and beneficial for cancer diagnosis.

62 Modulation of Phagocytic Activity of Alpha-Synuclein Stimulated Microglial cells by Anti-inflammatory agents

Kyra Brewer and Robert Haining
Georgia Gwinnett College, kbrewer1@ggc.edu

Nicotine has long been thought to be a carcinogen found in tobacco cigarettes and more recently E-cigarettes. Although public consensus shows a negative reception, recent *in vivo* and *in vitro* studies have supported the use of nicotine as an anti-inflammatory compound. In particular, its role in Parkinson's disease (PD) patients has been purported to be neuroprotective against PD. This is evidenced by epidemiological studies showing that smokers tend to have a lower incidence of PD. The degeneration of dopamine neurons during PD is concurrent with the release of pro-inflammatory cytokines that cause inflammation in the brain. This can reduce the neuroprotective effects of the microglia, by inhibiting their phagocytic response. With this in mind, we investigated the ability of nicotine and ibuprofen (a non-steroidal anti-inflammatory drug) to stimulate the release of anti-inflammatory cytokines and stabilize the phagocytic activity of microglia in an inflamed environment. We designed our experiment to model a typical PD patient. The BV-2 microglial cell line were first exposed to lipopolysaccharide (LPS; 1 μg/ml), then treated with varying doses and combinations of nicotine, ibuprofen or alpha-synuclein (α-synuclein). Phagocytic activity was measured using fluorescently-tagged *E. coli* particles and quantified using Image-J. Our experiments found that nicotine stabilized phagocytic activity in microglia incubated in neurotoxic environments induced by LPS and stimulated by α-synuclein. This supports the utility of anti-inflammatory compounds in the regulation of phagocytosis in microglia and their potential as a mechanism for therapeutic treatments of PD.

63 A Multi-approach Investigation to Evaluate Compounds that Mitigate Neuroinflammation

Gabriella Tyler, Viktor Cheban, Dr. Rashad Simmons, Dr. Pat Uelmen and Dr. Robert Haining
Georgia Gwinnett College, gtyler1@ggc.edu

Parkinson's disease is a progressive neurodegenerative disorder, which affects the basal ganglia and the activity of dopamine, a neurotransmitter in the brain. This interruption of dopamine appears to provide an explanation as to the loss of motor function by those who have Parkinson's disease (PD). 1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) is a prodrug to MPP+, a known neurotoxin which induces Parkinsonian symptoms to those exposed to it. The goal of this study was to: 1) to investigate the potential for nicotine and velvet bean extract to protect against MPTP-induced neurotoxicity and 2) to establish a zebrafish (*Danio rerio*) model to study these effects of nicotine and L-DOPA from velvet beans. Using high performance liquid chromatography, the concentration of velvet bean L-DOPA, a precursor to dopamine, was determined. In cell culture studies, the effects of nicotine or velvet bean extract on reducing neuroinflammation was then investigated. In behavioral experiments, the effects of nicotine and MPTP are being investigated. Reports from the American Academy of Neurology suggest that people who smoke cigarettes are ~44% less likely to develop Parkinson's disease, compared to those who have never smoked this research can help elucidate nicotine's putative role in mitigating inflammation associated with PD.

64 Optimization of the expression and purification for protein-based MRI contrast agent

Ballanah Torbett and Oluwatosin Ibhagui
Georgia State University - Center for Diagnostics and Therapeutics, ntorbett1@student.gsu.edu

Magnetic Resonance Imaging (MRI) is a non-invasive imaging technique with no ionizing radiation. This enables high resolution, and comprehensive images of biological treatment processes in pathological conditions, with detailed anatomic and dynamic 3D information of organs and soft tissues. It is, however, less quantitative and lacks required sensitivity. The availability of contrast agents with high relaxivity, sensitivity, and stability is important to improve the sensitivity of detection with MRI, extending its application to brains, behavior, and disease progression monitoring. ProCA32.collagen, a collagen-targeted protein-based MRI contrast agent developed for molecular MRI, meets the aforementioned need and has been found to possess 10-fold higher relaxivity, stability, and low injection dosage compared to contrast agents such as Magnevist. Addressing the clinical relevance of our contrast agent, this study reports our purification effort of ProCA32.collagen through optimized clone selection, glycerol stock generation, transformation, expression, and purification. We hypothesized that the selection and amplification of the best clone capable of expressing our target protein at the exact molecular weight, with the ability to produce a higher soluble/insoluble ratio of cell lysate, and with optimal yield, is critical to reproducibility and safety for our contrast agent. It is also essential to provide enough material for biophysical studies, like metal binding. Likewise, large protein quantities are important for animal studies, and preclinical and future clinical applications. By selective antibiotic resistance, we generated a fourteen-colony agar plate, expressing and purifying each colony. Of these fourteen, nine were selected by SDS-PAGE for significant protein expression. Furthermore, of the nine clones selected, SDS-PAGE showed that only seven had a significant protein amount, and clone nine had the best soluble:insoluble ratio of 85:15 percent. It is currently being used for development of optimized purification conditions for ProCA32.collagen, with two random clones as the control.

65 Expression and Purification of ProCA32collagen1 for Molecular Magnetic Resonance Imaging

Carlos Ramirez-Morales and Olawutosin, Ibhagui
Georgia State University - Center for Diagnostics and Therapeutics , cramirezmorales1@student.gsu.edu

Magnetic Resonance Imaging (MRI) has been widely applied for both brain disease and organ behavior studies. It has advantages for monitoring slow progression and detection of fibrosis and metastasis, with 3D high resolution deep tissue imaging without using ionizing radiation. MRI, however, requires contrast agents for contrast between normal and pathological tissues. Collagen is a great disease biomarker that is over-expressed in various diseases including liver fibrosis, and tumors, which can also be tied to brain diseases relating to collagen 4. Early diagnosis of organ fibrosis can prevent major clinical consequences, like cirrhosis, organ transplant, and hepatocellular carcinoma (HCC). Therefore, there is an unmet medical need to develop MRI contrast agents with desired sensitivity and collagen specificity to achieve high contrast to noise ratio, high relaxivity, high gadolinium metal binding affinity, and proper in-vivo properties with reduced toxicity. The development of collagen targeted protein-based MRI contrast agent ProCA32.collagen, achieved previously by our lab, is expected to meet these needs. In this study, we report the expression, purification and characterization of ProCA32.collagen for MRI. A yield of 50 mg/L was reported for the expression and purification. Some conditions for the bacterial expression of the protein include overnight growth, addition of 250 µl of IPTG per liter, and induction from an OD of 0.6 to 0.8. Conditions for purification include using a buffer of pH 8, anion exchange chromatography with a positively charged column, and use of the chelating agent EGTA. The purified protein will be used to perform relaxivity, metal-binding studies, and diagnostics for different types of diseases including brain tumor and liver cancer. This contrast agent will provide a powerful tool for quantitative assessment of fibrosis in several organs by monitoring and quantifying collagen expression in the organ of interest.

66 Action of nitrite on chlorite dismutase

Lauren Ekeleme and Dabney Dixon
Georgia State University, aekeleme1@student.gsu.edu

Chlorite dismutases are heme proteins that efficiently decompose chlorite (ClO^-) into chloride (Cl^-) and oxygen (O_2). Chlorite dismutases are under consideration as enzymes to treat chlorite in the environment. As nitrates can also be present, it is important to understand the products from the reaction of chlorite dismutase with nitrite. Several important heme proteins undergo covalent modification at the heme with nitrite. For example, myoglobin reacts to give a nitrite group at the 2-vinyl position, while horse radish peroxidase forms the 4-vinyl derivative. Because these derivatized hemes are very difficult to isolate and characterize, we have used horse heart myoglobin to conduct preliminary studies. The reaction between 0.078 M nitrite and myoglobin at pH 5.7 gave a new colored species; the spectral changes were fit to a first-order reaction with a half-life of 7.3 h; these data matched those in the literature. To extract the hemin, we compared the acid acetone and 2-butanone methods. The former was more successful, with as much as 77% of the heme recovered from the myoglobin extraction. Evaporation of the acetone (bp 56 °C) can lead to polymerization of the solid heme. To circumvent this, we added an equivalent amount of DMSO (bp 189 °C) before removing the acetone by evaporation or under vacuum. With this technique, the heme is always in solution; a 97% recovery has been achieved. pH titrations of the Fe(III) heme show different spectral species under acidic and basic conditions, as expected from the literature. The nitrohemins are less stable than hemin itself. Once the extraction techniques have been refined, we will move on to recovery of the nitrohemin from myoglobin and then to the determination of the product from chlorite dismutase.

67 The Anti-Inflammatory Properties of Nicotine on Dopaminergic Neurons via Microglial Mediation

Hannah Staley and Robert Haining
Georgia Gwinnett College, hstaley@ggc.edu

Microglia are the primary immune cells in the brain which function like macrophages and can undergo phagocytosis. In diseases such as Alzheimer's and Parkinson's, inflammation in the brain can sometimes cause microglial cells to function improperly, resulting in failure to remove plaque-causing agents from neurons, or excessive removal of neuronal cells and debris. As nicotine has shown certain neuroprotective effects, it is in question as to whether it could have a positive effect in preserving the integrity of microglial activity, and subsequently on neurons under inflammatory conditions. To better understand the effects of nicotine and other potentially neuroprotective compounds on microglial and neuronal cell health, BV2 microglial and MN9D dopaminergic cell lines were studied. In a target-transfer assay, BV2 cells were pretreated with nicotine and/or LPS, a known pro-inflammatory agent. Conditioned media from BV2 cells was transferred to MN9D cells, which were then studied via cell viability assays. In addition, ELISA assays detecting the presence and concentration of IL-6, a pro-inflammatory cytokine, emitted by microglia were performed. Preliminary results revealed that BV2 microglia may be playing a role in mediating nicotine's anti-inflammatory effects by exhibiting a reduction in release of IL-6 after treatment with nicotine. These findings highlight the importance of microglia in maintaining healthy conditions for neuronal cell function and postulate that nicotine may be a novel agent in the management of Parkinson's disease.

68 Can Physiological Concentrations of NaCl and KCl Increase Oxidative DNA Damage that is caused by Photoactive Polycyclic Aromatic Hydrocarbons?

Victoria Michel-Milian and Mohammad S. Safiarian
Georgia State University, vmichelmilian1@student.gsu.edu

Many over-the-counter dietary supplements and environmental pollutants contain anthracenes and other polycyclic aromatic hydrocarbons (PAHs) that are phototoxic to living organisms. When these compounds bind to DNA, photo-oxidative DNA damage is often generated. Our past research has shown that DNA damage of this type can be dramatically enhanced by concentrations of NaCl and KCl that exist in the cell nucleus. This presentation focuses on a previously studied 9-aminomethyl anthracene and three new polycyclic aromatic hydrocarbons that damage DNA when irradiated with ultra-violet light (350 nm, pH 7.0, 22 °C). It is possible that the phototoxicity of these compounds involves photo-damage to DNA that is made worse by physiologically relevant conditions of salt. We hope to identify the minimal structural features that a PAH must possess to exhibit such a salt-induced effect. It is possible that NaCl and KCl play a role in the occurrence of skin burns or cancer caused by the exposure of certain PAHs to ultraviolet light from the sun.

69 Arterial Contractility Regulation by Simvastatin

Farzana Zerin
Mercer Univeristy, farzana.zerin@live.mercer.edu

Statins belong to HMG-CoA reductase inhibitor class of lipid-lowering drugs with a range of lipid-independent pleiotropic effects. Long-term use of statin has been reported to influence vascular function and organ perfusion. However, no studies have investigated direct effects of acute statin application on fresh isolated arteries and its relevance for arterial contractility regulation. This application arises from our novel preliminary finding that simvastatin has a biphasic effect on aorta – causing vasoconstriction at therapeutic concentrations (0.001 – 0.1 μM) and vasodilation at supratherapeutic concentrations (> 1 μM), respectively. The hypothesis of this proposal is that simvastatin directly controls myocyte [Ca2+]i and arterial contractility by influencing both Ca^{2+} entry and Ca^{2+} release pathways in arterial myocytes, independently of HMG-CoA reductase. Wire myography was used to conduct this research. The overall goal of this research is to investigate underlying mechanisms of simvastatin-mediated arterial contractility regulation, which may have great value in statin pharmacotherapy.

70 Carolacton Analogs for CH Functionalization and Biological Testing

Elana Shaw, Wenbin Liu, Taylor Hari and Ashley Diaz
Emory University, elana.shaw@emory.edu

Carolacton is a natural product that has been found to selectively perturb pathogenic *S. Mutans* biofilm. A simplified carolacton analog with an aryl sidechain was synthesized to probe the natural products ability to serve as a substrate for C-H functionalization. Preliminary assays show regiospecific and enantioselective functionalization at the most accessible secondary C-H bond. These simplified and functionalized analogs will also be tested for biological activity.

71 Characterization of Immune Checkpoint Inhibitor Associated Myocarditis in Mouse Models and Possible Abatacept Therapy

Emmanuel Eziakor and Wouter Meijers
Vanderbilt University, eeziakor41@gmail.com

Immune checkpoint inhibitors (ICIs), a class of immunotherapy drugs that upregulate T-cell immune responses, have revolutionized oncology therapy. ICIs primarily target the immune checkpoint proteins, cytotoxic T-lymphocyte antigen-4 (CTLA-4) and programmed cell death protein 1 (PD-1), two mediators of T-cell inhibition. Despite the success of ICIs, studies have demonstrated their association with myocarditis (inflammation of the heart). We recently utilized Pdcd1-/-Ctla4+/- and Pdcd1-/-Ctla4+/+ mice models that mirror ICI associated myocarditis and discovered an association between ICIs and increased heart weight, which we attribute to cardiac hypertrophy (enlarged cells). The purpose of this experimental study is to further characterize ICI associated myocarditis and to determine if hypertrophy is evident. We hypothesize that the mice models will have elevated systolic blood pressure (SBP) and heart rate (HR). We also hypothesize that arrhythmia and hypertrophy will be evident in the mice models and that abatacept, an autoimmune disorder drug, will normalize the HR and SBP of our Pdcd1-/-Ctla4+/- mice. In this study, we examined the HR and SBP of the mice models and a group of Pdcd1-/-Ctla4+/-mice treated with 200 µg of abatacept for four weeks. An electrocardiogram (ECG) of a Pdcd1-/-Ctla4+/-mice was taken. Additionally, we extracted cardiac tissue samples from the mice models, performed immunofluorescence, and assessed cardiomyocyte size using ImageJ. Data analyzed using a Two-Sample T-Test Assuming Unequal Variances revealed significantly lower SBP ($P< 0.05$) and significantly higher HR ($P< 0.05$) in our mice models when compared to the control mice. Abatacept increased the SBP ($P< 0.05$) and decreased the HR of our Pdcd1-/-Ctla4+/+ mice, essentially normalizing the SBP and the HR. There were no significant differences in the average heart cell area for each group, ruling out hypertrophy's role in our mice models increased heart rate. Additionally, ECG data revealed arrhythmia. Overall, these results provide a platform for characterization and diagnostic tool development for immune checkpoint inhibitor associated myocarditis and reveal abatacept's therapeutic potential.

72 SDG Effects on Oxidative Stress and Inflammation in LPS-Treated Human Macrophages

Asha Murrell, Ayanna Fourte, Bakare Awakoaiye and Kelly Jordan-Sciutto
Spelman College, amurrel1@scmail.spelman.edu

Human Immunodeficiency Virus, commonly known as HIV can enter the brain via cells of the monocytic lineage. Infection and activation of macrophages/microglia cells leads to activation of inflammatory and oxidative stress pathways and subsequent neuronal damage in the central nervous system (CNS). This damage can cause a spectrum of cognitive impairments known as HIV-Associated Neurocognitive Disorders (HAND). Macrophage activation is also seen in many other neuroinflammatory disorders. Many studies have unsuccessfully targeted broad anti-inflammatory and antioxidant therapies to alter the deleterious effects of macrophages during disease state. Secoisolariciresinol Diglucoside (SDG), a flaxseed ligand, has been shown, through previous studies, to possess anti-inflammatory/antioxidant properties and activate the endogenous antioxidant pathways. We hypothesize that SDG has the ability to change the harmful phenotype of human macrophages during disease states through the use of the endogenous antioxidant response pathway thus preventing neuronal damage. In order to prove this hypothesis, human macrophages were treated with Lipopolysaccharide (LPS) or HIV in the presence of SDG for various time points. Whole cell lysates were collected, and Western Blotting was performed to assess changes in downstream proteins of the endogenous antioxidant response pathway. Based on preliminary data, proteins downstream of the endogenous antioxidant pathway are increased in the presence of SDG compared to LPS treated or HIV infected macrophages. With the success of this project, we believe that SDG may be a new therapeutic agent for neuroinflammatory disorders such as HIV-Associated Neurocognitive Disorders.

73 Glycine Betaine Exclusion from Carboxylate Surface

Sarah Choi and Amy Yoone
Middle Georgia State University, jonathan.cannon@mga.edu

In order to keep enough water in their cells when experiencing stress, many organisms build up osmolytes. Osmolytes not only help to retain water, but maintain cellular environments through stabilizing macromolecules and counteracting denaturants. Two models have sought to explain and predict the effects of osmolytes based on their interactions with biopolymer surfaces. A significant difference between the models exists because of contradictory data regarding the interactions of osmolytes with negatively charged biopolymer surface. We are examining discrepancies in measurements of the interactions of the glycine betaine with carboxylate groups. We have repeated published measurements of glutamate solubility in the presence and absence of glycine betaine using inexpensive equipment and data from over a dozen different undergraduate researchers. The discrepancy between the glycine betaine-carboxylate interaction data appears to be anomalous measurements of the solubility of glutamate in the presence of glycine betaine. We have extended previous studies by measuring the effects of pH on glycine betaine-glutamate interactions.