UNDERGRADUATE RESEARCH SYMPOSIUM SUMMER 2019

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ARTS & HUMANITIES

BIOLOGICAL SCIENCES & ENGINEERING

PHYSICAL SCIENCES & ENGINEERING

SOCIAL SCIENCES



JUDY AND BOBBY SHACKOULS HONORS COLLEGE AUGUST 2 , 2019 GRIFFIS HALL



MISSISSIPPI STATE UNIVERSITY JUDY AND BOBBY SHACKOULS HONORS COLLEGE

WELCOME

The Shackouls Honors College is pleased to sponsor the summer 2019 Mississippi State University Undergraduate Research Symposium. Prizes for academic areas are being partially supported by Phi Kappa Phi. The Shackouls Honors College has provided summer research support to some of the students presenting with additional funding from the Mississippi State University Office of Research and the National Strategic Planning & Analysis Research Center (NSPARC). Other students are being supported by the National Science Foundation and the National Institutes of Health.

We view the encouragement and support of undergraduate research for all students to be part of our core mission. Just as a good liberal education broadens the mind, provides students with a common core of knowledge, and familiarizes them with the basic methodologies of the various academic disciplines, undergraduate research allows students to dive deeply into important ideas and topics in a rigorous and creative way, paving the way for future intellectual work and exploration whether in the academy, business, or other life arena. Undergraduate research also allows students to see how disparate areas of their fields fit together to form an intellectual whole.

Enjoy the student posters and presentations and come away knowing more than when you entered our doors.

Sotis Popentin

Dr. Seth F. Oppenheimer Professor of Mathematics Associate Dean for Academic Affairs Shackouls Honors College



MISSISSIPPI STATE

Mississippi State University: Our State's Land-Grant Research Flagship

We are honored to welcome you to Mississippi State University's Summer, 2019 Undergraduate Research Symposium. Undergraduate students are an integral part of the multifaceted research underway at Mississippi State.

Every day, our faculty, staff, and students are conducting fundamental to applied research that provide innovative solutions, creative works, and new scholarship that address pressing local, state, regional, national, and global needs.

As a result of this work, MSU is the leading institution in our state for research that falls within its land-grant mission. Strengths across all colleges and research centers have led to our institution being categorized by the Carnegie Foundation as a "very high research activity" institution. The Carnegie Foundation has also recognized Mississippi State with its Community Engagement Classification.

Pursuing research opportunities is a critical part of academic life on our campus, and our students are recognized for their commitment to discovery, creation, and exploration in our labs, studios, library, research farms, and beyond. We are pleased that members of our faculty are committed to providing undergraduates with meaningful roles in the overall research enterprise, and promoting interdisciplinary research as an important component of scholarly activity.

Undergraduate research gives our students opportunities to apply classroom knowledge to new areas of interest, and helps them develop skills, collaborate with faculty and peers, and gain confidence. It is exciting to see the results of their efforts on display at today's symposium.

Again, welcome to the symposium, and thank you for your contributions to and interest in research at Mississippi State University.

Julie Jordan, Ph.D. Interim Vice President for Research and Economic Development



The Honor Society of Phi Kappa Phi (PKP) has a long and distinguished history. Currently, there are over 300 chapters of PKP scattered all across the world, from Maine to Hawaii and the Philippines, and from Alaska to Puerto Rico and beyond. During the 1996-97 academic year, PKP celebrated the 100th anniversary of the founding of The Honor Society of Phi Kappa Phi, and we are now in the second century of its recognition of - and service to - learning. The MSU chapter is in its 70th year of membership next year. Due to PKP's prestigious recognition and support of learning, the MSU Chapter is proud to also financially support the Summer 2019 Undergraduate Research Symposium in Griffis Hall at Mississippi State University. The symposium displays the importance of research for success as a student and beyond!

Summer 2019 Undergraduate Research Symposium Schedule

Poster Session: Griffis Hall (First, Second, and Third Floors)

1:00 pm - 3:30 pm

Project #:	Category:	Poster Location:
01	Arts and Humanities	First Floor
02 - 49	Biological Sciences and Engineering	First, Second, and Third Floors
50 - 90	Physical Sciences and Engineering	Third Floor
91 - 97	Social Sciences	Third Floor

<u>Award Ceremony - Griffis Hall, Forum Room - 401 (Fourth Floor)</u> 4:00 pm

Moderator:

Dr. Seth F. Oppenheimer, Professor of Mathematics, Associate Dean for Academic Affairs, Shackouls Honors College, Mississippi State University

Symposium Subject Area Awards:

Representative of The Honor Society of Phi Kappa Phi, Mississippi State University

This symposium would not be possible without the hard work of the judges who work under time pressure to try to determine which excellent project is just a bit more excellent than the others. If you see a judge, thank him or her.

Student Presenters

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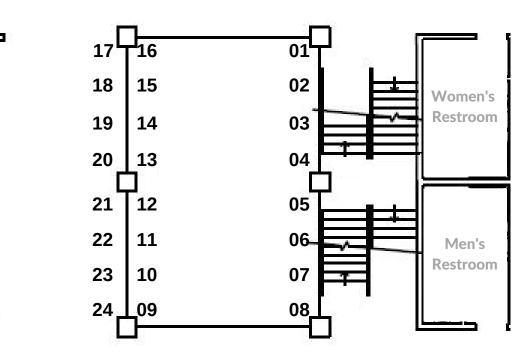
Map of Griffis Hall

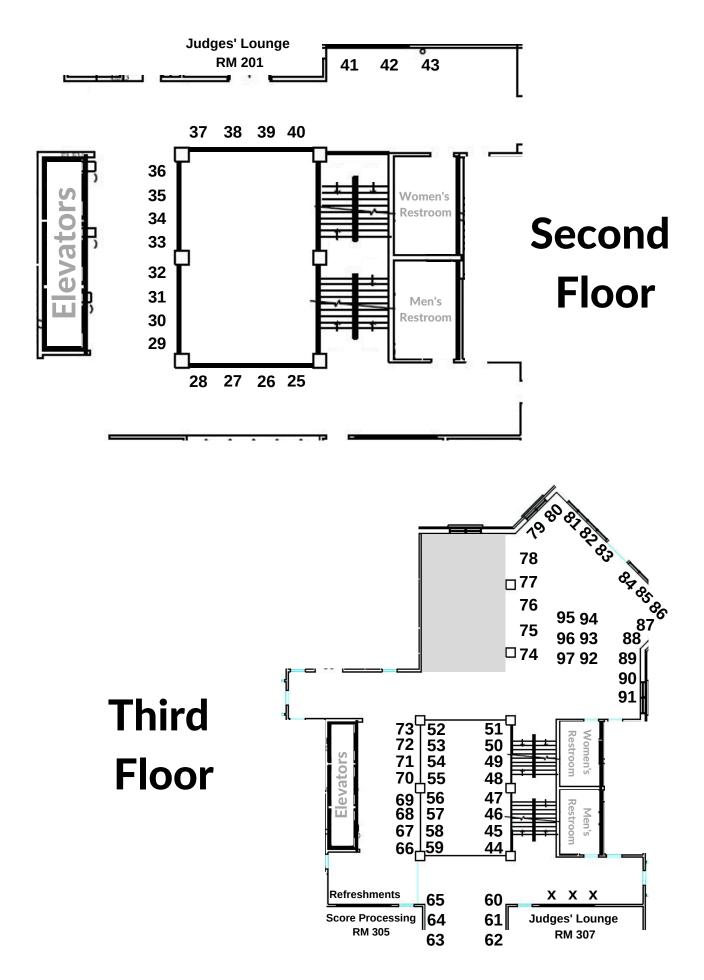
Poster Category Key:

01	Arts and Humanities
02 - 49	Biological Sciences and Engineering
50 - 90	Physical Sciences and Engineering
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First Floor

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Abstracts

02

Name: Javad A'arabi Major: Microbiology Faculty Advisor, Affiliation: Chinling Wang, Department of Basic Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Wenyuan Yang, Yue-Jia Lee, Hsin-Yi Lu

Adopting Lactobacillus Species and Organic Acids as Alternative Treatments to Necrotic Enteritis

Necrotic enteritis (NE), caused by *Clostridium perfringens* (CP), is a re-emerging disease that costs a six-billion-dollar deficit to the global poultry industry. Low level usage of antibiotics added to animal feed (as a growth promoter) has been shown to be an effective measure to control disease. Due to the extensive belief of antibiotic-resistant bacteria transferring to humans, many poultry companies have removed growth promoters from poultry feed, resulting in an increased incidence of necrotic enteritis. Therefore, an alternative treatment without using antibiotics to treat this disease is critical for the survival/profitability of the poultry industry. Lactobacillus species have been shown to improve the gut integrity of humans and animals to compete against pathogens. The hypothesis was that the use of beneficial bacteria can inhibit the growth of harmful bacteria in the chicken gut. The objective of this study was to evaluate the effectiveness of probiotics bacteria, Lactobacillus johnsonni and Lactobacillus salivarius, to protect chickens against CP. In the experimental design, broiler chicks were divided into four groups: A) positive control, B) L. Johnsonni treatment, C) L. salivarius and D) negative control. Groups A to C were challenged with CP. The results showcased that the L. johnsonni or L. salivarius supplement did not protect birds against the CP challenge. Orally giving probiotics daily seems to introduce stress to the birds and increase the susceptibility of CP, resulting in higher mortality and intestinal lesions than the positive control group (challenged but no probiotics). The conclusion is that neither L. johnsonii nor L. salivarius protects chickens against the CP challenge. A different methodology of administering the probiotics to avoid stress to chickens, such as mixing in feed, water, or a mixture of beneficial bacteria and organic acids, should be considered for future studies.

03

Name: William Acuff Major: Biological Engineering Faculty Advisor, Affiliation: Janice Chambers, Department of Basic Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Dr. Steven Gwaltney

Reactivation Effects of Novel Oximes on Rat Brain Acetylcholinesterase Inhibited by Metabolites of Phorate

Organophosphates (OPs), used as certain insecticides and nerve agents, pose a grave threat to military personnel and civilians alike due to their ability to inhibit acetylcholinesterase (AChE). The OP insecticide phorate (rat oral LD50 1.4-3.7 mg/kg) is particularly toxic. However, due to its agricultural nature, it is less vigilantly monitored than nerve agents, leading to easier access for nefarious uses. In vitro studies of phorate indicate that its metabolites, namely phorate-oxon (PHO), phorate-oxon sulfoxide (PHOxSx), and phorate-oxon-sulfone (PoSn) are the potent AChE inhibitors that cause toxicity. Additionally, phorate exhibits a lengthy delay of toxic signs in vivo; this property could be used by terrorists to cause panic in an exposed population. Traditionally, oxime drugs such as 2-PAM, in combination with atropine, have been used to treat OP poisoning. However, PHO is hypothesized to potentially inhibit AChE with an unusual ethoxy leaving group, yielding a phosphylated AChE that might not be readily reactivated by 2-PAM. Computational modeling is being used to determine the plausibility of this hypothesis. Additionally, the traditional oxime drug, 2-PAM, cannot penetrate the blood brain barrier. Recently MSU's novel substituted phenoxyalkyl pyridinium oximes (US patent 9,277,937) have been shown to reactivate inhibited AChE in the brain in animal tests. Preliminary in vivo results show an increase in survivability compared to 2-PAM when novel oximes were administered following lethal doses of phorate in rats. Additionally, our in vitro results show varying levels of AChE reactivation in rat brain preparations inhibited by PHO, PHOxSX, or PoSn. These results help broaden understanding of these novel oximes' therapeutic potential in relation to phorate and could lead to more effective antidotes to protect against potential phorate exposure. (Support: NIH U01 NS083430)

Name: Joy Adeyemo Major: Computer Engineering Home Institution: University of Missouri, Columbia Faculty Advisor, Affiliation: Jean-Francois Gout, Biological Sciences Project Category: Biological Sciences and Engineering REU/Research Program: Computational Biology REU

Error Rates in DNA Sequencing

DNA Sequencing is important for several reasons; for example, it provides valuable medical information that can give scientists an insight into mutations that cause diseases like cancer etc. Sequencing machines provide strings of base calls (A, T, C or G). These machines give a quality score which is a probability of erroneous base call for each base call. Sequencing machines make errors such as substitutions, insertions, and deletions. It would be helpful if there were specific numbers on how often these errors occur and if it differs depending on the machine being used. In order to get error rates, sequencing reads are mapped to a reference genome and these reads are found with discordant base calls at certain positions. These discordant base calls are likely to be sequencing errors. Two main programs are used: an in-house script and bwa. Bwa is used for mapping sequences against a reference genome. The in-house script is created to call sequencing errors. Also samtools is used for sorting, indexing, and creating alignments. Data collected so far shows that the error rate is in the range of 1 in 1000. Also, further research will study if these error rates correspond with quality scores.

50

Name: Suman Adhikari Major: Computer Science Faculty Advisor, Affiliation: Dr. Bryan Jones, Department of Electrical and Computer Engineering Project Category: Physical Sciences and Engineering Co-Author(s): Dr. Bryan Jones

A modular plugin-in architecture for CodeChat

The CodeChat plugin transforms source code into a web page, allowing software developers to view their source code as a beautiful and descriptive document by adding headings, formatting, hyperlinks, images, and diagrams. However, this plugin requires the use of a little-known text editor, Enki. To broaden its impact, this project proposes the creation of a modular plug-in architecture for CodeChat, enabling its use with a variety of text editors. A significant challenge to creating a modular plug-in involves bridging the services CodeChat provides, which are defined in the Python programming language, to the variety of programming languages which various text editors require. To accomplish this, this project employs Apache Thrift, which provides scalable cross-language service development. By describing the services CodeChat provides in a language-neutral format (a .thrift file), Apache Thrift can then generate code for a wide variety of different programming languages. Next, this project proposes development of a CodeChat server to provide the needed services and the creation of a JavaScript plugin client for Visual Studio Code (VSCode), a free and popular cross-platform text editor. After creating the plugin for VSCode, our next approach will be to develop plugins for other editors such as Visual Studio, Atom and Sublime. These editors employ different languages, so our work will only consist of providing the necessary interface between the CodeChat server and a supported language plugin client for the editor.

Name: Urita Agana

Major: Biochemistry

Faculty Advisor, Affiliation: Dr. Sorina C. Popescu, Department of Biochemistry, Molecular Biology, Entomology & Plant Pathology

Project Category: Biological Sciences and Engineering

Co-Author(s): Agana Urita, Setareh Nejat-van Warmerdam, Aline Badial, Maria Tomaso-Peterson, Sorina C. Popescu

Evaluation of the biological control activity of a Fusarium strain against the disease caused by the fungal pathogen Xylaria in crop plants

Taproot decline (TRD) caused by *Xylaria* sp. is currently a prominent disease of soybean in Mississippi. Previous research has revealed that the fungus is colonizing the soybean root at the time of germination and may continue throughout taproot development, impeding plant feeding during the vegetative period. Infected plants die in the late vegetative or early reproductive stages of development. Currently, TRD is managed through no-till or conservation tillage practices which are not effective to stop the spread of *Xylaria*. Since the fungus was found to overwinter on root stubble of soybean and other crops used in a rotation program, current management practices may be contributing to the widespread occurrence of TRD in MS.

Biological control of pathogenic microorganisms in crop plants is an environmentally safe and effective way of reducing or mitigating disease and minimizing yield loss through the use of natural enemies. The main goal of this project is to explore the potential of beneficial microorganisms (BMs) isolated from the plant rhizosphere to control TRD. As part of our experimental strategy, we will first test the effect of a non-pathogenic strain of *Fusarium (F #42)* on the growth of *Xylaria* on culture plates. Secondly, we will assess the potential of *F#42* to inhibit or block infection by *Xylaria* of soybean, corn, and cotton seedlings. Several parameters will be tested, including the timing of *Fusarium-Xylaria* co-cultivation in plates or seedlings assays, the size of the fungal inoculum, and the optimal conditions for potential protective activity of *F#42*. The effects of the treatments will be evaluated by measuring the diameter of fungal colonies after co-cultivation, the lengths and dry weights of roots and shoots of seedlings grown under various co-cultivation conditions. The results of three experiments (in vitro and in vivo) will be presented on this poster.

06

Name: Nathalia A. Alicea Maldonado
Major: Computer Science
Home University: University of Puerto Rico – Rio Piedras Campus
Faculty Advisor, Affiliation: Federico G. Hoffmann, Department of Biochemistry, Molecular Biology, Entomology & Plant
Pathology
Project Category: Biological Sciences and Engineering
Co-Author(s): Amanda Black, Brian Counterman
REU/Research Program: REU

Molecular Evolution of genes associated with longevity in Heliconius butterflies

The genus *Heliconius* is a species-rich assemblage of New World butterflies that are models for research in mimicry, speciation and the genetics of wing color patterns. In the current study, we explore their potential as a system to study longevity. Most adult butterflies are short-lived, with some living for just a week, and typical lifespans that are shorter than a month. By contrast, butterflies in the genus *Heliconius* have a lifespan close to 6 months, which is more than 12 times longer than the lifespan of average butterflies. Our main goal is to identify if any known longevity genes help explain this difference in lifespan and whether positive Darwinian selection is related to the observed increase in longevity. To do this, we first identified a list of aging- and longevity-associated genes in fruit fly, *C. elegans* and human available in the GenAge database. We then searched for orthologs of the genes in the list in a representative set of arthropod genes focused on butterflies from the Ensembl Metazoa and Lepbase repositories of genomic data. For each of these genes, we estimated phylogenetic trees to resolve orthology and then test for changes in the rate of molecular evolution in a maximum likelihood framework. We hypothesized that genes associated with longer lifespans in the three model species would be evolving under a different evolutionary regime in long-lived *Heliconius* butterflies relative to short-lived butterflies.

Name: Katelynn Annotti Major: Chemical Engineering Home University: Auburn University Faculty Advisor, Affiliation: Santanu Kundu, Dave C. Swalm School of Chemical Engineering Project Category: Physical Sciences and Engineering Co-Author(s): Madhubhashini Lakdusinghe REU/Research Program: Optoelectronic Materials REU

Color Change due to Self-Assembly of Poly(3-hexylthiophene) in Different Solvents

The curiosity in conductive polymers has grown over the last few years, sparking research into the ways to utilize the characteristics of such polymers, like Poly(3-hexylthiophene). The conductivity of the polymer results from the conjugation of the backbone, with sigma bonds creating the strength of the backbone and the pi bonds allowing for electrons to easily delocalize. Previous results indicate the conductivity of the polymer is linked to the crystallinity and the consequential formation of fibers and that the color change of P3HT polymer from orange to purple is an indication of self-assembly of molecules to form structures in solution. In this research, experiments were conducted with various solvents to determine the extent of color change as a function of time. The solvents in this analysis were benzene, chloroform, dichloromethane, tetrahydrofuran, toluene, styrene, and xylene. Using UV-Vis spectroscopy, each solution (of each solvent with P3HT) and its color was recorded and compared. Based on the results produced by the UV-Vis spectroscopy, over the course of thirty minutes, xylene, dichloromethane, tetrahydrofuran, and toluene revealed signs that structures were forming rapidly, while styrene and benzene, over the course of several hours, displayed a slight change in color indicating the formation of some structures. These self-assembled structures were visualized through transmission electron microscopic images (TEM). The conductivity of each of the solvents with P3HT is currently being measured to confirm that the color changed was indeed linked to the conductivity increase.

07

Name: Kadriana Armstrong Major: Biological Sciences Home Institution: Tougaloo College Faculty Advisor, Affiliation: Brandon Barton, Department of Biological Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Abby Jones, Jonathan Belanich, Heather Jordan REU/Research Program: REU- INFEWS: Food, Energy, and Water Security

Disentangling the Effects of Mass Mortality Events on Soil Food Webs

Death is a ubiquitous, natural life process that affects ecosystems, and has proven to be central to understanding ecological and evolutionary connecting trophic pathways. When a one, or a few individuals die, the remaining population continues to maintain functional roles and ecosystem processes. In contrast to individual deaths, mass mortality events (MMEs) involve the sudden death of many individuals. The increasingly frequent occurrences of MMEs cause a reduction in the afflicted population's ecosystem function causing both bottom-up and top-down effects via carrion-derived nutrients. In this experiment, we evaluated the importance of carcass biomass and functional group on necrophagous insects, carcass decay rate, soil chemistry and physical properties, and soil microbial composition. We have simulated the loss of two functional groups- scavengers and herbivores- to investigate the impacts different functional MMEs, as either 30kg (individual carcass) or 360kg (MME) of feral swine, the standardized carcass for this experiment, was deployed at various 10m² plots. We have collected soil samples from each of the sites in a randomized manner to ensure a wide breath of the microbes and arthropods were collected. The work we are currently undertaking is the creation and optimization of a work-flow process, beginning with the isolation and quantification of DNA from initial samples from prior to the induction of the experiment, as well as PCR amplification in order to ensure efficacy. All current soil samples will undergo processing to be amplified with PCR; first using a qPCR run to maximize DNA yield without overduplication. Prepared DNA will be built into libraries and sent for Illumina 16S Sequencing.

Name: Meghna Bajaj Major: Chemistry Home Institution: Alcorn State University Faculty Advisor, Affiliation: Keith Hollis, Department of Chemistry Project Category: Physical Sciences and Engineering REU/Research Program: REU

N-heterocyclic carbene (CCC-NHC) pincer complexes in OLEDs and as catalysts

Novel CCC-NHC backbones of symmetric ligand precursors have been synthesized and used to make metal pincer complexes. The symmetric ligand precursor was prepared by a copper coupling reaction between 1,3-dibromobenzene and imidazole. That product was alkylated with 1-chlorobutane, forming a dichloride disalt. Moreover, the dichloride salt was used to perform the metalation step using Zr(NMe₂)₄. The final Pt pincer complex was formed by transmetallation of the Zr complex using [PtCl₂(COD)] with CCC- NHC as backbone. This CCC-NHC pincer complex has proven to be photolytically stable, withstands high temperature which makes it a great candidate to qualify in the usage in Organic Light Emitting Diodes (OLEDs). These CCC-NHC ligands when bound to other metals can be used as catalysts in the Haber-Bosch process to reduce energy consumption. Our research is focused on producing several ligands (1,3-bisimdazolyl benzene, 1,3-bistriazolyl benzene, 1,3,5-triimidazolyl benzene, 1,3,5-triis(triazole) benzene) with various alkylation reactions (including alkylation with butyl chloride, neohexyl iodide and decyl chloride) and different metals to see the effects by activating with UV light. Also, the backbone is being altered to extend the light emitting ability of the complexes.

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Name: Kereikhan Bakhytkhanuly Major: Aerospace Engineering Faculty Advisor, Affiliation: Donghoon Kim, Ph.D., Aerospace Engineering Project Category: Physical Sciences and Engineering Co-Author(s): Daegyun Choi

Simulation and Analysis for the Planar Motion of a Spherical Unmanned Aerial Vehicle

As opposed to the majority of unmanned aerial vehicles (UAVs), the proposed spherical UAV possesses a spherical shaped outer body. The purpose of the spherical shell is to protect the inner body from damage and allow the vehicle to operate on the ground. One of the important concerns of the proposed design is the reduction of control surfaces. To achieve this, the concept of changing the center of gravity (CG) has been applied. The rolling motion on the ground as well as maneuvering in the air is performed by internally changing the CG, which produces momentum to drive the vehicle's motion. The total number of motors used in this design includes 3 actuators: a contra-prop to propel the SUAV body as a main actuator and 2 stepper motors to shift the CG. Regarding the motion on the ground, once the CG is moved, the tilted inner body provides force for a rolling motion. However, in flying motion, the vehicle attitude is changed through the variation of CG. In this work, the equations of planar motion for the spherical UAV are derived, and the proposed system is numerically simulated using MATLAB with application of PID control allowing SUAV behavior to be predicted and analyzed.

Name: Jaden Bennett Major: Mechanical Engineering Faculty Advisor, Affiliation: Lauren Priddy, Agriculture and Biological Engineering Project Category: Biological Sciences and Engineering Co-Author(s): Weitong Chen REU/Research Program: NIH R25 Bridges to Baccalaureate

Possibilities of Bone Scaffolding With 3D Printing

The current metal implants for treating large bone defects can cause stress shielding leading to implant failure and revision surgeries. The ideal scaffold would be biocompatible, biodegradable, and have mechanical properties similar to those of the native bone. We used 3D printing for scaffold production to insure repeatable and reliable models. First, biodegradable polylactide (PLA) scaffolds with uniform cubic pores were 3D printed with Makerbot Replicator Z18 (MakerBot Industries, LLC). Second, since the surface of PLA is hydrophobic, the scaffolds were then alkali treated (AT) for 6 hours with ammonia solution to improve the wettability (hydrophilicity) via hydrolysis of ester bonds and the introduction of hydroxyl functional groups. Third, nano-hydroxyapatite (nHA) was coated on AT-scaffolds to further enhance the hydrophilicity and surface roughness by interacting with the hydroxyl functional groups. Finally, to investigate the effects of alkali treatment and nHA coating on mechanical properties, compression testing was performed with Instron 5882 (Illinois Tool Works Inc.) at 1 mm/min and preload of 5N. Four groups of scaffolds (n=8 for each group) were prepared: PLA scaffolds (PLA), PLA scaffolds treated with AT (PLA/AT), PLA scaffolds coated with nHA (PLA/nHA), and PLA scaffolds both treated with AT and coated with nHA (PLA/AT/nHA). The results from compression testing showed that 6-hour AT significantly reduced the compressive stiffness, while nHA coating alone did not alter the stiffness. This mechanical data will help determine more optimal materials and suitable methods for using bone scaffolding in large bone defect surgeries

09

Name: Ellianna Blair

Major: Biochemistry (Pre-Vet)

Faculty Advisor, Affiliation: Dr. Carrie Vance, Department of Biochemistry, Molecular Biology, Entomology & Plant Pathology

Project Category: Biological Sciences and Engineering

Co-Author(s): Ellianna Blair, Carrie Vance, Mariana Santos-Rivera, Amanda Free, Victoria Jefferson, Florencia Meyer

Hematological and clinical evaluation of dairy cows with Bovine Respiratory Disease (BRD) caused by Mannheimia haemolytica

Bovine respiratory disease (BRD) associated with Mannheimia haemolytica is the principal cause of pneumonia in cattle. The first sign of this disease is the lack of appetite, followed by depression, increase in ocular and nasal discharge, fever (up to 107F) and coughing. Here we evaluated the course of infection overtime by challenging 5 six-month old Holstein calves with M. haemolytica aspirated directly to the lungs. Clinical assessments including temperature, heart rate (HR) and respiratory rate (RR) were measured during 4 baseline days, 11 days immediately after challenge, and then every other day until Day 21 post infection. In addition, Complete Blood Count (CBC) analysis was applied to blood samples collected on the same days as clinical assessments. Antibiotics were administered when the characteristic clinical signs of BRD appeared. Overall, there was an increase in HR, RR, White Blood Cells count (WBC), Red Blood Cell count (RBC), hemoglobin (HGB), and Hematocrit (HCT) immediately following the initial challenge day, then a decrease as the calves naturally recovered from the infection. Principal Component Analysis (PCA) was used to determine correlations between clinical signs and CBC results. None of the variables evaluated influenced the analysis during the baseline (non-infected) period. However, PCA indicated that temperature, HR, RR, HCT, RBC, and HGB were positively correlated in the animals during the infection with *M. haemolytica*. Further multivariate analysis will examine the relationship of these parameters with changes in haptoglobin and serum metabolites in blood plasma during infection. We were able to detect and evaluate clinical and hematological signs of BRD caused by *M. haemolytica*, contributing relevant information for future diagnosis strategies, therapeutic interventions and management practices during BRD infections.

Name: Raisa Bonner Major: Biological Sciences Home Institution: Skidmore College Faculty Advisor, Affiliation: Dr.Heather Jordan, Department of Biological Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Laxmi Dhungel REU/Research program: Computational Biology REU

Environmental Modulation of *Mycobacterium ulcerans* gene expression: Implications for Transmission, Virulence, and Pathogenesis

Buruli ulcer (BU) is a neglected tropical disease caused by Mycobacterium ulcerans, an environmental pathogen known to cause necrotic skin lesions that can lead to permanent consequences such as loss of limb and scarring, if left untreated. The disease has been reported in 33 countries with higher endemicity in West Africa and increasing incidences in Australia. The disease has been associated with wetlands and slow-flowing rivers with limited oxygen supply. Furthermore, there has been speculation that the increase in BU is caused by human activity such as deforestation, agricultural operations, and damming. The major virulence factor of M. ulcerans is mycolactone, a lipid exotoxin with immunosuppressive and cytotoxic properties. An exact mode of transmission of M. ulcerans is not well understood, however, various studies have suggested possible modes of transmission such as by cuts or abrasion, or biological or mechanical transmission through insect or mosquito vectors. In a study by Williamson et al. it was shown that BU is not established when introduced superficially through abrasion, however the disease becomes established when injected intradermally. This result suggests that sudden change in temperature and oxygen inside the body could lead to higher production of mycolatone contributing to disease. Based on this background information, we hypothesize that mycolactone expression is increased at microaerophilic conditions and at 370C. Further, there is limited information in the literature regarding global M. ulcerans gene expressions exposed to these conditions. Hence, in order to understand the effect of temperature and oxygen on mycolactone and global gene expression, we exposed M. ulcerans to aerobic, microaerophilc and anaerobic conditions at 30 and 37 degrees. Growth, mycolactone gene expression by qPCR and global gene expression by RNASeq was measured at 0, 24 and 48 hrs. Results showed mycolactone gene expression was increased under microaerophilic conditions. RNASeq analysis also showed global gene regulation upon exposure to 370C and microaerophilic conditions. The study provides data of the potential significance of mycolactone yielding a fitness advantage to M. ulcerans in the host or natural environment. Results will also lead to further elucidation of the source and reservoir of M. ulcerans in the environment, and of parameters leading to transmission, increased virulence and pathogenesis.

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Name: Avery Bouchillon Major: Biological Sciences Faculty Advisor, Affiliation: Michael S. Pratte, Psychology Project Category: Social Sciences Co-Author(s): Marshall Green REU/Research Program: NIH R25 Bridges to Baccalaureate

Mapping the Human Visual Cortex with functional Magnetic Resonance Imaging (fMRI)

Functional magnetic resonance imaging (fMRI) is used by cognitive neuroscientists to investigate the structure and function of the human brain. FMRI measures local changes in cerebral blood flow while an individual views a stimulus or performs some type of task. For example, the first cortical area of the brain that responds to visual information is known as the primary visual cortex (V1). V1 is located within the occipital cortex at the back of the brain, even though the exact location is different for every person. An important goal for learning how vision works is identifying where V1 and other visual areas are located within an individual person's brain. Neurons in V1 are sensitive to patterns of light and are highly organized such that each neuron responds only to a particular part of space, a property known as retinotopic mapping. These properties of V1 make it possible to map visual space by presenting a visual stimulus to individuals while measuring their brain activity with fMRI. Other parts of the brain are very sensitive to more complex stimuli, such as motion (i.e., medial temporal region) or shapes (i.e., lateral occipital complex). In addition to the early visual areas, other regions have

been found to respond only to categories of highly complex stimuli, such as houses (i.e., parahippocampal place area) or faces (i.e., fusiform face area). In this study, we use several standard procedures to identify the location of these visual regions within an individual's brain. Building detailed maps of an individual's visual cortex will allow us to investigate how these brain regions work together such that we can perceive and interact with the visual world.

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Name: Hunter Brown Major: Chemical Engineering Faculty Advisor, Affiliation: Dennis W. Smith, Jr., Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Eugene B. Caldona, David O. Wipf, Dennis W. Smith, Jr.

Facile fabrication of a superhydrophobic/superoleophilic surface via nanoparticle electroless deposition and perfluorinated polymer surface modification

Much recent research on superhydrophobic/superoleophilic material is geared toward simplicity of fabrication. In this study, a superhydrophobic surface was prepared by coating a copper metal sheet with silver nanoparticles via immersion in an aqueous AgNO₃ solution and subsequent dip-coating of the silver-coated sample with Nafion, which was followed by a drying at 120 °C. The entire fabrication process is simple and takes less than 40 min. The as-prepared coated sample has low surface energy and exhibited surface roughness with nano- and micro-hierarchical features. Due to its extreme anti-wetting property, the coating showed protective properties against corrosive media as evidenced by electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization measurements. Aside from being able to repel water, the coating, when applied onto a metal mesh also possessed superoleophilicity such that it is able to let oil pass through the mesh openings. Thus, the coated-mesh can act as a separation membrane, which can be very useful in oil/water separation application.

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Name: Kice Brown Major: Chemistry Home Institution: Mississippi College Faculty Advisor, Affiliation: Keith Hollis, Department of Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Sriloy Dey REU/Research Program: REU

Using Metal-Organic Frameworks for Breaking the Oxo Wall

The quest for efficient, clean energy has become a major area of research in recent years. Specifically, transition metaloxygen complexes are being targeted as catalysts for splitting water into oxygen and hydrogen. This process of reduction, in turn, oxidizes the catalyst forming a metal-oxo bond. Late transition metal-oxo complexes could be used as more efficient catalysts for splitting water than current transition metal complexes; however, these novel complexes with tetragonal symmetry are predicted to be thermodynamically unfavorable by Gray's oxo-wall. Gray's rule states all elements past group 8 on the periodic table are prevented from forming metal-oxygen double bonds. Our research is focused on synthesizing 1,2,4,5-tetra(1-imidazolyl)benzene as a precursor for the synthesis of metal-organic framework (MOF). The MOF has a rigid structure that preserves the required tetragonal symmetry of the complex; preventing two pincer complexes from reacting with one another to form a dimer. The dimerized complexes are less reactive with a symmetry that is not ideal for catalysis. The resulting MOF will be further coordinated to a late transition metal, producing a CCC-NHC pincer complex within itself that is capable of forming this previously unobtainable metal-oxygen double bond.

Name: Christian Brush
 Major: Computer Science
 Faculty Advisor, Affiliation: Scott Rush, Wildlife, Fisheries, and Aquaculture; Cindy Bethel, Computer Science and Engineering
 Project Category: Biological Sciences and Engineering
 Co-Author(s): Caleb Aldridge
 REU/Research Program: ORED Undergraduate Research Program

A web-based interface designed to promote biological conservation and education within Mississippi

We developed a web application based herpetological atlas for Mississippi—implementation anticipated late 2019. Specifically, we developed an integrated backend spatial database attractive to non-expert users that includes access to maps of geographic ranges for amphibian and reptile species by county. We are currently developing life history information on the diverse species showcased within this atlas. A graphical user interface (GUI) is being designed to operate in web-based and mobile-based applications. This friendly GUI is intended for use by teachers and researchers, as well as the general public for information and research purposes. Development of these tools provides co-learning opportunities between K-12 STEM classes and university students working in human-computer interaction and wildlife conservation. This co-learning environment can provide a means to enhance features within the computerbased platform, from its applicability to the user experience. Additionally, this computer-based infrastructure will function as an information hub to support conservation decision making, providing decision makers with up-to-date species status information.

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Name: Jordan Bryant

Home Institution: East Mississippi Community College

Faculty Advisor, Affiliation: Dr. Krishnan, Biochemistry, Molecular Biology, Entomology & Plant Pathology
 Project Category: Biological Sciences and Engineering
 Co-Author(s): Jordan Bryant, Kennadi Johnson, Christina Comino, Eadie Keenan
 REU/Research Program: NIH R25 Bridges to Baccalaureate

Development of a Drosophila model of Spinocerebellar ataxia Type 1 (SCA1) Disease

Spinocerebellar ataxia type 1 (SCA1) is a condition characterized by progressive problems with movement. Patients affected by SCA-1 develop an adult onset devastating pathology characterized by peripheral axonal motor, sensory neuropathy, distal muscular atrophy, pes cavus and steppage gait. The main goal of this summer research experience program was the development of a powerful genetic model to investigate pathogenesis of SCA-1 disease. The fruit fly, Drosophila melanogaster, is an organism extremely useful for studies on human biology, health and a wide range of pathologies including neurodegenerative diseases. This is because Drosophila genes controlling fundamental cellular functions, such as cell growth and death, are quite identical to those found in human cells. In this work, we developed a Drosophila model of SCAN- 1 disease by applying a well-known genetic approach. This focuses on the screening of several fly lines with UAS constructs for expression of abnormal polyglutamine repeats. The selected fly line which exhibits normal ataxin gene encoding for polyglutamine repeats. This approach would create a fruit fly model that mimics the human pathological condition. Subsequently, genome-wide transcriptome analysis of this SCAN-1 fly model will get insight into the mechanism of the disease. The identification of the steps of the SCAN-1 pathological cascade in turn will help the development of therapies targeting key molecules acting in these steps.

Name: Joshua Burcham Major: Chemistry Faculty Advisor, Affiliation: David O. Wipf, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Hellen Stephanie, Todd MIsna, David Wipf REU/Research Program: Chemistry undergraduate summer research

Fluoride removal by asymmetrical capacitive deionization using ion-selective biochar electrodes

Fluoride contamination in water systems due to industrial and farming activities has been an emerging global concern. Capacitive deionization (CDI), which employs a pair of oppositely charged porous electrodes to remove ions from water, has been known as a cost-effective technology for water desalination. This study aims at exploring the feasibility of activated biochar as a low-cost carbon-based electrode material for capacitive deionization of fluoride ions. The removal capacity was enhanced by grafting sulfonic and amine functional groups to the activated biochar to develop cation and anion selectivity. This reduces the co-ion effect in which half of the energy applied to the porous electrode is used to repel the oppositely charged ions. Physical and electrochemical characterizations was performed to investigate the morphology and capacitive behavior of the ion-selective biochar electrodes. A 3- D printed CDI cell was used with NaF solution fed to the cell by a peristaltic pump. The operating voltage was 1.2 V to avoid water electrolysis. The amount of fluoride ions removed from water was investigated using a fluoride ion-selective electrode. A fluoride removal capacity of 8.5 mg g⁻¹ was found. This result is beneficial to advance biochar practical applications in fluoride removal by means of capacitive deionization.

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Name: Cherish Burge
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Home Institution: Mississippi College
Faculty Advisor, Affiliation: Dr. Jonas King, Department of Biochemistry, Molecular Biology, Entomology & Plant
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Project Category: Biological Sciences and Engineering
Co-Author(s): Austin Drury, Travis van Warmerdam
REU/Research Program: REU – Computational Biology

Using Hidden Markov Models to Categorize Illumina Genomic Data

Analyzing metagenomic data can provide many challenges such as genome assembly and annotation. These challenges can be solved by separation and identification of individual sequence reads. Hidden Markov models (HMMs) are a class of probabilistic graphical models that allow predictions to be made about a sequence of unknown variables from a set of observed variables using a multi-step process. This tool can be used by building predictive HMMs generated for each taxonomic unit of interest. Genomic data can then be assigned to the appropriate taxonomic unit using these models. A script was written to help build the models by counting the number of times each combination of six bases occurred in a genome; then, probabilities were calculated based on those counts. Another script was written that scored the reads based on those probabilities. The reads were grouped into corresponding categories based on the maximum scoring model and the standard deviation of scores. Testing was performed to determine the accuracy in building the models. The computational cost, of both time and memory, of the building as well as the scoring, was also tested. Preliminary tests illustrate that the model seems to be effective at categorizing the individual sequence reads into their appropriate taxonomic unit of interest accurately and efficiently.

Name: Sydney Canaday Major: Chemistry Faculty Advisor, Affiliation: Dr. Todd Mlsna, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Achala S. Liyanage REU/Research Program: REU

The removal of pharmaceuticals from contaminated water by magnetized Douglas fir biochar

Contaminated water by pharmaceutical compounds is a growing environmental concern. Magnetic Douglas fir biochar has become an emerging solution to the growing pollution to our water sources. In a series of experiments, magnetized Douglas fir biochar (MBC) was used as an absorbent for the removal of acetylsalicylic acid, caffeine, and ibuprofen from aqueous solutions. MBC was produced by precipitating an iron oxide solution onto the surface of the biochar. This was followed by the treatment of sodium hydroxide. The surface morphology of the magnetized biochar was examined by scanning electron microscopy, point of zero charge, and surface area measurements. Different parameters were implemented to determine how well the magnetized biochar functioned as an adsorbent under varying conditions. These varying conditions include pH, initial concentration of the contaminant, contact time, temperature, and mass of adsorbent. MBC suspensions in contaminated solutions were shaken and then magnetically removed. After the removal of the magnetized biochar, the remaining solutions were analyzed using UV-visible spectroscopy. According to the data, it was discovered that it took less than five minutes to reach the equilibrium for maximum adsorption. The kinetic data was correlated to pseudo-first order and pseudo-second order adsorption models. The equilibrium adsorption data also was analyzed using the Freundlich and Langmuir isotherm equation models. Based on the high adsorption in a short amount of time, MBC can be considered as an eco-friendly and inexpensive method for the removal of pharmaceuticals from contaminated water.

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Name: Lily Cao Major: Chemistry Home Institution: University of Florida Faculty Advisor, Affiliation: Joseph Emerson, Chemistry Department Project Category: Physical Sciences and Engineering Co-Author(s): James Cope, Sean S. Stokes REU/Research Program: 2019 Summer REU: Food, Energy, and Water Security

Analysis of Copper Catalyzed Chan-Evans-Lam Coupling Reaction Conditions with Aryl Boronic Acid and Imidazole Derivatives

The Buchwald-Hartwig amination coupling reaction involves the coupling of N-nucleophiles with aryl halides to produce products that are commonly used in pharmaceuticals. This reaction is typically performed with the use of palladium catalysts. However, alternative catalysts that produce higher yields and are less toxic are being researched. The Chan-Evans-Lam (CEL) coupling reaction produces similar products with the use of copper salts as catalysts. Copper catalysts are inexpensive and less toxic and thus are a desirable alternative to palladium catalysts. This investigation will compare the effectiveness of a copper 1,10-phenanthroline catalyst to a newly synthesized copper 4,5-diazofluoren-9-one catalyst to produce C—N aryl bonded coupled products. The reaction was performed by mixing imidazole and boronic acid in a solvent with the addition of a catalyst. The organic product was separated and analyzed under a GC/MS and LC/MS to determine the yields of desired product and formation of other side products. A study will be done to optimize the effectiveness of the CEL coupling reaction under different reaction conditions. The following variables that will be tested include solvent, time, temperature, equivalency of reactants, concentration of catalyst, presence of base, and presence of water. Currently, results indicate that the copper 4,5-diazofluoren-9-one catalyst. Further investigation will be done on the other reaction conditions as well as different methods to increase yields of the coupled product.

Name: Gerardo Carreon Major: Chemical Engineering Home University: Texas A&M University Faculty Advisor, Affiliation: Jason Street, James Wooten; Department of Sustainable Bioproducts Project Category: Biological Sciences and Engineering REU/Research Program: REU-INFEWS

Treatment of Wood Pellets to Minimize or Prevent Off-Gassing

The industry of bio-product sustainable energy is growing in European countries who receive imports of more than six metric tons per year valued at ~\$800 million from the United States. The problem that has come under investigation is the off-gassing of wood pellets during sea transportation that has resulted in various deaths of ship workers. These regretful deaths have been associated with off-gassing of wood pellets which result in oxygen-depleted air and an increase in concentrations of carbon monoxide, carbon dioxide, hydrocarbons and other volatile compounds. The main concern is the levels of the toxic and potentially fatal gas carbon monoxide.

This research consisted of treating southern yellow pine with different processes and chemicals to study the effects on its off-gassing by testing the air composition with gas chromatography throughout four to five days. The experiment was set up to resemble transportation conditions. Air-tight sealed mason jars were placed in a water bath at 55oC. The methods tested on southern yellow pine were: methanol soaked, 1:1 potassium hydroxide and methanol solution, bio-oil soaked, heat autoclaved, steam exploded, acetic anhydride soaked, bio-oil and 1:1 potassium hydroxide and methanol solution, and treatment with the antioxidants tert-Butylhydroquinone (TBHQ) and butylhydroxyanisole (BHA). Results show a significant decrease in the levels of carbon monoxide in the processes involving heated autoclaved and steam exploded material.

The process that causes the off-gassing is not well understood and further research is needed to be able to counteract it. However, the results of this experiment show the processes of steam explosion and heat autoclave are promising solutions to pursue, showing a significant reduction from the control group. The steam exploded material saw a high removal rate of fatty acids in the wood, supporting the idea that the majority of wood off-gassing is a result of the fatty acids oxidizing.

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Name: Cade Cockrell Major: Aerospace Engineering Faculty Advisor, Affiliation: Donghoon Kim, Aerospace Engineering Project Category: Physical Sciences and Engineering

CO₂ Sensor Mobilization for Occupancy Detection

Efficient energy has quickly become one of the world's largest concerns with worries of limited fossil fuel resources, pollution, and costly utility bills. With air conditioners being one of the largest energy consumption units installed in residential and commercial buildings, having control over them could significantly benefit businesses or the average home owner. Coupled with a CO₂ sensor, communication between an autonomous vehicle and the main air conditioner unit allows for smarter operation of air conditioning systems and will result in a more comfortable, energy efficient environment. Mobilizing the CO₂ sensor could provide useful information such as mapping the CO₂ profile for a given room. By moving the sensor and tracking its position, identification of CO₂ rises correlated with human occupancy can be achieved. The data acquired from mapping the CO₂ and detecting human occupancy can be communicated to a main unit as input data used to control the air flow and temperature for any space.

Name: Leonna Conley Major: Biochemistry Faculty Advisor, Affiliation: Dr. Colleen Scott, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Daijun Feng REU/Research Program: Center for Selective C-H Functionalization Chemistry Summer Undergraduate Research Program

Synthesis of 3,6-Unsubstituted Diketopyrrolopyrrole (DHDPP) and the C-H Functionalization at 3,6-Positions

N,N'-dialkyl diketopyrrolopyrrole, more frequently referred to as DPP, is one of the most commonly used compounds in organic electronic devices such as organic field effect transistors (OFETs) and organic photovoltaics (OPVs). In such organic devices, DPP serves to transfer electric charges. DPP is furthermore utilized in organic light-emitting diodes (OLEDs) as well as fluorescent probes due to its distinguished fluorescent properties. However, the conventional synthesis of DPP can only give aromatic flanked DPP compounds, consequently limiting molecular structure design in the real applications. Furthermore, the conventional synthesis cannot tolerate electron deficient aryl groups. In this regard, we have designed and prepared 2,5-dialkyl-3,6-hydrido-1H,2H,4H,5H-pyrrolo[3,4-c]pyrrole-1,4-dione (DHDPP) that incorporates hydrogen atoms at its 3,6-positions, which will allow us to perform C-H functionalization with electron deficient aryl groups.

DHDPP was synthesized using simple reaction conditions. A new neon blue fluorescent spot was observed using thin-layer chromatography (TLC), which was later confirmed to be the product by 1H NMR analysis. The product was unstable in air. To prevent or limit the rapid decomposition of DHDPP, acetonitrile, the most commonly used solvent, was degassed using nitrogen to remove any traces of oxygen. We will also investigate the electronic effect of the R-group on the amide nitrogen on the stability of the DHDPP compound.

Once stabilization is achieved, the C-H functionalization will enable us to develop various donor acceptor and n-type materials, which will expand DHDPP's domain in structure design. After observing the reaction conditions of small molecules produced by the coupling with DHDPP, direct arylation polymerization will be conducted to create such donor acceptor materials and n-type polymers that cannot be produced by any other structures. Upon polymer development, their optoelectronic properties as well as their functionality in such organic devices will be observed and analyzed.

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Name: William Davis Major: Chemistry Faculty Advisor, Affiliation: Amanda Patrick, Chemistry Project Category: Physical Sciences and Engineering REU/Research Program: Chemistry REU

Characterization of Synthetic Monomers by High-Resolution Mass Spectrometry

This work aims to develop a method to determine the exact mass (EM) of a series of novel analytes. The EM of the analytes is needed to corroborate the other characterization methods. To develop a robust method, ionization conditions will be systematically changed to optimize signal stability and intensity and to evaluate the appearance of different characteristic ions (e.g., molecular ion, protonated analyte, sodiated analyte). The ionization sources evaluated include electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI). The EM of a series of ((perflurocyclohex-1-en-1-yl)oxy)phenyl monomers has been measured using APCI mass spectrometry. The series includes monomers that have a ketone group and those that do not have a ketone group. The monomers without ketones especially pose an issue as they are harder to ionize via protonation and little to no signal by the more common ESI mass spectrometry, making APCI optimization especially important here. Good signal was obtained using a methanol-water 3:1 solvent system and a flow rate of 50 μ L/min. Acidification was also tested with no clear advantage. For each mass measurement, the mass error was calculated. In the analysis of bis (PFCP-AR-BP), bis(PFCP-AQ-BP), and bis(PFCP-AR-BP), [M+H]⁺ error was below 5 ppm with some being less than 1 ppm. Bis(PFCP-AR-BP) does not have a ketone and the intensity was one and two order of magnitude less than bis (PFCH-PE-BP) and bis(PFCP-AQ-BP) respectively. While the protonated analyte was the most intense characteristic ion in each case, there was also a minor M⁺⁺ ion, which was of a higher relative intensity for bis(PFCP-AR-BP). Ongoing work aims to investigate parameters controlling the relative intensity of the M⁺⁺ versus [M + H]⁺ ions,

evaluate alternative charge carriers (e.g., Na^+ , Li^+) as an alternative method to make ESI competitive with APCI, and measure high-resolution mass spectra for additional monomers using the developed method.

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Name: Katie Evans Major: Microbiology Faculty Advisor, Affiliation: Shecoya White, Department of Food Science, Nutrition, and Health Promotion Project Category: Biological Sciences and Engineering Co-Author(s): Diana Wilson, Jessa Goodeaux

Shelf-Life Stabilization of Grape Tomatoes Using Zein/Essential Oil Composite Film

Public concern over chemical food preservatives has pushed research to examine new forms of natural active packaging: food packaging that contains active compounds such as antimicrobials to keep food fresh. Zein, a natural corn protein, is able to form a safe food coating in which active compounds can be easily incorporated. The present study was designed to determine the best application of a zein film coating on the shelf-life of grape tomatoes, whether applied directly to product packaging or directly applied to the product itself. Three zein films were engineered: 20% thyme essential oil (EO), 10% thyme EO, and one without thyme EO. Grape tomatoes were purchased at a local grocery store. The tomatoes were divided into six groups: 20% thyme EO film on tomatoes, 20% thyme EO on container, 10% thyme EO on tomatoes, 10% thyme EO on container, traditional zein coating on tomatoes, and no coating (control). Seven containers of tomatoes in total were used in the study, with two controls used to ensure an accurate baseline. Depending on group designation, either the plastic container or the tomatoes themselves were manually coated with approximately 20g of the assigned zein film. Tomatoes were then held at room temperature for nine days. Moisture loss and visual appeal were examined at regular intervals. Tray 6 (control) had the least overall moisture loss of 3.09%, while Tray 7 (also control) had the most overall moisture loss with 10.01%. All containers with a thyme EO zein coating had similar reduction in moisture loss, with the exception of Tray 3 (20% thyme coating on tomatoes) which showed decreased moisture loss. Trays 1, 3 and 6 all retained visual appeal. This study shows that an active zein film applied to the tomato container can have similar shelf-life extending properties as directly coated tomatoes.

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Name: Isidora Fereday Major: Biological Sciences and Microbiology Faculty Advisor, Affiliation: Dr. Justin Thornton, Biological Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Keun Seok Seo, Joo Youn Park

Engineering Bacteriophage Delivery of an Antimicrobial CRISPR/Cas9 System to Streptococcus pneumoniae

Streptococcus pneumoniae is a gram-positive, facultative anaerobe and is the most common cause of pneumonia, meningitis, and otitis media. As antibiotic resistance becomes an increasing concern, there is demand for novel treatments for bacterial infections. One such innovative solution is phage therapy, which uses bacteriophages to treat bacterial infections. The CRISPR (clustered regularly interspaced short palindromic repeats) and CRISPR-associated Cas9 genes are used as a genome editing system in bacteria. The CRISPR/Cas9 system can be targeted to a specific sequence of DNA and will cut the DNA at that location. We hypothesize that by integrating a CRISPR/Cas9 system into the genome of a temperate pneumococcal phage, we will develop a system for specifically clearing *S. pneumoniae*. We have established a CRISPR/Cas9 system that is targeted to the pneumolysin (*ply*) gene, which is a key virulence factor of pneumococcus. Cleaving the chromosome at the *ply* locus gene will effectively neutralize the pathogen. To generate the CRISPR/Cas9 system, synthetic oligos specific to the ply gene (spacer sequence) were cloned into the *BbsI* site of pKS1 vector that contains a promoter, leader sequence, DR, and spacer region) was amplified from pKS2 and cloned downstream of the genes for the tracr-RNA and Cas9 (originating from Streptococcus pyogenes SF370) to generate pKS4. Non-essential gene segments from *S. pneumoniae* temperate phage MM1 along with an erythromycin cassette for selection were cloned into pKS4 to flank the CRISPR/Cas9 system, thus resulting in creation of pKS5 and allowing for homologous recombination into the

pneumococcal chromosome. Successful integration of this system into the genome should result in progeny phage bearing CRISPR. Engineered phage will then be used for *in vitro* and in *vivo* assays for clearance of *S. pneumoniae*.

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Name: Isabella Ferrebee

Major: Secondary Education and Speech Home Institution: East Mississippi Community College Faculty Advisor, Affiliation: Heather Jordan, Biological Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Rebecca Waters REU/Research Program: NIH R25 Bridges to Baccalaureate

Effects of Bacterial Supplementation to Black Soldier Fly Waste Conversion and Ammonia Reduction

Globally, scientists are facing problems resulting from overpopulation, among which are how to reduce waste while also increasing both food supply and energy. A solution for these various problems is insect farming. Black soldier fly (Hermetia illucens, BSF) larvae are the ideal insects, as they are easy to rear, consume waste, do not carry disease, and do not sting. Additionally, they contribute to environmental sustainability by reducing greenhouse gases and wastes, fertilizing soil, and can be converted into biofuel. BSF larvae are rich in proteins and lipids, making them a wholesome food source for animals and humans alike; however, BSF larvae waste conversion yields low-level ammonia emissions. In this experiment, the bacterium Pseudomonas putida was added to BSF larvae's diets to determine its effects on insect growth and ammonia production. Pseudomonas putida is ideal because it is a nitrogen fixer and can degrade various organic substances, including plastics. The goal of this experiment was to increase growth of larvae while also decreasing undesirable ammonia. Over the course of nine days, different doses of Pseudomonas putida were incorporated into the diets of BSF larvae, with controls receiving water rather than P. putida. Six replicates of 100 larvae were given one dose of P. putida at the start of a 9-day trial, and three of these received a second dose two days prior to the end of the trial, to test a dosing effect. Waste and larvae were weighed throughout the experiment, and the larvae were counted, to determine waste conversion and mortality rates, respectively. The ammonia production was also determined using an ammonia assay kit. Results of these data demonstrate the utility of bacterial supplementation for increasing BSF larvae efficiency in waste conversion and further reducing ammonia outputs.

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 Project Category: Physical Sciences and Engineering
 Co-Author(s): Robert W. Lamb, Hunter Shirley, Chance M. Boudreaux, Nalaka P. Liyanage, Elizabeth T. Papish, Jared H. Delcamp

Electrocatalytic Reduction of CO₂ to CO using Ruthenium-Centered Pincer Complexes

The reduction of CO₂ to CO to rid the atmosphere of greenhouse gases while simultaneously creating a fossil fuel substitute greatly benefits both the environment as well as human sustainability. This reduction can be achieved via photochemical and electrochemical catalysis with a ruthenium-centered CNC pincer complex. Combinations of different ligands with the pincer have varying efficiency for production of CO versus H₂, presumably due to different active catalysts. However, the exact reason for these different catalytic behaviors is unclear. The energetics of the catalytic cycles were studied using DFT to understand how changes in the coordination sphere create catalysts with variable efficiency and effectiveness which will lead to more intelligent catalyst design.

63 Name: Megan Finney Major: Civil Engineering Faculty Advisor, Affiliation: Alireza Ermagun, Civil and Environmental Engineering Project Category: Physical Sciences and Engineering

Performance Analysis of Public Transit in and out of Campus

This study measures the performance of Starkville-Mississippi State University Area Rapid Transit (S.M.A.R.T) and compares the efficiency of S.M.A.R.T both in and out of the Mississippi State University (MSU) Campus. S.M.A.R.T is an operating transit system utilized not only by students and faculty of MSU, but also residents and visitors of Starkville. This system is comprised of eleven separate routes, six of which serve the campus. The routes provide swift and user-friendly access to popular destinations around Starkville including lengthy paths to the Wise Center and GTR Airport and shorter paths such as MSU's Central and Greek loops. Similarly, the fleet of buses is distributed rationally in which paths with the strongest demands receive the greatest amount of buses and drivers. We retrieved the ridership, number of fleet, number of drivers, and the operation cost of each route between 2016 and 2018. Using the data envelopment analysis, we measure and rank the performance of each route over time. Overall, the results unravel the performance of each route and assist city officials and transit authorities in allocating budget and improving the performance of S.M.A.R.T in and out of campus. This further helps meet the mission of S.M.A.R.T, which is providing an efficient public transportation service.

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Name: Nathan Frey
Major: Chemistry
Faculty Advisor, Affiliation: Charles Edwin Webster, Chemistry
Project Category: Physical Sciences and Engineering
Co-Author(s): Robert W. Lamb, Eric Van Dornshuld, Kelsie E. Krantz, Wenlong Yang, Paul Miller, Diane A. Dickie, Robert J. Gilliard, Jr.

Examining the Electronic Properties of Twisted Pyrene Compounds

Polycyclic Aromatic Hydrocarbons (PAHs) are arenes that typically deviate from planarity, thereby forming bowl-shaped and/or twisted structures. In this computational study, the electronic properties of five pyrene-containing PAHs have been studied. Three of these compounds contain two diazaborolidines and two compounds contain two N-heterocyclic germylenes (NHGes)—one of which contains an NHC coordinated to each germanium and one contains two coordinatively unsaturated germaniums. The geometric differences and fluorescent properties will be compared and discussed. Nucleus-independent chemical shift (NICS) values were computed at the center of mass of each five or six-membered ring [NICS(0)] using the B3LYP/BS1 level of theory (BS1 is defined as the 6-311+G** basis sets for C, H, N, F, and B and 6-31G* basis set for Ge). Molecular orbitals were analyzed for each compound. Time-dependent DFT (TD-DFT) computations were also performed to produce the simulated UV-Vis spectrum for each compound.

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Name: Justin Giles Major: Biological Sciences Home Institution: Tougaloo College Faculty Advisor, Affiliation: Dr. Steven R. Gwaltney, Department of Chemistry Project Category: Biological Sciences and Engineering Co-Author(s): Jerrano Bowleg

Substrate-induced changes in dynamics and correlated motions of PIN1: A molecular dynamics study

Pin1 is an essential peptidyl-prolyl isomerase (PPIase) that catalyzes *cis-trans* prolyl isomerization in proteins containing pSer/pThr-Pro motifs. It possesses an N-terminal WW domain that targets pSer/pThr-Pro motifs and a C-terminal PPIase domain that catalyzes prolyl isomerization. Recently, Pin1 was shown to modify the conformation of phosphorylated histone H1 and stabilize the chromatin–H1 interaction by increasing its residence time. This Pin1–histone H1 interaction

plays a key role in pathogen response, in infection, and in cell cycle control; therefore, anti-Pin1 therapeutics are an important focus for treating infections as well as cancer. To understand the Pin1–histone H1 interaction fully, we investigated how both the Pin1 interact with four histone H1 substrate peptide sequences (H1.4, H1.4₁, H1.4₂, H1.4₃). To achieve this, we utilize molecular dynamics (MD) simulations of Pin1 with and without the peptides derived from the human histone H1.4 protein. From experimental evidence, these peptides exhibit a range of values as well as differing degrees of inter-domain interaction, allowing a systematic exploration Pin1-substrate interactions. The goal of this study is to investigate the changes in structure, molecular motions and free energy upon substrate binding to Pin1. We would hope that the results of this work would allow for a better understanding of the structure-dynamics relationship of Pin1 and histones.

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Name: Jessa Goodeaux

Major: Food Science and Technology
 Faculty Advisor, Affiliation: Shecoya White, Department of Food Science, Nutrition, and Health Promotion
 Project Category: Biological Sciences and Engineering
 Co-Author(s): Katie Evans, Jailyn Smith, Derris Burnett
 REU/Research Program: CALS MAFES Undergraduate Research Scholars Program

The Effect of Natural Polysaccharide and Citrus Oil Solution on the Shelf Life of Ready to Eat Deli Chicken

Due to the increased demand for natural strategies to control pathogenic bacteria and food spoilage, effective compounds for use as antimicrobials have been sought by food manufacturers. Ready-to-eat meats are particularly a concern since they may be consumed without further cooking or processing and are known to be highly susceptible to the growth of pathogenic microorganisms. Substances derived from citrus fruits alone or combined with other natural antimicrobials have proven to inhibit growth or kill foodborne bacteria. In the present accelerated shelf-life study, the efficacy of a citrus based oil and antimicrobial polysaccharide solution were evaluated to determine deceleration rate of spoilage in readyto-eat deli chicken meat held at ambient temperature for 5 days. Chicken samples were subjected to the following treatments: orange oil combined with polysaccharide, polysaccharide alone, and control (no antimicrobial). Sensory and microbial evaluations were performed on Day 3 and Day 5. On Day 3, orange oil solution samples had an average bacterial count that was approximately 45% less than the control, and much more pungent odor than the other treatments. All samples were visually unaltered by the end of Day 3. By Day 5, the control samples had an average bacterial count that was 0.6 log CFU/g less than samples treated with the orange oil solution. Discoloration and rancid odor were observed in all the samples at the conclusion of the accelerated shelf life study. In conclusion, the ready-to-eat chicken deli meat treated with a citrus oil and polysaccharide solution proved to inhibit the growth of microorganisms within a 3 day time period. The effect of the solution declined between Day 3 and Day 5, which suggests that there is an optimal point of use that is less than 5 days.

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Name: Romans Grant Major: Chemistry Home Institution: Tougaloo College Faculty Advisor, Affiliation: Steven Gwaltney, Department of Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Jerrano L. Bowleg, Bidisha Sengupta

Ligand binding to a modified amyloid- β peptide: A molecular dynamics study

Amyloid- β peptides (A β) are protein deposits that can aggregate to form fibrils through Amyloid Precursor Protein (APP) catabolic pathway. The proteolysis of APP resulting in 42 residues of A β_{42} is commonly associated with Alzheimer's disease (AD). Effective medicinal approaches are limited to the developmental stages of the disease which are usually assessed post mortem - often the late stage. Current studies on AD focus on the intra- and intermolecular mechanism of monomeric A β that binds to form fibrils. Herein, molecular dynamics simulations of 100 ns were performed to study the dynamics of both the natural and modified A β_{42} at three different temperatures. Also, in this study, we explore the binding of three

Morin-like compounds to the A β_{42} peptide to understand the inhibitory mechanism of aggregation at three different temperatures. We would like to understand how temperature affects the binding affinity and the binding modes. This study may help in the design of new drugs that will inhibit the aggregation of A β_{42} to serve as an effective treatment for Alzheimer's disease.

66

Name: Abigail Grantham

Major: Chemical Engineering - Bachelors Faculty Advisor, Affiliation: Dr. Santanu Kundu, Chemical Engineering; Dr. Bill Elmore, Chemical Engineering Project Category: Physical Sciences and Engineering Co-Author(s): Katie Elmore

Enzymatic Polymerization of Epoxidized Oleic Acid

Oleic Acid is one of two distinct fatty acids found in cottonseed oil. It is easily obtained due to cottonseed oil's wide availability. Here, an attempt has been made to synthesize non-crosslinked polymers starting with oleic acid using enzymatic polymerization process. The resultant polymer will have applications in many areas and will also be attractive because of the renewable starting material and the possible biodegradability of the polymer. Oleic Acid is selected here as the single carbon-carbon double bond present in this molecule can be converted into oxiranes using epoxidizing reaction. The epoxidized oleic acid (EOA) can then be used for the polymerization reactions. After drying the EOA (using molecular sieves and anhydrous calcium hydride), dried toluene and the enzyme catalyst (Novozym N435) have been added to the EOA. The resultant mixture was then heated under Argon atmosphere. The resulting polymer was characterized using differential scanning calorimetry, thermogravimetric analysis, and gel permeation chromatography.

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Name: Monica Gurung Major: Civil Engineering Home Institution: Virginia Tech Faculty Advisor, Affiliation: Dr. Ashli Brown, Chemistry Project Category: Physical Sciences and Engineering REU/Research Program: REU-INFEWS Summer Research Program

The evaluation of adsorbents for the removal of aflatoxin M1 from contaminated milk using biochar

Aflatoxin is a hepatocarcinogenic naturally occurring compound produced by a fungus (*Aspergillus flavus*) and affects both humans and animals. Most humans get exposed to aflatoxin by consuming dairy products, grains, nuts, and many other agricultural products which have been infected by the fungus. When animals consume grains that are contaminated with aflatoxin B1, an enzyme found in the liver converts it to aflatoxin M1, which is secreted through mammary glands of lactating animals. Aflatoxin M1 is highly regulated in the United States allowing only 0.5 part per billion (ppb) of aflatoxin in milk. A lot of research has been done to eliminate aflatoxin from our food, but it still remains a huge threat to our health. This research Project investigates using a modified Douglas Fir biochar to remove aflatoxin M1 from milk. Biochar, charcoal produced from plant matter, has a very high absorption capacity and can be used as an economical filter alternative. The biochar was modified using methanol has been proved to bind and remove tetracycline from aqueous solutions. Since the chemical structure of aflatoxin M1 contain similar functional groups to tetracycline, we designed a methanol-modified biochar from the removal aflatoxin from milk and other contaminated liquids, such as beer and coffee. We used Liquid chromatography-mass spectrometry (LC-MS) and ELISA (enzyme-linked immunosorbent assay) methods to determine the aflatoxin binding capacity of our modified biochar.

Name: Ashley Hall Major: Biological Sciences Home Institution: Spelman College Faculty Advisor, Affiliation: Cyprianna Swiderski, Clinical Science Project Category: Biological Sciences and Engineering Co-Author(s): Christa Frodella REU/Research Program: Computational Biology REU

Investigation of the de novo lung transcriptome of horses with pasture-associated severe equine asthma

Severe equine asthma (SEA) is characterized by reversible airway obstruction, non-specific airway hyper-responsiveness and chronic neutrophilic airway inflammation. Two different forms of SEA exist: barn-associated and pasture-associated severe equine asthma. This experiment focuses on pasture-associated SEA, which affects horses grazing grass pastures in the southeastern United States during hot humid conditions. Our prior analyses have identified differences in innate immune effector mechanism in diseased versus control horses. To further test this hypothesis and identify transcripts that may be incorrectly annotated or missing from the current equine genome assembly (EquCab3.0), we first constructed a comprehensive de novo lung transcriptome (Trinity) from mRNA-sequencing data derived from serial lung biopsies of pasture-associated SEA (N=6) and control horses (N=6) during both seasons of disease exacerbation and remission (150pb, 40 million paired end reads/sample). Next, reads from the aforementioned mRNA sequencing data were mapped to our de novo transcriptome with Bowtie2 and quantified using Salmon. Differentially expressed genes (DEGs) were then analyzed using DESeq2. These results were then contrasted to DEGs that were similarly derived from the same pipeline with the exception of read alignment to the recent equine genome assembly (EquCab3.0). The results of this investigation will be informative not only regarding the pathogenesis of pasture-associated SEA, but also regarding the utility of the current equine genome assembly to predict relevant disease biology.

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Name: Dalton Hall Major: Biochemistry Faculty Advisor, Affiliation: Dr. Laura H. Downey, School of Human Sciences Project Category: Social Sciences Co-Author(s): Kristy Terp

Qualitative Analysis of Technology Usage in SNAP-eligible Participants in Mississippi

With most people having access to the Internet and various technological outlets, it's important to incorporate these advances and new norms in health promotion social marketing strategies. Social marketing is a broad-based approach to nutrition education and an approved technique for SNAP-Ed. Formative research was conducted to comprehend the various ways technology is consumed by SNAP-eligible participants and how to better incorporate technology in SNAP-Ed. The purpose of this research is to qualitatively analyze responses from current and former SNAP participants within 18 geographically dispersed focus groups throughout the state of Mississippi and to inform SNAP-Ed on anecdotal ways to implement social marketing to SNAP-eligible participants. After two different independent researchers analyzed the focus group transcripts, the data was condensed with special regard to questions regarding technology, mass media, and social media. The following four questions were then highlighted from the data: where people get information about healthy eating and cooking, where people get health information, would people be interested in an online class with reliable health-related information, and would people be interested in a state-sponsored SNAP-Ed website. The results show that nearly all participants use the Internet to get most of their health information, specifically Facebook and Pinterest. To a lesser degree, many participants get their recipes from television channels like The Food Network. When asked about the idea of a state sponsored SNAP website, the results showed that most participants would be interested, and it would decrease the spread of misinformation. Additionally, multiple participants state their interest in free online classes that offer health information on their own times through popular publishing sites like YouTube. To conclude, the data indicates the importance of utilizing various technological outlets to promote nutrition education and to inform SNAP-Ed's social marketing campaigns.

Name: Ruby Hall Major: Chemistry Faculty Advisor, Affiliation: Joseph Emerson, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): James Cope REU/Program: MSU Chemistry Summer Research

Investigations of Variables for Chan- Evan- Lam Coupling with the Discovery of 4,7-di(1H-imidazol-1-yl)-1,10-phenanthroline

The Chan-Evans-Lam coupling, also known as CEL coupling, is a reaction that involves boronic acids being coupled to N--H or O—H containing compound through an oxidative coupling. In this project, an aryl boronic acids are being coupled to in the presence of a copper catalyst; similar to a Suzuki coupling. The Suzuki coupling reaction uses a palladium catalyst, which is more toxic and expensive than copper-based catalysts. The two catalyst that were compared in the CEL coupling reactions were $[Cu(Dafo)_2]$ and $[Cu(Phen)_2]$. After many trials, data show that $[Cu(Dafo)_2]$ has proven to be the better catalyst for CEL coupling reaction. However, trials involving the $[Cu(Phen)_2]$ catalyst has produced an unexpected result; the creation of a new complex. Under specific reaction conditions 4,7-di(1H-imidazol-1-yl)-1,10-phenanthroline is generated, which is a novel activation of the Phen ligand. Studies are still underway to learn more about this serendipitous reaction and its proposed structure.

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Name: Amanda Herzberg Major: Chemistry

Home Institution: Northwest Missouri State University

Faculty Advisor, Affiliation: Ashli Brown, Department of Chemistry; Todd Mlsna, Department of Chemistry; Timothy Schauwecker, Landscape Architecture; Darrell Sparks, Department of Biochemistry, Molecular Biology, Entomology & Plant Pathology

Project Category: Physical Sciences and Engineering

Co-Author(s): Dr. Glenn Crisler II, Roger Davis Jr., Monica Gurung, Casey Johnson

REU/Research Program: REU-INFEWS: Food, Energy, and Water Security

Treatment of Wetland/Forebay Bioreactor Design

Phosphorus in the form of phosphate is often applied by farmers to increase soil fertility, however phosphate that is not taken up by plants can make its way to bodies of water by storm water runoff or erosion. This build-up of phosphate then results in algal blooms and eventually dead zones (hypoxic zones). In order to prevent dead zones, phosphate runoff must be reduced. Two industrial coproducts, slag and modified commercial biochar, were studied to determine their phosphate removing capabilities as a nutrient filter layer. Biochar, a carbonaceous material, is the product of the pyrolysis of biomass. Upon metal oxide impregnation, biochar is effective at scavenging phosphate ions in aqueous and soil matrixes. Slag, a co-product of steel production, has also been shown to have an affinity for phosphate. To investigate the capacity of a filter constructed using these materials, a small scale study utilizing five gallon buckets was performed. Each bucket was fitted with a valve, compacted subsoil, a filter material (biochar, slag, or sand), and topped with a thin layer of topsoil and a sedge. Each month, these filters were filled to capacity using 5 ppm phosphate testing was done using a molybdenum blue colorimetric method and analyzed at 830 nm via UV-VIS. The amount of phosphate in solution was used to compare filter media.

Name: Baylee Holt Major: Biological Sciences Home University: Alcorn State University Faculty Advisor, Affiliation: Andy Perkins, Computer Science Project Category: Biological Sciences and Engineering REU/Research Program: Computational Biology REU

Comparison of Sequence Mapping and Differential Expression Softwares

It has been shown that the choice of software can affect the outcome of differential expression studies in RNA-Seq experiments. We investigated the effect of currently-popular sequence mapping and differential expression software choice on the outcomes of a selection of data sets to determine how prevalent these differences are and to what extent they may affect downstream analyses. We downloaded software HISAT2 with Stringtie and Salmon, which were used to map quality-filtered reads for several data sets. Differentially expressed transcripts were identified using edgeR and DESeq2, and the resulting gene lists were compared. We also investigated the differences in functional and pathway enrichment results between the various approaches. The results from this study may help researchers determine whether it is necessary to employ multiple alignment and differential expression workflows, and whether the effects are data-dependent.

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Name: Baleigh Hull Major: Architecture Faculty Advisor, Affiliation: Silvina Lopez Barrera, School of Architecture Project Category: Arts and Humanities Co-Author(s): Leah Kemp

Designing Affordable Housing in Mississippi

Rural communities across the United States are struggling to maintain a commercial and industrial tax base. Small towns in Mississippi are no exception, and are suffering to maintain public spaces, infrastructure, and their downtowns. The presence of vacant lots, empty store fronts, and abandoned buildings are signs of a declining community. In addition, a significant portion of the population experience barriers to access inclusive well-designed affordable housing. Historically, downtowns utilized their buildings to create a vibrant and unique environment using the existing vernacular architecture. The goal of this project is to develop a series of mixed use and adaptive reuse building typologies that can be replicated to improve the need for affordable housing throughout Mississippi. As part of this project we selected four towns in two different regions (the Delta and the Northeast) that have different demographics and socio-economic backgrounds to compare. Indianola, Sunflower, and Shelby were the towns selected for study in the Delta, and Ripley was chosen for the Northeast. These towns were found to have some of the highest poverty rates in Mississippi and could benefit the most from this project. Design proposals were developed for existing buildings and infill residential development; focusing on building typologies involving upper floor housing, mixed income housing, and multi-family housing. Existing buildings were selected based on location and architectural appeal. Vacant lots were chosen to show the impact of new development in the downtown. The hypothesis that guides this project highlights that downtown affordable housing development can help alleviate housing inequality and prevent urban decay.

Name: Madison Keller

Major: Animal and Dairy Sciences (Pre-Vet) Faculty Advisor, Affiliation: Keun Seok Seo, Department of Basic Sciences, College of Veterinary Medicine Project Category: Biological Sciences and Engineering Co-Author(s): Sunghyun Yoon, Nogi Park, Joo Youn Park REU/Research Program: EMCC-MSU Bridges to Baccalaureate Degree Program

The Use of the Map Protein as a Vaccine Adjuvant to Stimulate an Immune System Response

Staphylococcus aureus is an opportunistic pathogen of humans and animals. S. aureus can penetrate mucosal membranes and cause infections at almost any site in the body by secreting toxins and membrane proteins. The increasing resistance to antibiotics by S. aureus poses a major health threat, therefore it would be ideal to develop a vaccine to prevent infections. However, such efforts have been met with a limited success. Secretory immunoglobulin A (slgA) is a key component in mucosal immunity, which protect our mucosa from pathogens by neutralizing toxins and colonization factors. We tested human IgA levels against secreted toxins and membrane proteins and found that membrane proteins showed much less IgA response than secreted toxins. This suggests that natural S. aureus infections could not elicit an IgA response against membrane proteins. As membrane proteins play a key role in colonization at the mucosal membrane, it is important to induce IgA response to membrane proteins for prevention of S. aureus colonization at the mucosal membrane. Interestingly, a single protein approximately ~65 KDa in size showed very high IgA levels in all human sera tested. The protein identity was found to be Major Histocompatibility Complex Class II Analogous Protein (Map). As an adjuvant antigen can induce cytokine milieu that drive a specific immunoglobulin isotype switching, we hypothesize that the Map protein could be used as a vaccine adjuvant to induce IgA immune response. To this end, we amplified the Map gene from S. aureus strain LAC, the most common type of S. aureus found in human skins and cloned into the protein expression vector system. We hope to have a purified protein that is able to be used in animal trials, that way we can further study the effects of the immune system response to S. aureus when introduced to this adjuvant.

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Name: Eunbea Kim Major: Psychology Faculty Advisor, Affiliation: Danielle K. Nadorff, Ph.D, Psychology Project Category: Social Sciences

Comparing Cultural Differences in Sense of Control, Social Cohesion, and Depression Symptoms in Older Adults: A Comparison Between the U.S and Japan.

Previous research has shown that the social environment surrounding individuals is highly linked to their mental health in late-life (Bronfenbrenner, 1979). One highly influential factor to mental health is an individual's culture (e.g., individualistic versus collectivistic) (Hernandez et al., 2009). Asian cultures utilize a collectivistic perspective, and are more likely to value cohesiveness among individuals and a virtue of respect for elders. Although this culture seems beneficial to older adults due to its promoting social cohesion (Kang, Shaver, & Sue, 2003; Kwan Bond, & Singelis, 1997; Uchida & Ktayama, 2009), it is also associated with a lower sense of control, which can lead to feeling less independent (Markus & Kitayama, 1991). Both of these factors are related to mental health (Chou, 2004). The current study utilized data from Midlife in the United States and Midlife in Japan to examine cultural differences between U.S. and Japanese older adults in sense of control, social cohesion, and depression symptoms. Hypothesis 1: older adults in Japan would report lower perceived sense of control than those in U.S. Hypothesis 2: older adults in Japan would report higher levels of social cohesion (assessed via social support minus strain from family, friends, and spouse) than those in the U.S. Hypothesis 3: older adults in Japan would report higher levels of depressive symptoms than those in the U.S. The results of ttests showed no significant differences between two groups of older adults in sense of control. Regarding social cohesion, elderly in the U.S. (M=4.14, SD=2.26) reported significantly higher rates in comparison to those in Japan (M=1.87, SD=2.05, t(3569)=23.56, p<.01). For depression symptoms, older adults in the U.S. (M=10.11, SD=2.50) reported significantly higher perceived level of depression symptoms than those in Japan (M=3.82, SD=1.34, t(3949)=62.82, p<.01). Thus, cultural differences may impact older adults in social cohesion and depression symptoms.

Name: Connor Kitchens

Major: Geosciences/Environmental Geoscience Faculty Advisor, Affiliation: Varun Paul, Geoscience Project Category: Biological Sciences and Engineering

Soil as a Filter

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The idea of this experiment was to test if soils, when combined with certain substances, could be used as filters. The reason for researching this is to find a cheap, yet effective, way to filter water. This is important because there are many places across the world that do not have access to multi-hundred thousand- or million-dollar filtration systems, therefore they are left with water that does not meet safety standards. With a simple system like the one tested, this issue could be lessened. The design is not expensive, and it could easily be replicated in the field. It could be done with a cardboard box, or something more durable, if available. The only requirements for the apparatus are as follows: something to hold the soil, preferably a with coffee filter or similar material, and something to drop water into the soil. Consequently, the device to hold the soil must be big enough to accommodate the soil and a pour volume of water. The findings of this experiment are promising. On average, 80% of the additives that were in the water being filtered were removed. In some cases, it was 95-100% removal. In conclusion, with more research, this experimental design could help millions across the globe.

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Name: Justin Labonte
Major: Biological Sciences
Home University: East Mississippi Community College
Faculty Advisor, Affiliation: Bindu Nanduri, Department of Basic Sciences, College of Veterinary Medicine
Project Category: Biological Sciences and Engineering
Co-Author(s): Mary F. Nakamya, Moses B. Ayoola, Leslie A. Shack
REU/Research Program: R25 SRE Bridges to Baccalaureate

Identifying the intersection between two-component regulatory systems and polyamine metabolism in *Streptococcus pneumoniae*

Streptococcus pneumoniae (Spn) is a Gram-positive facultative anaerobe which occupies the normal microbiota of the human nasopharynx and can cause invasive diseases such as meningitis, pneumococcal pneumonia, and septicemia. The primary defense of Spn against the host immune system is the production of a protective polysaccharide capsule (CPS). Previous studies have shown that impaired polyamine synthesis results in reduced CPS in pneumococci. Preliminary data indicates that two-component regulatory systems (TCRS) could be a part of the polyamine regulatory network. Working towards unraveling this complex network, the purpose of this study is to characterize the impact of the deletion of two-component regulatory systems on CPS in *S. pneumoniae*. Total CPS was isolated from wild type and viable Δ TCRS TIGR4 and D39 and quantified by immunoblots using serotype specific antibodies. The results of the preliminary immunoblot assays (with two out of a total eleven viable Δ TCRS in TIGR4) did not show any impact on CPS. Evaluation of the rest of Δ TCRS is ongoing. We will also evaluate the impact of impaired TCRS on polyamine synthesis and transport gene expression. Upon completion of this project we expect to determine the link between polyamines and TCRS, if any. Project findings will contribute towards the understanding of the molecular mechanisms of capsule by polyamines, which is a novel mechanism that can be targeted for developing novel therapeutics for controlling this human pathogen.

Name: Khiara Lee Major: Biological Sciences Home University: Tougaloo College Faculty Advisor, Affiliation: Dr. Todd Mlsna, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Naba Krishna Das, Chanaka Navarathna, Charles U. Pittman, Jr REU/Research Program: INFEWS

Removal of Molybdenum from Contaminated Water using Douglas fir biochar/iron oxide composites

Molybdenum (Mo) is a naturally occurring trace element that is present in drinking water. It is most commonly found in the molybdate form in well water and breast milk and used in medical image testing. Recently, the EPA deemed Mo as a potential contaminant as it leads to bodily complications like gout, hyperuricemia and even lung cancer. In this work we have assessed sorptive removal of Mo using Douglas fir biochar (BC) and its iron oxide analogues (MBC). Adsorption was studied as a function of pH, equilibrium time (5 min-24 hours), different initial Mo concentrations (2.5-1000 mg/L), different temperatures (5, 25 and 40 C°) and equilibrium method (batch sorption and fixed-bed column). Preliminary data suggest that MBC is a potential candidate for Mo sorption. Adsorbents and Mo-laden adsorbents were characterized by BET, PZC, SEM, TEM, EDS, XRD and XPS. The adsorption was sought to be governed primarily by chemisorption mechanisms driven by the surface iron hydroxyl groups of magnetite particles. **Keywords**: Molybdenum, adsorption, biochar, magnetite, XPS

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Name: Rebecca Manns Major: Biochemistry Home University: Edinboro University Faculty Advisor, Affiliation: Dr. Nicholas Fitzkee, Chemistry Project Category: Biological Sciences and Engineering Co-Author(s): Kayla D. McConnell, Olivia C. Williams, Emily R. Chappell, Nicholas C. Fitzkee REU/Research Program: REU - INFEWS

Thermodynamics of Protein Binding to Gold Nanoparticles Monitored by Synchronous Fluorescence Spectroscopy and Dynamic Light Scattering

The intrinsic properties of gold nanoparticles (AuNPs) allow for their application in drug delivery systems, biosensing, and catalysis. The function of AuNPs rely on interactions that occur on the nanoparticle surface and can be disrupted by undesired proteinnanoparticle binding. Recognizing how different proteins bind to AuNPs can lead to a better understanding of AuNP function in biological systems and how protein adsorption can alter that function. Our goal in this work is to examine protein adsorption on AuNPs and how that adsorption alters AuNP function. Data were collected using UV-Vis, dynamic light scattering (DLS), and fluorescence instrumentation. The data allowed us to measure protein binding on the nanoparticle surface and determine the binding affinity of each protein. Data were also collected using polarized resonance synchronous spectroscopy (PRS2); these measurements were then used to examine how protein binding contributes to scattering and absorbance. We know that nanoparticles scatter light in the wavelength region of 500 to 600 nm, and the amount of light that they scatter can be directly related to their size. As the concentration of protein is increased in the solution with a constant nanoparticle concentration, the scatting cross section increased until it reached a maximum. The maximum corresponded to the binding curve created by the UV-Vis and the change in hydrodynamic radius measured by the DLS. This work reveals the principles behind protein-AuNP interactions, and it demonstrates how protein adsorption can alter the function of AuNPs.

71 Name: Sarah McClain Major: Biological Engineering Faculty Advisor, Affiliation: Dr. Xin Cui, Chemistry Project Category: Physical Sciences and Engineering

Development of New Ruthenium(II) Complexes with Facial K3 Tridented Ligands

Ruthenium catalysts have become a vibrant direction in organometallic chemistry for their selective transformations, the study of C-H functionalization, and their use as possible anti-cancer drug candidates. I have been synthesizing the ruthenium catalyst through a three-step process. The first step is to synthesize a new type of N,N,N-tridented ligand. This is done by a tandem reaction of 2- chlorobenzo[d]oxazole and n-butyl lithium. The next step is the synthesis of the ruthenium complex with and electron deficient R ring ligand. Subsequently, we create a κ^3 -ruthenium complex through metalation of the new ligand with the with electron poor arene-ruthenium complexes. With ruthenium being a relatively cost-effective precious metal species, this new ruthenium catalyst will be applied for catalytic C-H activation reactions, as well as being promising candidates for anti-cancer screening.

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Name: David Mees Major: Biological Sciences Faculty Advisor, Affiliation: Dennis Smith, Jr., Chemistry Project Category: Arts and Humanities Co-Author(s): Ketki E. Shelar, Charles U. Pittman, Dennis W. Smith, Jr.

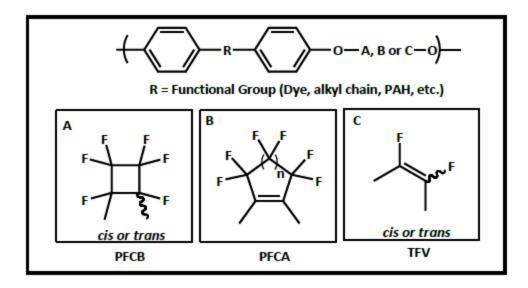
PFCB aromatic ether copolymers via Step growth polymerization and characterization

In our lab, we focus on semi-fluorinated polymers which includes fluoro-arylene vinylene ether (FAVE) polymers, perfluorocyclobutyl (PFCB), and perfluorocycloalkenyl (PFCA) aryl ether polymers.¹ The goal of my project is to perform step growth polymerization techniques to synthesize PFCB aryl ether homopolymers and copolymers with a variety of trifluorovinyl ethers (TFVE). Upon copolymerization, we will be able to analyze the variation in thermo-mechanical and chemical properties of the PFCB polymers. The synthesis of acenaphthylene diol-monomer occurs via double nucleophilic addition of *in-situ* generated Grignard phenyl TFVE-Br to acenapthenequinone. Obtained acenaphthylene diol-monomer undergoes deoxy-aromatization and oxidative ring cleavage in presence of TiCl₄ to give two monomers in optimum yield.² We aim to characterize these compounds by ¹H-NMR, ¹³C-NMR, ¹⁹F-NMR, DSC, TGA, GPC, HRMS, HPLC, FT-IR, SEM/TEM, EDX, AFM, rheology studies, M.P. and XRD (of monomers). Additionally, we are going to form films of the synthesized PFCB polymers.

The main goal behind my research project is to learn different reaction set-ups for organic synthesis and polymerization, to understand reaction mechanisms along with the reaction monitoring, and purification techniques.

References:

- 1. "Handbook of Fluoropolymer Science and Technology", Smith, Jr., D. W.; Iacono, S.; Iyer, S. Eds., John Wiley & Sons, **2014**.
- Farajidizaji, B.; Shelar, K. E.; Narayanan, G.; Mukeba, K. M.; Donnadieu, B.; Pittman, Jr., C. U.; Sygula, A.; Smith, Jr., D. W. Acenaphthylene Derived Perfluorocyclobutyl (PFCB) Aromatic Ether Polymers. *J. Polym. Sci., Part A: Polym. Chem.* 2019, *57*, 1270– 1274. DOI: 10.1002/pola.29388.



Name: Blaklie Mitchell Major: Biological Sciences Faculty Advisor, Affiliation: Dr. Mark Welch, Biological Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Jen Moss

Forensic Analysis of Iguana iguana in Cayman Islands Provides Warning of Invasion on Little Cayman

Iguana iguana, the Green Iguana, was originally native to Central and South America; however, due to trafficking, this species has been introduced to multiple islands within the Caribbean and Pacific as well as certain regions of North America. In much of this range, they have proven to be extremely invasive, and their invasion on some islands may pose a threat to other native iguana species, including the Grand Cayman Blue Iguana, Cyclura lewisi, and the Sister Islands Rock Iguana, Cyclura nubila caymanensis. The impact of the invasive Green Iguana on these natives has yet to be quantified. There are concerns that this species will compete for resources and that hybridization between the native and invasive species could further threaten endemic populations. Since hybridization can lead to a gradual form of genomic extinction, C. lewisi and C. nubila caymanensis could be lost even after other anthropogenic disturbances are remedied. My goal was to assess whether an invasive Green Iguana colony has been established on the island of Little Cayman, which hosts the critically endangered rock iguana species Cyclura nubila caymanensis. Using molecular markers, including nuclear microsatellites and mtDNA sequence data, the sibship and parentage of 14 Green Iguana hatchlings and 6 hybrid hatchlings recently found on Little Cayman were evaluated. Due to a lack of genetic variation in the molecular markers investigated, results were largely inconclusive. However, results from microsatellite genotyping suggested that a single individual did not dam both the Green Iguana and hybrid hatchlings. This finding demonstrates that this invasive species may have successfully colonized the island. Further characterization of this ongoing invasion will require the development of additional molecular markers that effectively capture adequate levels of genetic variability.

Name: Olivia Murtagh
 Major: Chemistry
 Faculty Advisor, Affiliation: Dr. Robert Phillips, Department of Chemistry, University of Georgia
 Project Category: Physical Sciences and Engineering
 Co-Author(s): Tung Dinh
 REU/Research program: Summer Undergraduate Research Opportunities at the University of Georgia

Crystallization Methods of Horse Liver Alcohol Dehydrogenase

Crystallization is an important process in determining the structure and mechanism of biological macromolecules, such as enzymes. However, crystallization is often a difficult and time consuming process, and results are not easily reproducible. A solution containing the macromolecule relies on several different variables, such as pH, temperature, concentration, and overall stability of the macromolecule, and must reach a supersaturated state in order to grow crystals. There are also numerous methods of crystallization, such as dialysis, vapor diffusion, and microcap dialysis. This research serves to demonstrate various crystallization procedures and techniques in the crystallization of horse liver alcohol dehydrogenase (HLADH) bound to a substrate and coenzyme. HLADH is a useful biocatalyst as it metabolizes primary and secondary alcohols to generate useful metabolites such as ketones and aldehydes. HLADH has a catalytic zinc site which reduces its coenzyme NAD+ to NADH using a hydride from an alcohol substrate. Five different crystallization methods with varying conditions were tested on purified HLADH, and two methods were proven to be successful in growing crystals. Previous experiments have obtained high resolution crystal structures of the apo-form of HLADH, but thus far it has been very difficult to grow useful crystal structures of the enzyme-substrate-coenzyme complex. Using x-ray diffraction, these crystallized enzymes containing both its substrate and cofactor will be analyzed to potentially provide more information on its specific mechanism and provide a more detailed structure.

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Name: Jacob Myers Major: Psychology Faculty Advisor, Affiliation: Danielle K. Nadorff, Ph.D., Psychology Project Category: Social Sciences REU/Research Program: NIH R25 Bridges to Baccalaureate

Custodial Grandparent Influence on Substance Use and Depressive Symptoms in a Nationwide Adolescent Sample.

Parents and caregivers play a vital role in their children's decisions to engage in substance abuse (Griffin et al., 2000). Previous studies have shown that custodial grandchildren (children raised by their grandparents) have a higher risk of developmental issues and mental health problems (Pruchno, 1999). This study evaluated whether children raised by custodial grandparents are at a higher risk of substance use than those in conventional parent-headed homes and multiple generational households (households that have at least one parent and one grandparent). Measures included reports of the primary caregivers of each child, the Kidscreen questionnaire (a health-related quality of life questionnaire for ages 8 – 18 years), and the frequency of tobacco and alcohol use as well as binge drinking frequency. Data was taken from the Health Behavior in School-Aged Children (HBSC) 2009-2010 dataset, which is a nationwide sample of 12,642 children ranging from 5th grade to 10th grade. Analyses of variance (ANOVAs) were run to examine the effect of caregiver type on depressive symptoms and substance abuse. Our results indicated that there were significant group differences in the rates of tobacco use (F(2,11535) = 11.259, p = .000), drinking alcohol (F(2, 11509) = 4.476, p = .011) and binge drinking (F(2, 11518) = 10.275, p = .000). Specifically, in each instance, children raised by grandparents were engaging in the highest rates of substance abuse. There were no significant differences in mental health scores by type of caregiver. Implications, limitations, and future directions will be discussed.

Name: Tymesha Nabors Home University: Alcorn State University Faculty Advisor, Affiliation: Dr. Deb Mlsna, Chemistry Project Category: Biological Sciences and Engineering REU/Research Program: REU

Analysis of effect of carbohydrates on the growth of Macrophomina Phaseolina

Macrophomina belongs to the Botryosphaeriaceae family of fungi and many members of this family are parasitic to plants. There are two species in this genus including Macrophomina limbalis and Macrophomina phaseolina. Macrophomina phaseoling is a pathogen that causes damping off, seedling blight, collar rot, stem rot, charcoal rot, basal stem rot, and root rot on agricultural crops such as soybean, sweet potatoes, and corn. *M. phaseolina* causes significant economic impact because it affects over 500 plant species with billions of dollars lost annually to this pathogen. After initial infections occur, the fibrovascular system of the plant roots and basal internodes of its host can be invaded reducing crop yields. This prevents proper nutrients and water transport throughout the plant. Results of infection can range from limited with small necrotic areas on plants, to plant death, depending upon plant stress during the M. phaseolina infection cycle. Cultural morphology of the pathogen includes black color and obvious production of visible but tiny microsclerotia. Germination of the microsclerotia happens all through the developing season when temperatures are in the range of 28°C and 37°C with the latter being more optimal for the pathogen and greater plant stress. Conducting biochemical or chemical studies (eg. Microbial Volatile Organic Chemicals-MVOCs) with fungi such as M. phaseolina require optimized growing conditions. Preliminary studies were conducted to develop standard protocols that were used throughout our experiments. This preliminary study was designed to evaluate the effects of select carbohydrates on fungal growth and timing (temporal) for optimized MVOC extraction protocols. The carbohydrates involved are glucose, fructose, galactose, sucrose, and maltose within a standard basal medium at 37°C and incubation period. Data collected and analyzed for this physiological study included radial growth of *M. phaseolina*, basal medium carbohydrate treated Petri plates and MVOC data for comparisons. We analyze the MVOC's using head space solid phase microextraction and GC-MS. All analyzed fungal growth and MVOC data will be reported and discussed.

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Name: Summer Nash Major: Chemistry Home University: Mississippi College Faculty Advisor, Affiliation: Dennis W. Smith, Jr., Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Eugene B. Caldona, David O. Wipf, and Dennis W. Smith, Jr. REU/Research Program: REU

Fluoroalkylsilane-modified polystyrene surface with superhydrophobicity and superoleophobicity

Surfaces that repel low-surface-tension liquids are of great interest owing to their practical importance and many technological applications. However, achieving the desirable liquid repellency is difficult as the surface must possess a low surface energy and an unusual roughness hierarchy that has re-entrant topographical feature in micron and sub-micron scales. This puts limits the types of substrates available and thus limits their applications. Many are prepared on nonmetallic surfaces, while common engineering metallic materials such as stainless steel (SS), are more industrially significant and practical. Hence, the fabrication of such surfaces remains a challenge. In this work, we report a simple architecting approach to fabricate a superhydrophobic/superoleophobic coating on a SS surface by drop-cast and dipping methods using precipitated polystyrene (PS), hydroxylated PS microbeads, and fluoroalkylsilane. Results showed that the prepared coating exhibited strong repellency towards water, highly concentrated strong acids, strong bases, salt solutions, hydrazine, ethylene glycol, and oil. The coating also displayed good thermal stability, a self-cleaning property, and stable static contact angles for water and oil even after a mechanical load was applied to it. All these advantages make the coating a promising material for oil/water proofing, corrosion protection, and oil sensing applications.

Name: Phuoc Nguyen Major: Electrical Engineering Faculty Advisor, Affiliation: John E. Ball, Electrical and Computer Engineering Project Category: Biological Sciences and Engineering Co-Author(s): Harish Chander, Ethan M. Stewart, David Saucier, Tony Luczak, Adam C. Knight, Brian K. Smith, Reuben F. Burch V, R. K. Prabhu

The Use of Soft-Robotic Stretch Sensors in Detecting Ankle Joint Kinematics during Unexpected and Expected Slip-Trip **Perturbations: A Pilot Study**

Soft robotic sensors (SRS) are flexible sensors that produce an output that changes when deformed. The unique nature of the SRS allows them to be mounted on a structure like the human body to locate and analyze movement. In this experiment, StretchSense SRS are specifically used to detect abnormal foot-ankle movements to prevent fall injuries. These unstable movements include unexpected slipping (US), unexpected tripping (UT), expected slipping (ES) and expected tripping (ET), which were tested on ten participants (five male and five female). Each participant, with two SRS mounted on each ankle, was asked to stand on a treadmill controlled by the researchers while their ankle movements, dorsiflexion (DF) and plantar flexion (PF), were recorded when the treadmill was activated. 3D motion capture data was also collected during these trials. A model was created utilizing the SRS data and motion capture data to determine the viability of SRS as a means for detecting trip and slip occurrences.

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Name: Ashleigh Nicaise Major: Biological Engineering Faculty Advisor, Affiliation: Barbara Kaplan, Center for Environmental Health Sciences, Department of Basic Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Evangel Kummari

Optimization of a PrimeFlow RNA Expression Assay to Evaluate Effects of the Environmental Contaminant, TCDD

The environmental contaminant 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) is known to bind to aryl hydrocarbon receptor (AhR), a transcription factor that induces gene expression, such as cytochrome P4501a1 (Cyp1a1). Upregulation of Cyp1a1 is a hallmark of TCDD exposure and indicates activation of AhR. Previous data from our laboratory showed TCDD upregulated the cell surface protein Fas ligand (FasL) on B cells. The purpose of this study was to optimize an assay in which TCDD's effects on AhR activation and FasL upregulation were evaluated simultaneously. This study includes three experiments using mouse splenocytes treated with TCDD or vehicle, and cell counts and target gene amounts were varied. QPCR was used as a positive control to show TCDD increased Cyp1a1 gene expression. The experiment using lower cell counts without increasing target genes and the one using higher cell counts with increasing target genes both showed the desired upregulation of Cyp1a1 and FasL, but use of higher cell counts without increasing target genes did not. These results demonstrate that the manufacturer's suggested target gene amount shows Cyp1a1 expression consistent with the QPCR positive control, and if cell counts are increased, the target genes need adjustment accordingly. This assay will allow accurate definition of the effects of TCDD.

Project funded by NIH R15 027650

Name: Kaitlyn Odom Major: Microbiology Faculty Advisor, Affiliation: Dr. Matt Ross, Basic Science Project Category: Biological Sciences and Engineering Co-Author(s): Abdolsmad Borazjani

Inhibition of Thromboxane A Synthase with Novel Small-Molecule Inhibitor WWL113

Thromboxane A2 (TxA2) is an inflammatory lipid hormone that is released by blood platelets and monocytes/macrophages. TxA2 is an unstable compound (half-life ~1 min) but it induces platelet aggregation and vasoconstriction of arteries. It can cause the aggregation of platelets within coronary and carotid arteries contributing to the development of heart attacks and strokes. Therefore, targeting the pathways that lead to thromboxane biosynthesis using pharmacological inhibitors might help to reduce these ischemic events. The goal of this study was to target the enzyme thromboxane A2 synthase (TXBAS), which is responsible for converting prostaglandin H2 (PGH2) to TxA2, with novel small-molecule inhibitors and determine whether its production could be blocked. TxA2 is non-enzymatically converted to a stable biologically inactive metabolite, TxB2, which can be measured by LC-MS/MS. Intact living human monocytic cells (THP-1 cell line) that express TXBAS were pretreated for 30 min with increasing concentrations of WWL113 or WWL229 (two small-molecule compounds we have shown to inactivate carboxylesterase 1, or CES1), then incubated with exogenous PGH2 and the levels of TxB2 was assessed. WWL113 but not WWL229 significantly decreased the production of TxB2. The concentration of WWL113 that inhibited 50% of the production of TxB2 (IC50) was ~0.1 uM. Recombinant human TBXAS protein was also overexpressed in COS-7 cells to verify that WWL113 was a bona fide inhibitor of this enzyme. These results suggested that WWL113, which had previously been reported to be a selective inhibitor of CES1 and to exhibit anti-inflammatory effects, can also target TBXAS. Thus, the benefiical effects of WWL113 observed in diet-induced obese mouse models might be related to its ability to block the production of proinflammatory TxA2. [supported by NIH 1R25GM123920-01A1, NIH R15GM128206-01]

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Name: Laura Olive Major: Chemistry Faculty Advisor, Affiliation: Dr. Charles Edwin Webster, Department of Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Dr. Eric Van Dornshuld

New insights into assessing the performance of DFT energetics on small oxygen/sulfur containing compounds

Using computational approaches, the structures and energetics of the skewed anticlinal geometries of X–O–O–Y, X–O–S–Y, and X–S–S–Y (where X,Y = H or Me), as well as the corresponding trigonal pyramidal isomers including X– O(O)–Y, X– S(O)–Y, X–O(S)–Y, and X–S(S)–Y were analyzed. Implementing post-SCF ab initio and 22 density functional methods in conjunction with 12 different correlation consistent basis sets of double-, triple-, and quadruple-zeta quality, the geometries were fully characterized. In general, the skewed anticlinal isomers are lower in energy than their trigonal pyramidal counterparts. However, two isomer pairs show qualitative relative electronic energy inconsistencies and exhibit significant basis set dependence.

Name: Taten Palmer Major: Landscape Architecture Faculty Advisor, Affiliation: Dr. Timothy Schauwecker, Department of Landscape Architecture Project Category: Biological Sciences and Engineering REU/Research Program: CALS URSP

Control of Chinese Privet as a Part of the Water Resources Management Plan for the Redbud-Catalpa Creek Watershed

As a part of the Undergraduate Research Scholars Program at Mississippi State University, we investigated the control of the highly invasive shrub Chinese privet (*Ligustrum sinense*) in the Catalpa Creek Watershed. The goal of our research is to provide management personnel with Standard Operating Procedures (SOPs) for invasive species management and to provide a cost-benefit information for each of the methods for decision-making purposes. Our research compared three published methods for control of chinese privet in the field: Cut Stump, Hack and Squirt, and Basal Bark Application methodologies. Eighteen cross-sections of the upper reaches of Catalpa Creek, all located on the HH Leveck Research Farm (South Farm), were sampled for Chinese privet cover in 2017. Chinese privet was a dominant plant species on the banks of Catalpa Creek. Using this data as a starting point, a privet treatment method was randomly assigned to each of 18 stream cross sections to implement the methods. The Cut Stump method was implemented by cutting through the circumference of the privet 12" or below on the trunk and then treating with herbicide. The Hack and Squirt method required a machete or sharp tool to cut around the circumference of the privet 12" or below on the trunk and then immediate application of herbicide on the cut area. The final method that we implemented was the Basal Bark method, with an application of triclopyr herbicide with an oil-based surfactant to the bottom 12" of the trunk. Based on reduction of privet cover and ease of application, the Cut Stump method would be the recommended option for reducing privet cover.

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Name: Aubrey Parrish Home Institution: Florida State University Faculty Advisor, Affiliation: Holli Seitz, Communication Project Category: Social Sciences

Effects of Body-Positive Marketing on Brand Success

Background: The body-positive movement has increased in popularity since its inception in the early 2000s when companies began to showcase a wide variety of body types in their advertisements, providing a sharp contrast to the unrealistically thin models that were typically portrayed in the media. It is important to determine if promoting the body-positive movement is an effective strategy for increasing brand sales and improving body satisfaction of the consumers. We predict that customers will be more willing to purchase brands that showcase diverse body types than those that showcase only one body type. We also expect that customers who are exposed to body-positive media images will have higher levels of body satisfaction than those who are exposed to other media images. Finally, we will investigate whether the effect of images on purchasing intention is mediated by body satisfaction and/or attitude toward the brand. Method: We will conduct an online survey-based between-subjects experiment with a 2 (Body positive orientation: High

Method: We will conduct an online survey-based between-subjects experiment with a 2 (Body positive orientation: High or low) x 2 (Brand) x 2 (Presence of model in image) factorial design. We will randomly assign 400 women between the ages of 18 and 30 to one of eight experimental groups. Each group will be exposed to ten Instagram images from a lingerie or swimwear brand with either high (Aerie, Savage X Fenty) or low (Victoria's Secret, Frankie's Bikinis) levels of body positivity. The groups will either be exposed to images of models or of just the clothing items. Following their exposure to the images, the women will be asked to rate their willingness to purchase from the brand, their levels of body satisfaction, and their attitude toward the brand.

Results: Preliminary results will be presented.

Name: Richard Perkins Major: Mechanical Engineering Faculty Advisor, Affiliation: Yucheng Liu, Mechanical Engineering Project Category: Physical Sciences and Engineering Co-Author(s): Wenhua Yang, Dr. Lei Chen, Caleb Yenusah

Finite Element Analysis of the Effect of Porosity on the Plasticity and Damage Behavior of Mg AZ31 and Al 6061 T651 Alloys

Porosity has been known to have a profound effect on a material's mechanical properties, often weakening the material. Highly porous metallic materials prove troublesome for supporting a load-based structure due to the voids that are present throughout the microstructure of the material. In this study, the previously developed ISV damage plasticity model is used to investigate the effect of the porosity on aluminum alloy 6061-T651 and magnesium alloy AZ31 through finite element analysis (FEA). It is determined that porosity has a profound impact on the strength of the aluminum alloy and much lesser effect on the magnesium alloy. Porosity is also shown to affect other properties of the materials, such as the hardness and pore growth.

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Name: Trey Pittman Major: Biochemistry Home University: Mississippi College Faculty Advisor, Affiliation: Keith Hollis, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Sriloy Dey REU/Research Program: Hollis Research Group

Synthesis and Characterization of Novel Symmetric CCC-NHC Pincer Platinum Complexes

During our research, novel CCC-NHC pincer platinum complexes have been synthesized. These complexes possess special photo-physical properties which are utilized in organic light emitting diodes (OLEDs). The photo stability of these pincer complexes in open atmosphere is greater than the commercially available alternatives. The complexes are also more energetically efficient compared to available LED and incandescent alternatives. The novel CCC-NHC pincer complexes are obtained through a 3 step process: (1) a copper coupling synthesis of differing ligand backbones (2) alkylation reaction to synthesize symmetrical ligand arms (3) metalation and transmetalation of ligand precursors to synthesize CCC-NHC pincer platinum complexes. These complexes emit light under long-wave UV radiation and are synthesized for potential use in OLEDs. Our research is focused on using different precursors to affect the emitted light. When altering of the pincer backbone and the arms of the ligand we can observe differences in the emitted light. Learning more about the CCC-NHC pincer complex properties could lead to new innovations in the organic light emitting device industry.

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Name: Allison Ratliff Major: Biochemistry Faculty Advisor, Affiliation: Dr. Gary Ervin, Biological Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Adrian Lazaro-Lobo

Variation in Germination of Baccharis halimifolia from native, expansive, and invasive populations

Introduction: Germination is one of the most critical stages of a plant's life, so rapid germination would be beneficial for expansion and invasion. The possible variation in germination from different distributional ranges of Baccharis halimifolia, a highly invasive dioecious shrub, was evaluated. This variation could happen due to the Evolution of Increased Competitive Ability hypothesis. Light and Salinity could affect this as well. Materials and Methods:

Seeds were collected from two populations in each distributional range: native (United States Gulf Coast), expansive (interior of the United States) and invasive (Spain). A total of 2,467 seeds were germinated in a growth chamber and treated to a regime of 16h of light and a day/night temperature of 24/18°C. They were subjected to three levels of salinity consisting of 0 (control), 10 (low salinity), and 20 (high salinity) g NaCl/L and two levels of luminosity (light and shade). Results and Discussions:

The expansive range yielded the best results in both light and dark environments when treated with low levels of salinity, which could suggest that there has been selection for individuals with faster germination. However, in stronger salinity the native range produced the best results which could be due to maternal plants being subjected to higher salinity in soils of coastal areas. The invasive range usually had the lowest germination rate, which went against the original hypothesis. This could be explained by the founder effect.

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Name: Claudia Reid Major: Biochemistry Faculty Advisor, Affiliation: Dr. Todd Mlsna, Department of Chemistry Project Category: Biological Sciences and Engineering Co-Author(s): Amali Herath, Charles U. Pittman, Jr

Polyaniline modified biochar to remove nitrate from aqueous systems

Helpful characteristics of biochar include the ability to increase soil fertility in dry environments and the ability to absorb and preserve nutrients in soil. Both aspects of use are available for low cost of production. The adoption of these uses of biochar have increased popularity of this product recently. Biochar has been proven to help improve the environment by decreasing the number of pollutants through its adsorptive properties. Douglas Fir biochar (DFBC) synthesized by fast pyrolysis method was modified with aniline to alter some of its properties. The modified biochar was then characterized by point of zero charge, BET surface area, thermogravimetric analysis and Scanning electron microscopy. Nitrates can potentially have a negative effect on the environment when an excess amount is present. The significance of this experiment is to optimize the parameters for nitrate absorption by aniline modified biochar. The adsorption studies of nitrate were conducted using Liquid Chromatography with a UV detector at 210 nm for DFBC and PANI-BC. The kinetic studies were carried out at pH 6 with three different concentrations of nitrate. Batch sorption studies for nitrate were performed by varying the concentration of nitrate at three different temperatures ranging from 10- 45 °C, and the data was fitted to different adsorption isotherm models for both types of biochar. PANI-BC exhibited a higher adsorption capacity for nitrate compared to the pristine DFBC.

Keywords: DFBC, PANI-BC, nitrate

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Name: Parker Reneau

Major: Chemical Engineering Home University: Louisiana Tech University Faculty Advisor, Affiliation: Todd Mlsna, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Sharifur Rahman REU/Research Program: Computational Biology REU

Reclamation of Phosphate Using Biochar Fe/Mg-LDH Composites

Phosphate serves an integral role in the environment and its stability. From soil nutrient levels to water treatment, phosphate ions need to be harvested and used efficiently. Inorganic phosphorus is a main nutrient needed for plants and must be introduced back into soil. Layered double hydroxides (LDH) precipitated onto biochar, a byproduct of biomass pyrolysis, makes invaluable sorbents. LDH can intercalate phosphate ions between the hydroxide layers. Biochar has a high surface area to volume ratio due to its porous exterior. This project aims to optimize phosphate ion adsorption via kinetic and thermodynamic studies, comparing the adsorption of LDH to LDH modified biochar, and characterizing the surface of the biochar. LDH was synthesized from iron (III) chloride and magnesium chloride with pH adjustments using

the Hanna pH/ORP Meter. The biochar and LDH were ground to a size of 125-300 µm. Sorption of LDH and LDH modified biochar were tested concurrently at varied pH. Using the UV-Vis spectrometer, this test delivered the concentration of phosphate remaining after adsorption via shaking in an industrial shaker. A kinetic study was run over 20 times with intervals ranging from 30 seconds to 24 hours to determine the time of maximum adsorption for both the LDH and the modified biochar. A thermodynamic study was conducted at three temperatures and varying concentrations to determine what temperature phosphate adsorption favored. Using the Brunauer, Emmett, and Teller surface area analyzer (BET) and X-ray photoelectron spectroscopy (XPS), the surface area and functional groups of the biochar-LDH composites were determined. These studies present data for the economic, environmentally friendly advances in phosphate reclamation efforts.

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Name: Matthew Rowland

Major: Agricultural Engineering Technology & Business Faculty Advisor, Affiliation: John Linhoss, Agricultural and Biological Engineering Project Category: Biological Sciences and Engineering

Evaporative rate of poultry litter at varying biochar inclusion rates

Elevated litter moisture in poultry houses can negatively impact bird welfare and performance through increased ammonia volatilization, poor footpad scores, and increased pathogenic microbial populations. Biochar (BC) as a litter amendment has been shown to increase litter water holding capacity, but little research has been conducted to evaluate how BC affects the evaporative rate of water from litter. This study examines water evaporation rates for pine shavings at varying BC inclusion rates. Evaporative rates were measured at air velocities of 0, 1.3, 2.5, and 3.8 m/s using four custom wind tunnels over a 101 hr period. BC inclusion rates were 0, 10, 20, and 100% by weight and initial litter samples were wetted to a starting moisture content of 25 or 50%. Mean moisture content for the 100% BC inclusion rates was significantly lower than the other inclusion rates (P<0.001) for both starting moisture contents, indicating a higher rate of evaporation. There was no significant difference in mean moisture content for the remaining BC inclusion rates. Litter samples in the 2.5 m/s wind speed treatment had a significantly lower mean moisture content than the other treatments (P<0.001). Overall, BC does not seem to negatively affect litter evaporative rates and BC inclusion rates of 10% and 20% by weight were as effective as fresh pine shavings at releasing water.

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Name: Melinda Rydberg
Major: Biochemistry
Home University: The College of St. Scholastica
Faculty Advisor, Affiliation: Bindu Nanduri, Department of Basic Sciences, College of Veterinary Medicine
Project Category: Biological Sciences and Engineering
Co-Author(s): Mary F Nakamya, Moses B. Ayoola, Leslie A. Shack
REU/Research Program: Computational Biology REU

Is a putative ornithine decarboxylase gene necessary for Streptococcus pneumoniae virulence?

The gram-positive human pathogen, *Streptococcus pneumoniae*, colonizes the nasopharynx and can lead to severe infections in the immunocompromised including pneumonia, septicemia, and meningitis. Existing therapeutic methods such as vaccines target only about 20% of pneumococcal serotypes, and antibiotic resistance is an increasing threat. Previous work from the Nanduri lab demonstrated the importance of polyamine metabolism—both biosynthesis and transport—and how it affects *S. pneumoniae* virulence. Polyamines such as putrescine, spermidine and cadaverine, are small polycationic hydrocarbon chains, that play a significant role in a multitude of cell processes due to their ability to bind to negatively charged molecules including DNA and RNA. It is understood that regulating the biosynthesis of particular polyamines can affect the expression of a capsule, an important virulence factor that is the target of current vaccines. Therefore, regulating the production of a capsule by altering polyamine synthesis could potentially contribute to the design of novel therapeutics. However, annotation of polyamine metabolism in pneumococcal genomes is incomplete. The focus of this study is to determine the role of a putative ornithine decarboxylase, ΔSP_0166, that catalyzes the

synthesis of putrescine, on pneumococcal virulence. Working towards this, we employed a markerless mutagenesis strategy that introduces a stop codon into ΔSP_0166 , disrupting the translation of this gene and ultimately polyamine biosynthesis. Disruption of this pathway is predicted to affect the production of capsule which will reduce pneumococcal survival in vivo. Markerless mutagenesis is accomplished through a series of PCR reactions to generate a product with a stop codon in ΔSP_0166 that is cloned into a plasmid used to transform *S. pneumoniae* to generate a mutant strain by homologous recombination. Further characterization of ΔSP_0166 will be carried out to verify its effect on capsule production.

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Name: Caroline Schaade

Major: Mechanical Engineering Faculty Advisor, Affiliation: Dr. Matthew Priddy, Mechanical Engineering Project Category: Biological Sciences and Engineering

TI-64 Porous Hip Implants to Reduce Stress Shielding

A common issue in current clinical orthopedic implants is that the implant stiffness often leads to device failure, causing patients to endure corrective surgeries. Implant stiffness causes stress shielding, which is a decrease in physiological loading of the bone and can lead to mechanical loosening of the prosthetic implant and osteolysis. A possible solution is introducing porosity into the device, which will reduce the overall stiffness of the device. However, in order to accomplish this, the geometry of the lattice structure affects the strength and stiffness of the hip implants. For example, depending on the orientation of layers of pore fibers, the greater the impact on pore size and the stiffer the implant becomes. In this study, a porous TI-64 hip implant was designed through additive manufacturing (AM), which allows for the implementation of customized shapes and geometry. Through a literature review performed this semester, it has been determined that the implant should be designed to withstand compression forces from two to eight times the body weight while closely matching the stiffness of native bone. Conducting this research will allow for the creation of spatiotemporal models of the relationship between porosity and stiffness and ultimately improve the implant industry.

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Name: Minjae Seo Major: Computer Engineering Faculty Advisor, Affiliation: John E. Ball, Department of Electrical and Computer Engineering Project Category: Physical Sciences and Engineering Co-Author(s): Thomas Benson

Pulse Rate Anklet

As the sporting goods business develops, it needs to be comfortable to help athletes' exercise. Heart rate is one of the vitals measured to make sure that athletes stay safe while consistently driving themselves to meet their physical goals. Current heart rate monitors take measurements from either a strap around the chest or a watch at the wrist. The devices at these locations can be uncomfortable, and the NBA and NCAAF regulation prohibit the use of any wrist attachments. The goal of the Pulse Rate Anklet is to measure the heart rate at the ankle with a device that is comfortable and does not restrict an athlete's performance. This collected data is crucial to inform the coach of the athletes' health status. The size should be small enough to fit on a wide range of body types and to not hinder an athlete's performance. The Pulse Rate Anklet should be accurate so that coaches and athletes can be confident in the measurements from the device. The five-hour battery life is important because the device needs to last for the entire workout or game. The Pulse Rate Anklet will use a photo plethysmography (PPG) sensor to measure the heart rate. PPG sensors work by shining an LED onto the skin and measuring the changing amount of light reflected into a photodiode. An accelerometer will be used to keep the heart rate measurement accurate while the athlete is in motion. The cypress microcontroller was picked because it can store the heart rate data in flash memory, and it is small enough to meet device size requirements. All of the heart rate data is shared to the viewing station and will be shown on a graph displaying a live readout of the user's heart rate.

Name: Katelyn Sette
 Major: Biochemistry
 Faculty Advisor, Affiliation: Russell Carr, Center for Environmental Health Sciences, Department of Basic Sciences
 Project Category: Biological Sciences and Engineering
 Co-Author(s): Juliet E. Ryan, Navatha Alugubelly, Shirley X. Guo-Ross

The Mechanistic Basis for the Species Difference in the Toxicity of the Insecticide Chlorpyrifos between Juvenile Rats and Mice

One of the most common classes of agricultural insecticides is the organophosphorus pesticides (OPs) which exert their toxicity through inhibition of brain cholinesterase (ChE) leading to hyperactivity in the nervous system. Currently, there is a growing concern that exposure to low levels of OPs induces negative impacts in developing children. The chemical most commonly linked to these issues is chlorpyrifos (CPF). Recently, we observed that there was a difference in susceptibility to CPF between juvenile mice and rat. The basis for this difference is unknown, but we hypothesized that it could be due to differences in detoxification mechanisms. In the blood, certain enzymes act as alternative binding sites which removes the chemical from circulation. To investigate this, 10-day old rats and mice were exposed daily for 7 days to corn oil or a range of dosages of CPF via oral gavage. Pups were sacrificed on day 16 and brain and blood were collected. The effects of CPF on juvenile rat brain ChE activity was greater than that observed in juvenile mice. In the blood, there were higher carboxyl esterase and ChE activities in the juvenile mice than in the juvenile rats. The level of inhibition of these enzymes was also found to be higher in rats than in mice following oral exposure to the same dosages of CPF. The higher level of inhibition in rats indicates that the protective function of these enzymes is overwhelmed faster in rats than in mice. This allowed more compound to reach the brain and inhibit ChE resulting in higher toxicity in rats as compared to mice.

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Name: Abigail Sharp Home University: The George Washington University Faculty Advisor, Affiliation: Dr. Todd MInsa, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Hasara Samaraweera REU/Research Program: REU - INFEWS

Phosphate Removal by Various Lignite Adsorbents

Low quality lignite coal has been engineered into coal char - a green adsorbent for polluted water remediation. Since the lignite material is not fully carbonized, it can be modified to adsorb phosphate fertilizers from agriculture wastewater. To prepare the coal char, the lignite is pyrolyzed after varied treatments in a muffle furnace under nitrogen. In this study, the lignite was prepared with three different treatment modifications including: lignite that was pyrolyzed with salt and base; lignite that was not pyrolyzed with salt and base added, and lignite char that was pyrolyzed with salt and base added. The efficiency of each lignite coal char was investigated in regard to contact time of the adsorbent with phosphate ranging from 5 minutes to 24 hours, pH levels between 2 to 12 and initial concentration of 100 ppm to 500 ppm of the phosphate solution. The goals of this study were to characterize the adsorbents, optimize the adsorption parameters and identify the best coal char material.

Name: Patrick Sheridan Major: Chemistry Faculty Advisor, Affiliation: Joseph Emerson, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): James Cope, Sean S. Stokes REU/Research program: 2019 Summer REU: Food, Energy, and Water Security

Investigating the Catalytic Potential of Copper Triflate and Copper Iodide

Copper based catalyzes present a green and cost-effective alternative to palladium and other transition metalbased processes. The literature has shown that both copper(I) and copper(II) compounds can be effective in replacing more toxic and expensive traditional metal catalysts in a variety of coupling reactions. One particular example is the Chan-Evans-Lam coupling reaction which uses copper(II) catalysts to couple boronic acids with amines and alcohols. While this reaction has reported moderate yields in the literature, current methods struggle to obtain more significant yields. In addition, copper(I) is being used to attempt a decarboxylative coupling reaction using copper(I) iodide to couple an alkenyl or alkynyl carboxylic acid to an aryl boronic acids instead of halides. Here, we report our current efforts to better understand these processes.

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Name: Jeffrey Shipman Major: Biological Sciences Home University: Fayetteville State University Faculty Advisor, Affiliation: Bindu Nanduri, College of Veterinary Medicine, Department of Basic Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Mary F Nakamya, Moses B. Ayoola, Leslie A. Shack **REU/Research Program:** Computational Biology REU

Role of nspC and galt2 genes in capsule biosynthesis in Streptococcus pneumoniae

Streptococcus pneumonia is a gram positive opportunistic bacterial pathogen that causes otitis media, septicemia, meningitis and pneumonia. This ability of S. Pneumoniae to cause disease is based on its virulence factors including capsule, which is the target for current pneumococcal vaccines. Polyamines are poly cationic hydrocarbons found in all living organisms and are necessary for regulation of various biological functions. Our previous results demonstrate that impaired polyamine biosynthesis results in reduced capsule in pneumococci, possibly due to impaired galactose catabolism. In this study using a markerless mutagenesis strategy, we will evaluate the impact of the deletion of nspC and galt2, genes from polyamine synthesis, and galactose metabolism pathways on capsule synthesis and virulence of S. pneumoniae TIGR4. After confirming the gene deletions by sequencing, we will characterize the growth, total capsule. We expect our results to confirm or refute our expectation that nspC and galt2 adversely affect capsule synthesis, there by resulting in reduced virulence of pneumococci.

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Name: Jacob Smith Major: Chemistry Faculty Advisor, Affiliation: Dr. Charles Webster, Department of Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Robert W. Lamb, T. K. Hollis

Reactivity and Relative Energies for CCC-Rh^I-NHC Pincer Complexes and the Reduction of Dinitrogen to Ammonia

The CCC-Rh¹ -NHC pincer complex is extremely nucleophilic due to the electron donation of the CCC ligand framework. Since the CCC-Rh¹-NHC complex has a center that is extremely electron dense, ligand-based reactions may be feasible due to strong back bonding into a coordinated ligand antibonding orbital. Multiple ligands, such as dioxygen, carbon dioxide, and carbonyl complexes, were used to test the general reactivity and stability of CCC-Rh¹ - NHC complexes using density

functional theory computations. One reaction of particular interest is the activation and reduction of dinitrogen (N_2) to ammonia.

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Name: Annie Snyder
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Project Category: Biological Sciences and Engineering

Adsorptive removal of aqueous arsenic (V) from contaminated water using Latin American bamboo biochar: a systematic study.

Bamboo biochar, an economic and sustainable material, originating from discarded culms of a native Latin American species (*Gudua chacoensis*), was evaluated for the sorptive removal of As(V) from water. Two biochars were compared; raw biochar (BC) which was produced using slow pyrolysis at 700 °C for 1 h, and its chemically co-precipitated iron-nano particle dispersed analogue (BC-Fe). The surface properties of the adsorbents were examined by SEM, PZC and BET. Fixed-bed column sorption was carried out at different pH's (5, 7 and 9), and breakthrough curves were used to describe its performance. The regeneration of the beds was evaluated by employing 1M solutions of ammonium sulfate, potassium hydroxide, and potassium phosphate. The effect of competing ions on As (V) adsorption onto BC and BC-Fe was tested in the presence of ten different ions (sulfate, phosphate, nitrate, chloride, acetate, dichromate, carbonate, fluoride, selenite, molybdate) at three different concentrations (0.01 mM, 0.1 mM, 1 mM). The adsorption capacity and the ability of BC and BC-Fe to provide water free of arsenic (V) was evaluated using a natural contaminated water from a domestic drinking faucet in Altamirano, near Buenos Ares, Argentina in both batch and fixed-bed column studies. As (V) quantification was done using ICP-MS instrument. This bamboo biochar can be considered as an environmentally friendly and cost-effective adsorbent candidate to provide arsenic (V) free water.

Keywords: bamboo, Latin America, As(V), breakthrough, competitive

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Name: Hailey Spillers Major: Biochemistry Faculty Advisor, Affiliation: Dr. Sorina C. Popescu, Department of Biochemistry, Molecular Biology, Entomology & Plant Pathology Project Category: Biological Sciences and Engineering Co-Author(s): Thualfequar Al-Mohanna, Setareh Nejat-van Warmerdam

Biochemical and functional characterization of plant thimet oligopeptidases in the context of the plant systemic acquired immunity

Plants defend themselves against pathogen infection by activating an immune response. One type of response effective against pathogens is the systemic acquired resistance (SAR). SAR is a 'whole-plant' resistance response analogous to the innate immune response of animals and humans. Previous research in our lab has demonstrated that two thimet oligopeptidases (TOP1 and TOP2) play a role in the plant immune response, modulate cellular redox homeostasis, and are critical components of the SAR. We determined that TOPs bind the phytohormone salicylic acid (SA), which inhibits peptidolytic activity. My project explores the predicted redox-mediated regulation of TOP1 and TOP2 and their role in the accumulation of salicylic acid (SA) in plants deficient in each or both TOPs. In the first project, we quantified the number of cysteine residues and disulfide bonds in TOPs.

TOP1 and TOP2 vary in the number of cysteine residues in their sequences, and we predict that they also vary in the number of intramolecular disulfide bridges. Cysteine has important structural, biological, and functional importance in proteins, and often, the presence or absence of disulfide bridges directly affects the protein's structure and function. LowpH and high-pH discontinuous systems were used to separate and quantify cysteine residues through gel electrophoresis. In the second project, we quantified free and total hydrolyzable SA in Arabidopsis plants deficient in the expression of TOP1, TOP2, or both genes. Elevated levels of total SA in Arabidopsis tissues indicates a response to the pathogenic attack and the onset of SAR. Through the quantification of available cytoplasmic, unconjugated SA, it is possible to determine the amplitude of the defense response in infected plants and the role of each TOP gene in SA synthesis and accumulation. High-performance liquid chromatography (HPLC) was used to quantify endogenous SA in various mutants of Arabidopsis, and statistical methods were used to analyze data.

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Name: Yashaswin Sridhar Major: Psychology Faculty Advisor, Affiliation: Dr. Michael R. Nadorff, Department of Arts and Sciences Project Category: Social Sciences Co-Author(s): Courtney J. Bolstad, B.S

Prevalence of Depression among Individuals Living with Animals

The Internet is filled with articles that list psychological benefits of owning pets, and anecdotal reports from pet owners also support that pets can have antidepressant effects. Of the total American population, 67% of households own pets, and 6.7% of adults suffer from depression, so a connection between pet ownership and depressive symptoms could impact millions of people. However, empirical research on the antidepressant benefits of pet ownership has shown mixed findings, and much of this research has notable limitations. The current study aimed to provide much needed fundamental research regarding the rates of depression among individuals who live with animals compared to those who do not. We analyzed data from the National Health and Nutrition Exam Survey collected between 2005 and 2006. The participants in this study included 3162 non-institutionalized, U.S. citizens, 18 years of age and over. Participants answered questions regarding the status of animals living in their house and completed a depression screening measure, the PHQ-9. The PHQ-9 places respondents into five severity categories based on their total score. A chi-square analysis was conducted to compare the rates of the various depression severities between participants who lived with animals and those who did not. The results revealed that the rates of depression were marginally higher across all five categories for individuals who were not living with animals, however, this difference was not significantly different. On the surface, it appears that individuals have similar rates of depression regardless of whether they live with pets or not. If pets do provide psychological benefits to their owners, interventions should be developed to leverage this effect as our results show many pet owners are impacted by depressive symptoms. Future research should attempt to replicate our findings by using additional large data sets that measures both depression and pet ownership status.

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Name: James Stevens

Major: Biochemistry

Faculty Advisor, Affiliation: George Popescu, Institute for Genomics, Biocomputing, and Biotechnology Project Category: Biological Sciences and Engineering

Identification of kinase gene families in seven plant species using a Random Forest classifier

Gene families are groups of genes of originating from a single ancestral gene, typically sharing similarities as well as conserved domains and structure. We have recently developed GeneFamilyRF, an integrative method that employs ortholog clustering, Hidden Markov Models, and motif identification through presently existing methods to measure factors that indicate familiar relationships among genes. We are using this method to study the evolution of kinase gene families (kinomes) of seven plant species. The Arabidopsis kinome is currently the only one to be fully characterized, featuring over 1000 genes. The families considered in our kinome analysis are Receptor-like Kinases(RLK), Cyclin-Dependent Kinases(CDKs), all families in the Mitogen-activated protein kinase cascade(MAPK, MAP2K, MAP3K, MAP4K), SnRKs, AGCs, NEKs, AURORAs, and SHAGGY-LIKE families. The most challenging kinase families in our experiments were RLKs and CDKs. We had to implement additional enhancements that have enabled the analysis of the Leucine-Rich Repeat Receptor-Like Kinase (LRR-RLK) and Cyclin-dependent Kinase (CDK) families. LRR-RLKs feature 2 motifs, the Leucine-Rich Repeat and the kinase domain, requiring multiple motif analysis, while CDKs require MEME with differential enrichment to find a motif not shared with other kinases. We are currently adding to GeneFamilyRF methods for multiple protein motifs and novel motif identification through MEME, allowing the analysis of families with multiple or less characterized motifs. Another dimension of work is to add divergence rate estimates to be used for classification of gene families.

Name: Katherine Strickert Major: Chemistry Home University: The College of Wooster Faculty Advisor, Affiliation: Nicholas C. Fitzkee, Department of Chemistry Project Category: Biological Sciences and Engineering Co-Author(s): Ryan B. Williams REU/Research Program: REU - INFEWS

Does Binding to a Nanoparticle Change a Protein's Structure?

Gold nanoparticles (AuNP) have become increasingly prevalent in medicine and biotechnology due to their applications in drug delivery and biosensing. In biological fluids, proteins will bind to the surface of the gold nanoparticles, forming a protein corona, which can interfere with the AuNP's intended function. Whether this binding process affects the secondary or tertiary structure, and thereby the function of the bound protein, is a current area of investigation. Hydrogen-deuterium exchange (HDX) is the process during which labile hydrogens are replaced by deuterium. This process occurs spontaneously for the amide protons in a protein when a deuterated solvent is present. This phenomenon is particularly useful when utilized in conjunction with NMR spectroscopy for analyzing protein structure, as buried hydrogens and hydrogens in secondary structure will be resistant to HDX. If proteins on AuNP surfaces have an altered structure, the HDX rates are expected to change. In this work, we are investigating a protein relevant to biofilm formation (the Amidase domain from S. epidermidis autolysin E, or Ami). Ami is known to bind other surfaces, and we are interested in how it behaves on an inert AuNP surfaces as a model for protein binding. We are measuring HDX rates for the free and surface-bound Ami protein using real time NMR spectroscopy. These rates can be compared to determine whether structural perturbation occur when this protein interacts with surfaces. This work will potentially lead to two scientific advances: First, it will inform scientists interested in using AuNPs in biomedical applications. Second, it will lead to a deeper understanding of how biofilm-relevant proteins interact with surfaces generally.

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Name: Emily Sykes Faculty Advisor, Affiliation: Dr. Carley Morrison, School of Human Sciences Project Category: Social Sciences Co-Author(s): Brice Fortinberry

Which Leadership Competencies are Teachable and Qualities that are Inherent?

Non-profit organizations are often strained for resources even though they make a considerable contribution to local communities. Nonprofits need volunteers to function effectively, but there is limited research on the competencies needed for volunteer leaders. There is even less literature on which of these competencies are teachable and which inherent. This study, using Delphi methodology, aimed to establish a set of teachable skills and inherent qualities that organizations can use to develop selection criteria and leadership programming for volunteer leaders. At the conclusion of three rounds of iteration, a list of 41 leadership related items were not only divided into two categories: teachable skills and inherent qualities but also rated on how important they are for volunteer leaders to possess.

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Name: Amber Travis Major: Biological Sciences/Microbiology Faculty Advisor, Affiliation: Dr. Thornton, Biological Sciences Project Category: Biological Sciences and Engineering

Classifying the Activity of SP1466 Protein in Streptococcus pneumoniae

Streptococcus pneumoniae (pneumococcus) is the leading cause of community-acquired pneumonia and otitis media. It commonly colonizes the upper respiratory tract of healthy individuals, but it can lead to diseases such as pneumonia, bacteremia, or meningitis, particularly in high risk populations such as infants, immunocompromised individuals, or the

elderly. Protein SP1466 is a putative hemolysin that is part of the core genome. SP1466 is a predicted hemolysin with homology to type III family of hemolysins. The majority of research done on type III hemolysins has been in bacteria including *Bacillus* and *Vibrio*. The purpose of this study is to identify the potential role of SP1466 in pneumococcal colonization/pathogenesis. We have utilized a gene deletion technique employing splicing by overlap extension PCR (SOEing PCR) to create an isogenic mutant lacking SP1466 in the TIGR4 strain of *S. pneumoniae*. This mutant possesses an erythromycin cassette in the place of the *sp1466* gene. We are also attempting to clone and express SP1466 using the pET21b *E. coli* expression vector. We have designed primers and successfully amplified the gene by PCR for restriction digestion and eventual ligation into pET21b. Once the protein is expressed, the cells will be exposed to epithelial cells, white blood cells, red blood cells, etc. to determine if SP1466 possesses cytotoxicity. Characterizing the function of SP1466 in *S. pneumoniae* will provide novel information about this potential virulence factor.

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Name: Joshua Waldbieser Major: Computer Science Home Institution: Mississippi College Faculty Advisor, Affiliation: George Popescu, Ph.D., IGBB, MSU Project Category: Biological Sciences and Engineering Co-Author(s): Tony Arick, Jared Cole, Corrinne Grover REU/Research Program: Computational Biology REU

Cross-Species Gene Annotation Using RNA-Seq Data

Genome annotation is a challenging task in eukaryotes, and a critical step in their functional analysis. Typically, annotations are generated using *ab initio* methods after genome assembly is completed, or improved using gene finder algorithms trained on existing gene models and gene expression information (mapped from RNASeq data). However, many challenges remain for species lacking genomic resources. Given the rapid expansion of genome sequence information in a few target genomes, the capacity to generate accurate genomic annotations in plants is growing significantly. To take advantage of the available genomic data, new algorithms, methods, and pipelines that build on existing genome information to annotate distant species are being developed. BRAKER2, one such pipeline, was designed to automate much of this process.

Here we proposed to determine the accuracy of BRAKER2 gene predictions on non-model organisms using the plethora of resources available for a model species. We assessed the accuracy of gene predictions as a function of species divergence. We chose several publicly available datasets from species at various evolutionary distances from our initial reference species (*Arabidopsis thaliana*) to use for testing. The sensitivity and precision of the gene models predicted by BRAKER2 using these datasets compared against the existing *A. thaliana* annotation were used as the measure of annotation accuracy. We determined a quantitative measure of species divergence using chloroplast phylogeny. After completing the experiment with A. thaliana, we repeated the process, but with reference to *Gossypium raimondii* and *Zea mays*.

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Name: Peyton Wall Major: Microbiology Faculty Advisor, Affiliation: Joseph Emerson, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): James Cope REU/Research Program: MSU Chemistry Summer Research

Synthesis and Preliminary Catalytic Trials associated with a Copper(II) Complexes Based on a Tetradentate Carbene Ligand

Carbenes are neutral carbon atoms that have a valence of two, but also contain lone pair of electrons that can be used for bonding with metal ions. Carbenes are generally not stable in solution, however carbenes can be effectively stabilized within a metal-ligand complex. In some cases, ligand systems with strong sigma donation properties (like carbene donors)

have been used in conjunction with palladium for organometallic catalysis, including Suzuki type cross-coupling reactions for C—C bond forming reactions. Here we describe our efforts to generate and characterize a tetradentate ligand with two carbene C donor atoms and the related copper coordination complex as an organometallic catalyst. Copper-based catalysts have a huge economical advantage over palladium-based catalyst, where our goal is to generate a cheap, sustainable catalyst for C—C and C—N bond forming reactions.

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Name: Seth Walters Major: Physics Faculty Advisor, Affiliation: Ben Crider, Physics and Astronomy Project Category: Physical Sciences and Engineering

Application of GEANT4 for Efficiency Modeling of an Implantation Detector System used in Beta-Decay Studies of Exotic Nuclei

Beta decay is a radioactive decay process that is a highly sensitive and selective means for assessing the properties of highly unstable, neutron-rich nuclei (or exotic nuclei) when there are only a small number of atoms available for study. One method of performing beta decay studies involves the implantation of radioactive ions of exotic nuclear species directly into a detector. Following implantation and subsequent decay, event by event reconstructions using spatial and temporal information allow for the unique identification of the parent and daughter decays. A feature of performing beta decay studies using an implantation detector is that one cannot determine the absolute efficiencies of the detectors via calibrated, radioactive source measurements alone. Instead, source measurements must be reproduced in simulation where the origin of the source is moved physically inside the detector in order to reproduce the experimental conditions for implantation. A new CeBr₃ implantation scintillator is being developed for usage in a new, highly versatile gamma-ray detector array at the National Superconducting Cyclotron Laboratory (NSCL). The detector arrays are currently being designed and built at NSCL. This work reports on the first efforts to characterize these new detector arrays inside of the GEANT4 simulation toolkit. Preliminary results modeling the system and understanding detector efficiency will be presented.

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Name: Michael Wan Major: Chemistry Faculty Advisor, Affiliation: Joseph Emerson, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Dr. Sean Stokes, James Cope

Copper(I) Catalysis of Iodobenzene and Indole using Amino Acids and Water

Amino acids are an inexpensive alternative to chiral ligands typically used in catalytic processes. There are twenty amino acids that are found abundantly in nature and 19 of them have a chiral center, which could provide a cheaper alternative to the many other chiral ligands used for catalysis. Because each of the amino acids has its own unique structure, each amino acid behaves differently as a ligand. Currently amino acids have not been studied in this scope to a vast extent, thus this study is aimed at testing if amino acids could be used as reliable ligands for aqueous copper-based transformations. In this study, indole and iodobenzene will be coupled using a copper(I)-amino acid architecture in hopes to produce N-phenylindole. Instead of the predicted coupling of the two reactants, the iodobenzene coupled to the amino groups of the ligand. This project is focused on the deconvolution on the possible competing side reactions with the ligands in water and our attempts to minimize them.

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Project Category: Biological Sciences and Engineering
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REU/Research Project: REU

A versatile Fe-Ti oxide/biochar composite adsorbent for contaminant removal from water

Biochar is a form of charcoal that is rich in carbon. It contains the ability to improve water quality, absorb nutrients and preserve nutrients in soil while increasing soil fertility. Other positive characteristics include its low production cost and its porous structure that makes is very effective at retaining water and other nutrients. Basically, it is an environmentally friendly solution to many problems in the environment. Biochar is made from plant material via pyrolysis. This work is the first report on Fe-Ti oxide/biochar (FTOBC) composite for sorptive removal of contaminants from aqueous solutions. Nano Fe-Ti oxides were dispersed on a high surface area Douglas fir (~700 m 2 /g) (BC) by a modified chemical co-precipitation method using FeCl 3 and TiO(acac) 2 salts followed by a base and high temperature treatment (~400 °C). FTOBC consists of three phases; iron oxide, titanium oxide and biochar that ca n adsorb different contaminant classes including heavy metals, anions, oxy anions and organics. Preliminary sorption studies for the removal of Methylene blue (MB), Fluoride (F⁻), chromate/dichromate (Cr⁶⁺) and lead (Pb²⁺) in simulated waters for both BC and FTOBC were performed. Adsorption was studied as a function of pH, equilibrium time and initial adsorbate concentration and temperature. Preliminary data suggest that FTOBC has a potential to simultaneously adsorb MB, F⁻, Cr⁶⁺ and Pb²⁺. BC, FTOBC and adsorbate-laden FTOBC was characterized by PZC, BET, SEM, TEM, EDS, XRD, TGA, DSC and XPS.

Keywords: Fe-Ti oxide, biochar, methylene blue, fluoride, chromium, lead

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Name: Cameron Watson Major: Chemistry Faculty Advisor, Affiliation: Dr. Debra Mlsna, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Lisa Smith, Maggie Leake, Dr. Debra Mlsna REU/Research Program: REU-INFEWS: Food, Energy, Water Security

Supporting Student Engagement in General Chemistry: Effect of Switching Lab Partners and Group Quizzes

Collaborative learning has been said to be very helpful for students and their education as it requires students to be more interactive with other students. The process of working in groups may even encourage students to interact more outside of class and could help increase grades. We performed two different experiments focused on collaborative learning with first-year, undergraduate students in chemistry courses at Mississippi State University. The first experiment focused on the effect that switching laboratory partners every three labs had on student performance. We studied student performance by examining students' laboratory quiz grades, datasheet grades, student Likert-scale surveys, and observational results. The second project focused on the impact that group quizzes have on student interactions and student academic performance within a General Chemistry classroom. We examined students' group quiz grades, individual quiz grades, exam grades, and student Likert-scale surveys. Results from these studies will be presented.

Name: Colton Watson Major: Chemistry Faculty Advisor, Affiliation: Todd Mlsna, Department of Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Chanaka Navarathna

Sorptive removal of 1,4 dioxane using Douglas fir biochar

1,4 dioxane is a small, carcinogenic molecule that can be commonly found in consumer goods such as cosmetics and hygiene products. Its ability or inability to be removed from waste water via absorption was previously unknown. Biochar is an inexpensive and green absorbent that typically has a high surface area. This allows biochar to be used in sorptive removal of contaminants from water. Herein, for the first time we report the adsorptive removal of simulated dioxane waters using a Douglas fir biochar (~700 m²/g S.A). An LC-UV (at 200 nm) method for dioxane determination in water (using acetonitrile and water gradient) was optimized. Effect of initial solution pH, equilibrium time and initial dioxane concentration were studied. Preliminary data suggest that the Douglas fir biochar has the potential to purify water of dioxane. The dioxane-laden adsorbents were characterized using FT-IR, EA and XPS. **Keywords:** dioxane, cosmetic, biochar, adsorption, LC-UV

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Name: Dakota Williams Major: Civil Engineering Faculty Advisor, Affiliation: Andy Perkins, Computer Science and Engineering Project Category: Biological Sciences and Engineering REU/Research Program: NIH R25 Bridges to Baccalaureate

A Pipeline to Compare Differential Expression Workflows

A number of software programs are available for RNA-Seq alignments and identification of differentially expressed transcripts. These programs have been shown to sometimes produce dissimilar results, meaning researchers will often to want to run several programs to be sure of the results and compare lists of differentially expressed transcripts. We built an integrated pipeline that can run several of these programs and compile their results in an easy to understand manner. From raw RNA-Seq reads, this pipeline will use *Hisat2* and *Salmon* for read alignment and then perform differential expression analysis using *DESeq2*, *EdgeR*, and *Limma*. Once all six analysis workflows have been processed, the results will be compiled into a visualization that will show how the results from various programs overlap, as well as how they diverge. This approach should give researchers a clearer and more robust picture of the results of the differential expression analysis, and the effect of the choice of software on their particular experiment.

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Name: John Williams Major: Chemistry Faculty Advisor, Affiliation: Todd MIsna, Chemistry Project Category: Physical Sciences and Engineering Co-Author(s): Chanaka M Navarathna, Achala S Liyanage, Akila G Karunanayake, Felio Perez, Charles U. Pittman, Jr

Soprtive removal of Selenates and Selenites using Douglas fir biochar/metal oxide/hydroxide nanocomposites

Selenium is present in soil in both Selenite (SeO3²⁻) and Selenate (SeO4²⁻) forms. Selenium is an essential element for metabolism regulation in animals and counteracting environmental stresses in plants. High concentrations (> 2ppm) of these compounds in water results in toxicity, as they can alter protein structure and inhibit their function. Biochar allows an inexpensive and relatively simple avenue for water purification and soil remediation via adsorption. Four different biochars; Raw biochar (BC), magnetite modified biochar (MBC), 3:1 Fe:Mg LDH (FMBC3) and 1:1 Fe:Mg LDH (FMBC1) were assed for sorptive removal of both Selenite and Selenite. Each biochar was equilibrated with aqueous solutions of Selenite or Selenate (at different pH, equilibrium time and concentration) and Se contents after sorption were analyzed using ELAN

DRC II ICP-MS. Adsorbents and Se-laden adsorbents were characterized using PZC, BET, SEM, TEM, EDS, XRD and XPS. Preliminary data suggest that all four adsorbents are potential candidates for Se reclamation from water. The complete understanding of the Se sorption Chemistry allows industrialization of this process to use in large scale water treatment. Se-laden biochars can also be used in soil amendment for Se deficient soils. **Keywords:** selenium, magnetite, biochar, soil, adsorption

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Project Category: Biological Sciences and Engineering
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REU/Research Program: NIH R25 Bridges to Baccalaureate

Expression of c-Fos in Central Brain Regions Following Repeated Developmental Exposure to Low Levels of Chlorpyrifos

The organophosphorus insecticides chlorpryifos (CPF) is one of the most widely used pesticides in the world. CPF exerts its acute toxicity through the inhibition of acetylcholinesterase (AChE) and the subsequent accumulation of acetylcholine causing hyperexcitation of the nervous system. However, developmental exposure to lower dosages, CPF does not inhibit AChE but alters the metabolism of the neuromodulatory endocannabinoid anandamide (AEA) in the brain through the inhibition of fatty acid amino hydrolase (FAAH). AEA accumulates and overstimulates the cannabinoid receptor (CB1) inducing either inhibition in some regions or excitation in other regions. The purpose of this study was to identify regions in the central brain where neuronal excitation is occurring following repeated developmental exposure to CPF using c-Fos as a marker for neuronal excitation. To investigate this, rat pups were orally exposed from postnatal day 10 (PND10) to PND16 to either corn oil, 0.5, 0.75, or 1.0 mg/kg CPF. An additional group was treated 0.02 mg/kg PF-04457845 (a specific inhibitor of FAAH) as a positive control. Rats were sacrificed 12 hours after the final treatment and brains were collected and sliced using a cryostat to isolate specific regions of the brain. Immunohistochemistry was then performed on these specific regions to determine c-Fos expression. Staining detected expression of c-Fos in the retrosplenial agranular cortex, which is involved in differentiating between perceptual and memory functions, and the thalamic nuclei, mainly the paraventricular nucleus. This is involved in the stress response and the xiphoid nuclei which reduces the importance of threats thereby dampening the response. (Supported by 1R25GM123920-01A1)

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Name: Jackson Wolfe Major: Aerospace Engineering Faculty Advisor, Affiliation: Donghoon Kim, Department of Aerospace Engineering Project Category: Physical Sciences and Engineering Co-Author(s): Sepehr Zangeneh

Development of a Three-Dimensional Environment Mapping System

Three-dimensional mapping has been a popular and intense subject of research for a long time. With the rapid development in technology, specifically LIDAR (Light Detection and Ranging), it has never been easier to map a surface or an object with high precision, such as the layout of a room. The problem with most commercial threedimensional LIDAR systems is cost, with some systems reaching up to \$78,000. Such systems also usually have a narrow field of view and a limited scan range. The main goal of our three-dimensional LIDAR is to bring down the cost of such a system to something that more people can afford while also adding the ability to do a full 360- degree scan and still maintaining that similar level of accuracy and precision. Other goals include portability and the ease of use for end users. To achieve this, we decided to vertically mount a two-dimensional LIDAR (RPLIDAR by Slamtec) to a rotating platform. The rotating platform is made up of 3 main pieces that were designed in SolidWorks and 3D-printed on an Ultimaker S5. A two-pole stepper motor and a Raspberry Pi 3B+ module are used to rotate the platform at small angular increments. To control the quality

and the speed at which the 3D model is made, the amount of each increment is changed. There are several challenges with this design. The main hardware related issue is making sure the stepper motor is stepping at the correct rate to accurately record data. Some of the data related issues include data acquisition, data transmission, and data plotting. All of these issues will be addressed with various tests of the system. Most tests will consist of placing the system in a space of known dimensions and then comparing the data plots to the known dimensions.

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Name: Melissa Wood Major: Biological Sciences Home University: Knox College Faculty Advisor, Affiliation: Mark Welch, Biological Sciences Project Category: Biological Sciences and Engineering Co-Author(s): Andy Perkins REU/Research Program: Computational Biology REU

Population level transcriptomic comparisons of Helianthus annuus L.

Helianthus annuus L., known as the common sunflower, has many applications in agriculture as a crop for its seed, oil, forage for livestock, and aesthetics. It is grown across many latitudes, which makes it an ideal plant for studying genetic variation, and thus phenotypic variation between populations spanning different geographical and climatic regions. Heritable differences such as growth rate, leaf size and bloom time are observed in changing latitudes. We obtained high quality RNA-seq data from 95 individual sunflowers from a total of 6 distinct populations at 2 different latitudes, Oklahoma and Kansas, grown in a common garden experiment. Using read coverage tables created in mapping these data to the sunflower reference genome, differences between the transcriptomes and gene expression of the two sets of populations will be analyzed. Transcriptomic variation observed in this study may, upon further investigation, lead to a deeper understanding of genetic adaptation and selection for *H. annuus* populations spanning many climates.

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Name: Ethan Worch Major: Electrical Engineering Faculty Advisor, Affiliation: Sathish Samiappan, Electrical Computer Engineering Project Category: Physical Sciences and Engineering

Feature Selection of Hyperspectral Imagery using Naturally Inspired Metahearistic Algorithms for Agricultural Applications

Hyperspectral imaging captures hundreds of spectral bands and can differentiate subtle targets. It has many important agricultural applications; however, the potential of this rich information suffers Hughes Phenomenon which requires having a larger training set as the number of bands increases. For this reason, selecting a subset of bands will both reduce the dimension and alleviate Hughes phenomenon. The optimal combination of the bands used in classification can greatly influence the accuracy of the produced classification map, but there exist many methods by which to select the bands to be used. Projection based feature reduction such as principal component analysis is not a very viable candidate as it tends to alter data as it is projected which makes feature selection the natural choice. Feature selection can be accomplished either by using metrics or by using heuristic methods. In this research, different naturally inspired metaheuristic methods will be tested for their speed and accuracy in band selection. Better band selection can lead to an increase in the accuracy of the applications of hyperspectral imaging such as advanced vegetation analysis and crop disease identification.

Name: Melanie Xia Major: Computer Science Home University: University of Miami Faculty Advisor, Affiliation: Dr. George Popescu, IGBB Project Category: Biological Sciences and Engineering Co-Author(s): Himangi Srivastava, Marilyn Warburton REU/Research Program: Undergraduate Research in Computational Biology

Analysis of chromosomal variation and transcriptional reprogramming in A. flavus resistant maize

The Aspergillus flavus strand, NRRL3357, is known to produce a carcinogen known as aflatoxin. The infection of major agricultural crops, such as maize, contributes to significant crop losses annually. Furthermore, inadequate screenings of maize products are detrimental to mammalian health, most notably liver cancer in human populations. One of the most viable methods of combating this issue is to selectively breed a resistant line of maize with a susceptible line of maize to produce a variety that is both resistant to *A. flavus* and is capable of producing high yields. We are conducting a comparative study of transcriptomes from two lines of maize-Mp719 resistant and Va35 susceptible- inoculated with two fungal strains- aflatoxin producing NRRL3357 and non-aflatoxin producing NRRL 21882 (commonly used to resist infection from toxic strains of *A. flavus*)- to identify transcriptional reprogramming changes and resistance pathway modifications between breeding lines.

The analysis includes mapping RNASeq reads to references B73 maize genome and A. flavus genomes while preserving the unmapped reads for the subsequent de novo transcriptome assembly. One key objective is to investigate structural chromosome variation in the maize varieties to identify genes that regulate defense mechanisms against aflatoxin. Further quantification of the transcriptome assembly will allow us to identify the active areas in the genome and observe changes between treatments. Finally, differential expression analysis will help us identify significant changes in gene expression associated with the pathogen infection.



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