

Arkansas INBRE Research Conference

Arkansas IDeA Network of Biomedical Research Excellence

Schedule of Events

Friday, November 2, 2018

12:00 p.m. to 1:30 p.m.	Registration (Chancellor Hotel Atrium, 2 nd floor). Graduate Program Information available from 12:00–1:30.
1:30 p.m.	Opening Session, chaired by Professor Feng Wang, Chemistry, University of Arkansas. (Chancellor Hotel, Eureka Springs Ballroom)
1:35 p.m. to 3:00 p.m.	Invited faculty presentations
3:00 p.m. to 3:15 p.m.	Set-up time for student orals
3:00 p.m.	Official hotel check-in
3:15 p.m. to 5:00 p.m.	Undergraduate oral presentations (Chancellor Hotel, Biology – Eureka Springs Ballroom; Chemistry – Bella Vista Room; Physics – Petit Jean Room). (12 minute talks with 3 minutes for questions)
5:15 p.m. to 6:15 p.m.	Faculty Discussion Group and Reception (Chancellor Hotel, Lounge and Restaurant, First Floor)
5:15 p.m. to 6:15 p.m.	Student Discussion Group and Reception (Chancellor Hotel, Atrium)
6:30 p.m.	Banquet (Fayetteville Town Center) Your nametag is your ticket in!
7:15 p.m.	Featured Speaker: Dr. Christopher Mason

Saturday, November 3, 2018

7:30 a.m. to 8:00 a.m.	Poster Set-up begins (Hillside Auditorium & Physics Bldg.)
7:30 a.m. to 10:00 a.m.	Conference Registration (Upper Hillside Lobby)
7:45 a.m. to 9:30 a.m.	Continental breakfast (Upper Hillside Lobby and Physics)
7:45 a.m.	Poster judges receive assignments (Upper Hillside Lobby for Biology, Chemistry) (Physics Building for Physics)
8:00 a.m. to 9:00 a.m.	Poster Session A (Hillside and Physics)
9:00 a.m. to 9:15 a.m.	BREAK – Remove Session A posters. Put up Session B posters. (Note that breakfast ends at 9:30.)
9:15 a.m. to 10:15 a.m.	Poster Session B (Hillside)
10:30 a.m. to 11:45 a.m.	Workshops and Tours (UA Campus, various locations)
11:55 a.m.	Award presentations & conclusion, Hillside Auditorium 202

Registration Information

The INBRE registration desk will be open:

- Friday – 11:00 p.m. to 5:00 p.m., Chancellor Hotel Atrium (2nd floor)
- Saturday – 7:30 to 10:00 a.m., Hillside Auditorium, Upper Lobby

Travel Subsidies are no longer being given.

Lodging will be at the Chancellor Hotel, 70 N. East Avenue, Fayetteville, AR 72701 and at the Holiday Inn Express, 1251 N. Shiloh Drive, Fayetteville, AR 72704

Parking: Friday parking is complimentary in the Municipal Parking Garage, third level only (first level card access for registered guests of the Chancellor Hotel). Parking in the parking garage behind the Town Center is free between 12:30 pm and 9:00 pm Friday.

Saturday parking is free on the UA campus in designated yellow-sign lots and parking decks. Please see the map at end of program.

Arkansas INBRE

The Arkansas IDeA Network of Biomedical Research Excellence (Arkansas INBRE) is funded by a grant from the National Institute of General Medical Sciences (NIGMS), under the Institutional Development Award (IDeA) Program of the National Institutes of Health (NIH). The IDeA program was established for the purpose of broadening the geographic distribution of NIH funding for biomedical and behavioral research. Currently NIGMS supports INBRE programs in 23 states and Puerto Rico.

The Arkansas INBRE builds on the successful Arkansas Biomedical Research Infrastructure Network (BRIN) program that was established in 2001 under a grant from NCRR. The Arkansas BRIN established a statewide network that links Arkansas institutions of higher education to establish and maintain a statewide infrastructure in support of growing efforts to build capacity for biomedical research in Arkansas. <https://inbre.uams.edu/>

Arkansas INBRE Research Conference

The Arkansas INBRE Research Conference is sponsored by Arkansas INBRE and is hosted by the departments of biological sciences, physics, and chemistry and biochemistry, Fulbright College of Arts and Sciences, University of Arkansas.

Conference Planning Committee

Dan Lessner, Christian Tipsmark, Ravi Barabote, biological sciences
Denise Greathouse, Roger Koeppel, Feng Wang, Leslie Johnson chemistry and biochemistry
Reeta Vyas, physics

INBRE Steering Committee

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Biotechnology Core Leaders
Joshua Sakon, UAF
Alan Tackett, UAMS

Poster Session and Awards

Display

Poster set-up begins at 7:30 a.m. Saturday in Hillside Auditorium, Lower Level; and Physics Building.

Session A – 8:00 a.m. to 9:00 a.m.
9:00–9:15 BREAK. Take down Session A posters.
Put up Session B posters.
Session B – 9:15 a.m. to 10:15 a.m.

Presenters are expected to be present during the scheduled time. Business or business casual dress is encouraged. *See index and abstracts in this program for numbers and Session assignments.*

Awards

Prizes will be awarded to the top oral and poster presentations by undergraduate students in each discipline. The awards will be presented Saturday at 11:55 a.m. in Hillside Auditorium Room 202. Presenters must be present at the awards presentation to receive an award.

Judging Rules

Each undergraduate oral presentation and poster will be judged by at least two judges, selected from various institutions. To avoid a possible conflict of interest, no judge will evaluate a presentation from his/her own institution.

Awards will be given in each of the three disciplines – physics, biology, and chemistry and biochemistry. Only oral talks and posters with undergraduate participation, and where a sole designated presenter is an undergraduate student, will qualify for awards.

Featured Speaker

Planetary-scale and Space-based Genomics for Improving Astronaut Health

Christopher E. Mason,
Ph.D.



Dr. Christopher Mason is an Associate Professor in the Department of Physiology and Biophysics, Weill Cornell Medicine.

ABSTRACT: The avalanche of easy-to-create genomics data has impacted almost all areas of medicine and science, from cancer patients and microbial diagnostics to molecular monitoring for astronauts in space. Recent technologies and algorithms from our laboratory and others demonstrate that an integrative, cross-kingdom view of patients (precision metagenomics) holds unprecedented biomedical potential to discern risk, improve diagnostic accuracy, and to map both genetic and epigenetic states. Leveraging these data, the global profile of the world's urban systems (MetaSUB.org) is being created to track the intra-city and inter-city shifts in antimicrobial resistance (AMR) markers. Finally, these methods and molecular

tools work together to guide the most comprehensive, longitudinal, multi-omic view of human astronaut physiology in the NASA Twins Study, which lay the foundation for future long-duration spaceflight, including sequencing, quantifying, and engineering genomes in space.

The Mason laboratory is working on a ten-phase, 500-year plan for the survival of the human species on Earth, in space, and on other planets. To that end, they develop and deploy new biochemical and computational methods in functional genomics to elucidate the genetic basis of human disease and human physiology. They focus on novel techniques in next-generation sequencing and algorithms for tumor evolution, genome evolution, DNA and RNA modifications, and genome/epigenome engineering. They work closely with NIST/FDA to build international standards for these methods and ensure clinical-quality genome measurements and editing. They also collaborate with NASA to build integrated molecular portraits of genomes, epigenomes, transcriptomes, and metagenomes for astronauts, which help establish molecular foundations and genetic defenses for long-term human space travel.

Dr. Christopher Mason completed his dual B.S. in Genetics and Biochemistry (2001) from University of Wisconsin-Madison, his Ph.D. in Genetics (2006) from Yale University, and then completed post-doctoral training in clinical genetics (2009) at Yale Medical School while jointly a post-doctoral Fellow of Genomics, Ethics, and Law at Yale Law School (2009). He is currently an Associate Professor at Weill Cornell Medicine, with appointments at the Tri-Institutional Program in Computational Biology and Medicine between Cornell, Memorial Sloan-Kettering Cancer Center and Rockefeller University, the Sandra and Edward Meyer Cancer Center, and the Feil Family Brain and Mind Research Institute.

Invited Faculty Presentations

Friday from 1:30 p.m. to 3:00 p.m. (Chancellor
Hotel, Eureka Springs Ballroom)

No registration required



Dr. Laura MacDonald, Ph.D.

Department of Biology
Hendrix College
(1:35 –2:00)

**TITLE: Collagen Increases Tumorigenic
Characteristics of Papillary Thyroid Cancer
Cells Harboring BRAFV600E Mutations**

Abstract: Thyroid cancer is the most common endocrine cancer, and incidence is increasing worldwide. Thyroid cancer can be classified as well-differentiated, poorly differentiated, or anaplastic. Of well-differentiated thyroid cancers, papillary thyroid cancer is most common, and is associated with activating BRAF mutations. While the genetic basis for thyroid cancer is well-understood, less is known about how the tumor microenvironment alters papillary thyroid cancer tumor cell behavior. Jolly and others reported that papillary thyroid tumors derived from cells harboring activating BRAF mutations and PTEN deletions were enriched with fibrillar collagen in mouse models. Additionally, they reported that upregulation

of collagen I and the cross-linking enzyme lysyl oxidase was associated with advanced disease and decreased survival in patients. In this study, we investigated whether growth on collagen enhanced tumorigenic characteristics of papillary thyroid cancer cell lines. Interestingly, cell lines grown in the presence of collagen displayed a more aggressive phenotype. Notably, these cells were more mesenchymal in morphology, had increased growth rates, were more resistant to apoptosis induction, and were less sensitive to small molecule inhibitors. These and other results suggest that presence of collagen in the tumor microenvironment increases tumorigenic behavior of tumor cells, which may play an important role in thyroid cancer progression.



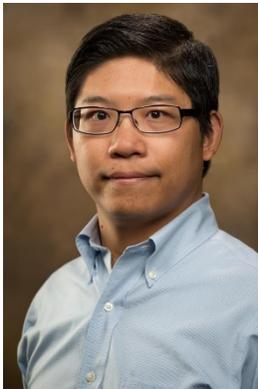
Dr. Irosha N. Nawarathne, Ph.D.

Department of Chemistry
Lyon College
(2:05 – 2:30)

**TITLE: TB or Not TB? That is Not the Only
Question**

Abstract Multi-drug resistant tuberculosis (MDR-TB) remains a public health crisis and a health security threat with 600,000 new cases with resistance to rifamycins (RR-TB), of which 490,000 had MDR-TB. Among reported MDR-TB patients, 6.2% were diagnosed with extensively drug resistant (XDR) TB. The rifamycins, long considered a mainstay of tuberculosis treatment, particularly rifampin (RMP) – the most effective first-line drug in

combination therapy, bind to the β subunit of Mycobacterium tuberculosis RNA polymerase (MTB RNAP) and block RNA synthesis. TB is fully curable using combination therapy that includes rifamycins; the average treatment cost per TB case is about \$0.045 million. However, numerous drug resistant strains (MDR and XDR-TB) disrupt interactions between rifamycins and modified MTB RNAP, via single mutations in the β subunit, leading to drug resistance. The financial toll of treating patients with MDR-TB and XDR-TB comes at a terrible price with greater drug resistance as the treatment time increases to 20-32 months and due to the lack of available therapeutics. Appallingly, the alternative TB drugs show life-threatening side effects. In our lab, we strategically explore the ways to find novel therapeutics for prevalent MDR/XDR-TB to prevent the global epidemic through multiple TB outbreaks and to reduce the financial burden. Certainly, there is more to our research story.



Dr. Yong Wang, Ph.D.

Department of Physics
University of Arkansas
(2:35 – 3:00)

TITLE: Watch to learn: Understanding the Spatial Organization and Dynamic Diffusion of Molecules in Live Bacteria

Abstract: Spatial organization and dynamic diffusion of molecules inside bacterial cytoplasm are vital for them because

transport and mixing of cytoplasmic molecules and resources primarily rely on diffusion due to the small size of bacteria and lack of active transport mechanisms. Although the diffusion of particles and molecules in various solutions and environments has been extensively studied both theoretically and experimentally, quantitative knowledge on the dynamic diffusion of biological molecules inside live bacteria remains relatively limited, due to the lack of temporal and spatial resolutions on single live bacteria. The recent development of super-resolution fluorescence microscopy in combination with single-particle tracking has provided powerful tools for understanding the organization of various cellular components and dynamics of cellular processes in live systems. In this talk, I will present our research on the organization and anomalous diffusion of the histone-like nucleoid-structuring proteins (H-NS) in *E. coli* bacteria, for which we achieved a spatial resolution of 20 nanometers and a temporal resolution of 30 milliseconds. In addition, I will describe how the ultra-high spatial and temporal resolution allows us to understand the antibiotic mechanism of silver ions and nanoparticles, which suppress the growth of and kill bacteria, opening new avenues to fighting against antibiotic-resistant microbes.

Student Oral Presentations

Undergraduates will give 12-minute oral presentations from 3:15 p.m. to 5:00 p.m. on Friday. All talks will take place at the Chancellor Hotel. Students were chosen based on abstracts and willingness to present an oral platform talk. Additional information, authors, and footnotes can be found in the complete list of abstracts in this program.

Biology Oral Presentations

(Eureka Springs Ballroom)
Tameka A. Jennings, Chair

Brandon Hogland, Harding University
(3:20 p.m.) Discovery of Novel antimicrobial peptides

Ruth Victoriano, UA Fort Smith
(3:35 p.m.) Antioxidant Assessment of Stilbenoid-rich Extracts from Peanut Hairy Roots

Jonathan Jenkins, Hendrix College
(3:50 p.m.) Collagen Increases Apoptotic Resistance in Papillary Thyroid Cancer Cell Lines Harboring BRAFV600E Mutations

Hannah Zang, Lyon College
(4:05 p.m.) Mutational analyses of a factor promoting cytoplasmic ribosome maturation in *S.cerevisiae*

Grace Young, UA Little Rock
(4:20 p.m.) Using DOPE-FISH Microscopy to Image Ecologically Important, Multi-Taxon Bacterial Communities

Taylor Hill, UA Pine Bluff (4:35 p.m.)
Identifying Gar, Catfish, Red Snapper, Tuna, Carp, and Sea Bass Using DNA Barcoding in Mice Treated with Cranial Radiation and Sulforaphane

Chemistry and Biochemistry Oral Presentations (Bella Vista Room)

Susanne Striegler, Chair

Emily N. H. Tran, University of Central Arkansas
(3:20 p.m.) Squaramide-based anti-parasitic drugs toward the discovery of novel treatments for American trypanosomiasis

Madison Perchik, Rhodes College
(3:35 p.m.) The Effects of Proton Abstraction on the Binding Selectivity of Ligands in the Phenylalanine Hydroxylase Active Site

Anna Pinson, Harding University
(3:50 p.m.) Identification of Oxidative Enzymes in the Metabolism of Synthetic Cannabinoid 5F-AKB-48

Fernanda Hernandez Sanchez, University of the Ozarks
(4:05 p.m.) Chemical Approaches for Investigating Cancer Growth Inhibition and Male Contraception by DEC-TEC and PROTAC

Benjamin D. Justice, Arkansas Tech University

(4:20 p.m.) Human Glioblastoma Multiforme Growth Retardation by Inhibition of Cystine Transport

Jordan Trant, Lyon College (4:35 p.m.)
Fighting Drug Resistant Mycobacterium tuberculosis Using Modified Rifamycins

Physics Oral Presentations

(Petit Jean Room)

Hugh Churchill, Chair

Ariel Rogers, Truman State University
(3:20 p.m.) Single-Cell Investigation of the Effects of DC Electric Current on Bacteria

Levi Humbard, Pittsburg State University
(3:35 p.m.) Effects of Thickness Gradient on Magnetoresistance in a Co/Pt Multilayer

Arturo Morales Barrios, John Brown University
(3:50 p.m.) The Slip-Stick Behavior of the Friction Force on a Body on an Inclined Plane

Lucas A. Blake, Southern Arkansas University

(4:05 p.m.) Gas Sensing in a Microresonator System Using Non-Adiabatic Tapered Fibers

Jack Freeland, University of Arkansas
(4:20 p.m.) Mechanical Energy Based Amplifiers for Probing Interactions of DNA with Metal Ions

Chris Klenke, Missouri State University
(4:35 p.m.) Molecular Dynamic Simulations to Study Tunnel Barrier Layer Formation in Ultra-Thin Film Alumina

Participating Institutions

Arkansas State University
Arkansas Tech University
Central Baptist College
Harding University
Henderson State University
Hendrix College
John Brown University
Lyon College
Missouri State University
Northeastern State University
Northwest Arkansas Community College
Oklahoma State University
Ouachita Baptist University
Pittsburg State University
Rhodes College
Southern Arkansas University
Truman State University
University of Arkansas at Fayetteville
University of Arkansas at Fort Smith
University of Arkansas at Little Rock
University of Arkansas at Monticello
University of Arkansas for Medical Sciences
University of Arkansas at Pine Bluff
University of Central Arkansas
University of the Ozarks

Saturday Workshops

INBRE participants are expected to attend a workshop as part of the program. All workshops and tours will take place Saturday at 10:30 a.m., in various locations on the University of Arkansas Campus

Registration for Workshops will be at Conference Registration Table

Workshop 1 – Chemistry “Leveraging Public Sequence Databases with Next Generation Tools!”

(Chemistry Building, Room 144)

Ben Busby, NIH/NLM/NCBI

This workshop will begin with a demonstration of new computational and visualization tools offered by NCBI and others in the bioinformatics community. Methods for extracting data from databases will also be demonstrated, particularly “edge computing,” or the practice of streaming data from where it is stored rather than downloading it, using magicBLAST as an example. We’ll also discuss other high-throughput ways to access data and metadata, such as the EDirect command line metadata API, taxonomic organization of SRA datasets, and online .bam visualization. We’ll also discuss how these data extraction mechanisms can be paired with community resources, and general frameworks such as Galaxy, CyVerse, Bioconda, and Bioconductor.

Workshop 2 – Preparing for Graduate School

(Chemistry Building, Room 132)

Colin Heyes, PhD, Dept. of Chemistry & Biochemistry, UAF

This workshop is targeted towards undergraduate students who are considering graduate school as a career. Topics to be discussed will include graduate school expectations and how to prepare for and select the right graduate school and program for you. A panel of faculty and graduate students will be available to share their tips, strategies, insights, and practical advice. We conclude with a Question and Answer session, with the possibility of breaking out into smaller groups based on specific interests.

Panelists:

Suresh Kumar, Professor of Chemistry and Biochemistry, UAF

Jessica Pickens, graduate student in Chemistry and Biochemistry, UAF

Perry Caviness, graduate student in Chemistry and Biochemistry, UAF

Doug Rhoads, University professor of Biology and director of the Cell and Molecular Biology (CEMB) program, UAF

Bryce Pelfrey, graduate student in biology, UAF

Workshop 3 – Molecular Modeling

(Chemistry Building Library, Room 225)

Peter Pulay, PhD, Dept. of Chemistry and Biochemistry, UAF

Limited to 12 participants or groups. If feasible, bring a computer, although this is optional.

Methods of molecular modeling on a personal computer will be addressed, with software available for distribution to up to 12 individuals or cluster teams.

Workshop 4 – Nanochemistry

(Chemistry Building, Room 147)

Jingyi Chen, PhD, Dept. of Chemistry and Biochemistry, UAF

Limited to 15 participants.

Nanochemistry plays an important role in many applications ranging from medicines to catalysis, electronics, energy conversion and storage. In this workshop, the emphasis focuses on the nano-chemistry in theranostics applications, in particular, the use of nanoparticles in disease diagnostics and therapy. An overview of nanomedicine will be presented, followed by a specific example based on the gold nanostructure nanoplatfrom.

Workshop 5 A Beginner's Workshop for Statistical Techniques for Medical Studies

(Gearhart Hall, Room 101)

Zhuoxin Sun, PhD (Senior Statistician, ECOG-ACRIN Cancer Research Group and International Breast Cancer Study Group, Senior Research Scientist, Frontier Science and Technology, Adjunct Associate Professor, Dept. of Math. Science, Univ. of Arkansas)

The workshop has a maximum enrollment of 20.

This workshop will begin with an introduction of some basic ideas about

clinical trials in medical research. It will cover different types of clinical trials conducted at various stages of drug development, principles to avoid bias in clinical trials, and ideas about determining the number of patients needed in a clinical trial. Two hands-on case studies with clinical data will be examined to demonstrate how to use some basic statistical techniques in clinical trials. The hand-on exercises will be performed with Microsoft Excel with the Data Analysis Addin.

Workshop 6 – Cellular Mechanisms of Salt and Water Transport in Fish

(Ferritor Building, Room 317)

Christian Tipsmark, PhD, Biological Sciences Department, UAF

The goal of physiological research is to understand the function of living systems from the level of the whole organism and its organs to that of the single cells and bio-molecules. This workshop highlights mechanisms and regulation of salt and water transport in fish and demonstrates some of the methods used in physiology. It will cover experimentations with whole animals and isolated tissues. Techniques demonstrated will include enzyme assays, specific mRNA and protein quantification and cellular localization of specific proteins with immunofluorescence.

Workshop 7 – Physics “Super-Resolution Fluorescence Microscopy”

(Physics Building, Room 133 and 115A)

Yong Wang, PhD, Physics Dept., UAF

Limited to 15 participants.

This workshop will briefly introduce the basics of super-resolution fluorescence microscopy based on single-molecule localization, which improves the spatial resolution of light microscopy from ~300 nanometers to ~20 nanometers (see 2014 Nobel Prize in Chemistry for more details). Attendees will have a chance to image an important universal regulatory protein – HNS – in *E. coli* bacteria, to localize individual HNS molecules, and to produce super-resolved images of HNS proteins in *E. coli* with a resolution of ~ 20 nanometers.

Workshop 8 – Physics “High Temperature Superconductor”

(Physics Building, Room 134 and 131)

Jin Hu, PhD, Physics Dept. UAF

The discovery of superconductivity is one of the major breakthroughs in Physics in the last century. The studies on superconductivity and related phenomena have been awarded several Nobel Prizes. This workshop will introduce this fascinating quantum phenomenon. Workshop attendees will then have the opportunity to synthesize the high temperature superconductor.

Workshop 9 – Physics: “A 2D How-to”

(Nano Building, Room 105)

Hugh Churchill, PhD, Physics Dept., UAF
Limited to 15 participants.

After a brief introduction to the field of 2D material research, I will demonstrate the now-famous “Scotch tape technique” that is used to peel apart atomically thin layers of graphene and many other 2D materials from 3D crystals. Workshop

attendees will then have the opportunity to try this themselves using tape, tweezers, and silicon chips, followed by “flake hunting” with a microscope.

Workshop 10 – Physics “Graduate Application”

(Physics Building, Room 132)

Reeta Vyas, PhD, Physics Dept., UAF
Limited to 20 participants.

Participants will learn about career options for physics graduates, dos and don'ts of the application process for Physics Graduate Programs in the US – importance of and preparation for GRE, course work, recommendation letters, assistantships, etc.

Workshop 11 – Visualizing Mitochondrial Dynamics

(Ferritor Building, Room 325)

Shilpa Iyer, PhD, Biological Sciences Dept., UAF

Limited to 10 participants.

The goal is to understand mitochondrial changes in healthy and diseased states. We will demonstrate techniques that will visualize and analyze images from multiple cell types corresponding to different mitochondrial diseases.

Abstracts

Presentations are posters, on Saturday, unless denoted as “Oral” for Friday afternoon.

Biological Sciences

Friday Oral Platform Session

ORAL – 3:20. Discovery of Novel antimicrobial peptides from the venom of the wolf spider, *Rabidosa rabida*. Brandon Hogland, Amber G. Hug, Ryan J. Stork. *Biology, Harding University, Searcy, AR 72143.*

The World Health Organization (WHO) and the Centers for Disease Control (CDC) have initiated plans to encourage the research and development of novel antibiotics. According to the WHO, pharmaceutical companies have stopped researching new antibiotics (Shrivastava, 2017). Yet, globally antibiotic resistance is increasing. The need to develop novel antibiotics is very clear. As microorganisms continue to develop resistance, it becomes even more important to find new answers (Neu, 1992). Researchers have been challenged to find antibiotics in the least likely places. Thus, antimicrobial research is once again becoming a central focus in pharmaceutical research due to the continued decrease in antibiotic susceptibility of antibiotics currently used to treat infection. With this new initiative in place, scientists are looking in soil, arthropods, other bacteria and fungi for answers to this new dilemma (Ageitos et al., 2017). Previous studies have indicated that spider venom contains proteins that are antimicrobial in nature. In our study, we chose *R. rabida* as the model vector for identifying new antimicrobial agents. *R. rabida* is native to most of central North America and in habitats with warm temperatures. This led us to hypothesize that the terrestrial wolf spider *R. rabida* has proteins capable of antimicrobial activity. After LRPC/MS analysis, 739 known peptides were discovered in the venom in addition, we found 9500 peptides not matching sequences in the UniprotKB database. Our next step is analyzing the unmatched peptide for novel antimicrobial peptides. We will then custom order these synthetic versions of these novel proteins and conduct antimicrobial assays against those organisms listed as increasingly drug resistant.

ORAL – 3:35. Antioxidant Assessment of Stilbenoid-rich Extracts from Peanut Hairy Roots. Ruth Victoriano, *Biology, UA Fort Smith, Fort Smith, AR 72904*, Patrick Roberto, Fabricio Medina-Bolivar, *Biology, Arkansas State University, Jonesboro, AR 72401.*

Oxidative stress, the imbalanced accumulation of reactive oxygen species (ROS), may lead to inflammation and oxidative damage of nucleic acids, lipids, and proteins. In humans, oxidative stress is associated with several illnesses including cancer and neurodegenerative disorders such as Parkinson’s and Alzheimer’s disease. Antioxidants present in our diet may counteract the effects of ROS. To this end, the long-term goal of this project is to develop novel plant-based antioxidant compounds that could be used as functional ingredients. The peanut plant produces antioxidant compounds known as stilbenoids and peanut hairy root cultures treated with elicitors can be used as a sustainable bioproduction system for these compounds. Specifically, the objective of this project was to assess the antioxidant properties of stilbenoid extracts produced in these cultures. Peanut hairy root cultures of cultivar Hull were treated with cyclodextrin alone or in combination with methyl jasmonate, hydrogen peroxide and magnesium chloride for 168 hours. Stilbenoids were extracted from the culture medium with ethyl acetate and analyzed by HPLC. Extracts from the combined elicitor treatment contained higher levels of stilbenoids including resveratrol and the prenylated stilbenoids arachidin-1, -2, -3, and -5. The antioxidant activity of the extracts was assessed with the 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay. Extracts produced from the combined elicitor treatment exhibited greater antioxidant activity than the extracts from the cyclodextrin treatment alone. Our studies suggest that the peanut hairy root extracts are a good source of antioxidant compounds that have potential use as nutraceuticals to improve human health.

ORAL – 3:50. Collagen Increases Apoptotic Resistance in Papillary Thyroid Cancer Cell Lines Harboring BRAFV600E Mutations. Jonathan Jenkins, Laura J. MacDonald, *Biology, Hendrix College, Conway, AR 72143.*

Thyroid cancer is the most common endocrine malignancy, and incidence is on the rise. Papillary thyroid cancer is the most common subtype, and is often associated with BRAF mutations. Recently, Jolly and others showed that papillary thyroid cancer tumors containing BrafV600E mutations and lacking PTEN recruit and stimulate proliferation of cancer associated fibroblasts. Additionally, these tumors are enriched in collagen. Lastly, upregulation of collagen in patient tumor samples correlates with progressive disease and increased mortality. Based on these observations, we hypothesized that collagen may increase apoptotic resistance in papillary thyroid cancer cell lines. To test this hypothesis, three papillary thyroid cancer cell lines were plated in the presence and absence of collagen and treated with staurosporine to induce apoptosis. Apoptosis was assessed through quantification of apoptotic nuclei through immunofluorescence

microscopy and assessment of PARP and Caspase cleavage through Western blotting. Cells grown in the absence of collagen and treated with staurosporine displayed significantly higher numbers of apoptotic nuclei as compared to cells grown in the presence of collagen. Additionally, cells grown in the presence of collagen displayed increased resistance to MEK inhibition and increased AKT activation, suggesting that collagen contributes to apoptotic resistance in an AKT dependent manner.

ORAL – 4:05. Mutational analyses of a factor promoting cytoplasmic ribosome maturation in *S.cerevisiae*. Hannah Zang, Alexander Beeser, *Biology, Lyon College, Biology, Batesville, AR 72503.*

The assembly of cytoplasmic ribosomes is an evolutionarily conserved process that consumes an immense amount of cellular resources and results from a complex spatiotemporal interplay between ≈ 80 ribosomal proteins (RP's) and 4 ribosomal RNA's (rRNA's) in three distinct subcellular compartments. Contributing to ribosome assembly are greater than 200 non-ribosomal proteins known as trans-acting factors (TAF's), that interact with various RP/rRNA subassemblies to promote their specific directional maturation towards, but which are not ultimately components of, translationally competent 80S ribosomes. TAF's are enriched for proteins with ATPase, GTPase and RNA helicase activity but many other TAF's have no predicted enzymatic activity and are thought to act as assembly "place holders" ensuring directional assembly. Most TAF's function within the nucleolus/nucleus, but several function cytoplasmically prior to ribosomal subunit joining. Of particular interest to us is the TAF encoded by the YVH1 dual-specificity phosphatase. Yvh1p is required for the cytoplasmic removal of Mrt4p, a TAF added to pre-60s complexes within the nucleus that is co-exported with pre-60S subunits. Cytoplasmic removal of Mrt4 is a prerequisite for the addition of the ribosomal stalk (consisting of RP's Po/P1/P2) present in translationally competent ribosomes. Accordingly, cells lacking Yvh1p fail to remove cytoplasmic Mrt4, precluding addition of the stalk and demonstrate profound translational defects. Deletion analyses have also established that the ability to remove cytoplasmic Mrt4p from pre-60S subunits maps to a cysteine rich domain (CRD), distinct from the dual-specificity phosphatase domain, but whose function remains unknown. To better understand the function of this conserved CRD, we have generated a large panel of loss of function mutants, which are described here. We have also made preliminary to better characterize the nature of the translational defects that arise from loss of Yvh1p function. A better understanding of Yvh1p's role in translation is warranted as the human ortholog of YVH1, Dusp12 is a candidate oncogene in aggressive human liposarcoma's

potentially implicating ribosome assembly and/or ribosome compositional heterogeneity in human disease.

ORAL – 4:20. Using DOPE-FISH Microscopy to Image Ecologically Important, Multi-Taxon Bacterial Communities. Grace Young, Scott Woolbright. *Biology, UA Little Rock, Little Rock, AR 72204.*

While DNA "barcoding" via next generation DNA sequencing has provided unprecedented "windows" into microbial community composition, such studies only provide lists of species in the community. However, microbes also form spatial interactions that cannot be predicted or studied using DNA sequencing alone. New techniques using FISH microscopy provide a means for investigating the spatial distribution of interacting microbial taxa. In conjunction with DNA barcoding studies in the Woolbright lab, I am using a new FISH technique known as double-labeling of oligonucleotide probes (DOPE-FISH) to look for unanticipated spatial interactions among bacterial taxa from a variety of ecosystems (freshwater, marine, terrestrial). Understanding the spatial structure of such communities is likely to have significant impacts on our understanding of how interactions among bacteria act to structure microbial communities with implications for research on harmful algal blooms (HABs) as well as a variety of other community- and ecosystem-level studies. To date, I have successfully employed DOPE-FISH on single-species lab populations of *E. coli*. We are currently in the process of extending our studies to other lab strains and to natural populations from a variety of ecosystems (aquatic, marine, terrestrial, etc.).

ORAL – 4:35. Identifying Gar, Catfish, Red Snapper, Tuna, Carp, and Sea Bass Using DNA Barcoding. Taylor Hill, Naterica Jones, *Biology, UA Pine Bluff, Pine Bluff, AR 71601*; Abigail S. Newsome, *Bioinformatics, Mississippi Valley State University, Itta Bena, MS 38941.*

Consumers deserve to know more about their seafood. Consumers need to know what kind of fish they are getting, how the fish were caught or farmed, and consumers should be able to trust the information on labels they buy in stores are accurate. Seafood's path from the fishing boat or farm to people's dinner plates is long, complex, and non-transparent. Because of seafood's traveling path, it is common for mislabeling and fraud. This project focused on checking to see if fishes' labels were correct and to see if carnivores, filter feeders, and omnivores had similar single-nucleotide polymorphisms. The samples used in this research were from Walmart in Greenwood, Mississippi. The DNA of the samples was confirmed by DNA sequencing. Using DNA barcoding to identify these samples will help confirm if fishes' labels bought at the Walmart in Greenwood, Mississippi are correct.

Biological Sciences

A – Saturday 8:00 – 9:00 Posters

B – Saturday 9:15 – 10:15 Posters

1A. Endosome-to-Golgi SNARE Mediation of Liposome

Fusion. Onika Olson, Jared Smothers, Kyoungtae Kim. *Biology, Missouri State University, Springfield, MO 65897.*

SNARE proteins mediate membrane fusion between the Endosome and Golgi. The v-SNARE (vesicular SNARE) Snc2 combines with the t-SNARE (target SNARE) complex composed of Tlg2, Tlg1, and Vti1 to create an active SNARE multiplex. The “zippering” of the assembled SNARE complex is thought to provide the force necessary to draw two opposing membranes into close enough proximity to destabilize and fuse the separate bilayers into one membrane. We utilized an in vitro fusion assay using FRET techniques to measure the fusion efficiency of Endo-TGN SNARES. For this, recombinant SNARE proteins were purified and reconstituted into liposomes containing fluorescent NBD and Liss-Rhodamine lipids. The methods used for proteoliposome construction as well as the future direction of measuring fusion efficiency will be discussed in the subsequent presentation.

1B. Site Directed Mutagenesis of Known Vps1

Ubiquitination Sites. Ryan Windish, Kyoungtae Kim. *Biology, Missouri State University, Springfield, MO 65897.*

Ubiquitination is a cellular process that is important for protein degradation. It occurs through a series of enzymatic reactions in which ubiquitin, a key factor ubiquitously expressed in eukaryotic organisms, tags the substrate proteins to be degraded via proteasomes. Vacuolar Protein Sorting 1 (Vps1), which is yeast’s homologue to mammalian dynamin, has five known ubiquitination sites. This protein is crucial to the retrieval of both Vps10 and Snc1, which play significant roles for intracellular vesicular trafficking pathways. We have performed experiments by mutating the known ubiquitination sites of Vps1 through site directed mutagenesis. A mutant strain harboring Vps1, K561N mutation displayed severe defects in the trafficking of Snc1 and Vps10, suggesting that the Vps1 ubiquitination sites are pivotal for their trafficking toward the Golgi and that proper turnover of Vps1 regulates these cargo trafficking processes.

2A. Assessing Cuticular Hydrocarbon Variation in

Rhagoletis pomonella. Melanie Beehler, *Biology and Chemistry, Lyon College, Batesville, AR 72503*, Jackson H. Jennings, William Etges, *Chemistry and Biology, UA Fayetteville, Fayetteville, AR 72701.*

Rhagoletis pomonella have provided a textbook example of sympatric speciation in the short time span of approximately 150 years. While genetics and transcriptomes of *Rhagoletis pomonella* have been studied (10), cuticular hydrocarbons have not been investigated. In this study, the Etges lab group was able to identify nearly half of the compounds present in the cuticular hydrocarbon profile. All identified compounds were either alkanes or methyl-branched alkanes. Multivariate Analysis of Variance (MANOVA) results reported significant effects of population, sex, and host plant on cuticular hydrocarbon profiles, including a significant population x sex interaction effect. These data provide evidence that apple-attacking flies have diverged from the original hawthorn flies in their hydrocarbons, which are known to mediate sexual isolation between other insect populations and species, and provides groundwork for further studies aimed at understanding what drives sexual isolation between these two types of flies.

2B. Effects of environmental stressors on regeneration in the Axolotl *Ambystoma mexicanum*. Allison Garrett, Madison McGraw, Maryline Jones, *Math & Science, Lyon College, Batesville, AR 72503.*

Axolotl, Ambystoma mexicanum, is a neotenus salamander retaining gills at the adult stage and threatened of extinction in the wild due to increased pollution and predation. This species is notable for its powers of scar-less tissue regeneration and remarkable resistance to cancer, making it a key model for biomedical research. Axolotls are used in particular to develop new technologies against aging, treat human trauma and in research against cancer. The axolotl’s ability to regenerate is strongly linked to its health which is sensitive to environmental stress such as water pH imbalances and onset of stress due to powerful tank filtration systems. Despite knowledge about best rearing practices, specific parameters for avoidance of stress in axolotl care that pertain to the propagation of higher rates of limb regeneration are largely unknown. This study examined the effects of stress factors such as water temperature and presence of substrate against the rate of tail regeneration. Axolotl larvae were exposed to a combination of heated/chilled water and presence/absence of substrate and rate of tail regeneration were measured over a 23-day period after tail amputation. The effect of substrate presence alone yielded no significant difference in the rate of tail regeneration between sample groups in either temperature condition ($p=0.351$). However, larvae in heated conditions displayed a significantly higher average rate of regeneration than those in chilled conditions ($p<0.001$). Our results provide new insights into the ways environmental stressors like temperature and habitat play a role in the metabolic and limb regeneration rates of this salamander.

3A. Exploring the Role of G-Quadruplex Structures in the Mitochondria. Sarah Gilmour, *Biology, Hendrix College, Conway, AR 72032*, Jun Gao, Kevin Raney, *Biochemistry and Molecular Biology, UAMS, Little Rock, AR 72205*.

G-quadruplex structures are unusual four-stranded secondary structures of nucleic acids whose biological function has been the subject of much investigation. Recent studies have shown that quadruplex-forming sequences are overrepresented in the mitochondrial genome. The objective of this project is to investigate the presence of quadruplex structure formation within the mitochondria and to explore some biological functions for these structures. To that end, the BG4 antibody, which is specific for quadruplex structures of DNA and RNA, was stably expressed in *S. cerevisiae* and human HeLa cell lines with a mitochondrial targeting sequence. We hypothesized that this antibody could bind to quadruplex-forming nucleic acids in the mitochondria in order to stabilize the structure and inhibit protein binding at the site of quadruplex formation. Immunofluorescence microscopy was used to visualize binding of the antibody in the mitochondria. Additionally, plating assays on *S. cerevisiae* cultures indicated a defect in mitochondrial function induced by BG4 binding, as cells expressing mtBG4 were unable to utilize glycerol as a carbon source. qPCR was used to determine BG4's effects on mitochondrial copy number, which showed that the BG4 antibody depleted mitochondrial DNA in yeast.

3B. A Comparison of Resting-State Networks as derived from fMRI in Patients with Parkinson's Disease and Healthy Controls. Journey Eubank, *Biology, Hendrix College, Conway, AR 72032*, Aaron Kemp, Linda Larson-Prior, *Psychology, UAMS, Little Rock, AR 72205*.

Parkinson's Disease (PD) is a neurodegenerative disease associated with extensive loss of dopaminergic cells. Classically defined as a movement disorder, PD is also associated with a variety of cognitive impairments. We used resting-state functional magnetic resonance imaging (rs-fMRI) to research functional connectivity (FC) of the brain in patients with PD and age-matched healthy controls (HC). Rs-fMRI provides an opportunity to study correlated patterns of activity in the brain, known as resting state networks (RSNs). A common method of identifying RSNs is through the use of Independent Components Analysis (ICA). This data-driven approach yields spatial maps of correlated brain regions without any a priori assumptions rather than a parcellated predetermined locale. Correlations across the timecourses of the independent components can then be statistically compared in a matrix to quantify the FC among RSNs and the differences between the PD and HC groups. Neuroimaging data included a 7-minute

rs-fMRI scan, a T1-weighted anatomical scan, and a B0 field map. Data were imported to the FSL processing suite (fsl.fmrib.ox.ac.uk/fsl/fslwiki/FSL). 32 subjects were analyzed. The study pipeline included, brain extraction, intensity normalization, slice time correction, and co-registration to each subject's T1 image. Individual subject data were then registered to the Montreal Neurological Institute (MNI) standard space image for group analysis. Post-processing utilized dual regression algorithm in FSL to analyze group differences of functional networks in PD versus HC. Differences were seen in broad networks between groups that included both motor and cognitive functions.

4A. Epigenetic interactions between methyltransferase SWN and chromatin remodeler PKL. Joey Dean, *Natural Sciences, Ouachita Baptist University, Arkadelphia, AR 71988*, Jiaxin Long, Joe Ogas, *Biochemistry, Purdue University, West Lafayette, IN 47907*.

The repressive epigenetic modification H3K27me3 (trimethylation of lysine 27 on histone 3) plays a substantial role in enabling tissue-specific gene expression. Much remains to be understood regarding the establishment and maintenance of H3K27me3-enriched chromatin. CURLY LEAF (CLF) and SWINGER (SWN) are histone-lysine N-methyltransferases that act in separate pathways to promote methylation of lysine 27 on histone 3. Recent work from the lab has revealed that the ATP-dependent chromatin remodeler PICKLE (PKL) acts in a common epigenetic pathway with CLF and indicates that it promotes maintenance of H3K27me3 by promoting chromatin assembly. Based on this precedent, we investigated the relationship between PKL and SWN and whether PKL and SWN act in a synergistic or common pathway. We hypothesize that PKL and SWN work in separate pathways, given previous findings that CLF and SWN act in separate pathways and that PKL acts in a pathway with CLF. To test our hypothesis, we are examining whether double mutant plants lacking SWN and PKL exhibit synergistic phenotypes relative to *swn* and *pkl-1* plants. The phenotypes we are examining include callus formation with varying concentrations of auxin and cytokinin, seed size, and penetrance of the "pickle root" phenotype, which results from expression of embryonic traits in the primary root. The results of these analyses clarify how PKL interacts with distinct K27 methylation pathways to contribute to gene expression and tissue differentiation in plants.

4B. Investigating the Role of Carbon Nano-Onion as an Extracellular Growth Matrix for PC12 Cells. Kayla Haberman, Rachel Bacon, Madison Crosby, Nathan Reyna, Casey Roark, *Biology, Ouachita Baptist University, Arkadelphia, AR 71988*, Rajshekhar A. Kore, Robert Griffin, *Radiation Oncology, UAMS, Little Rock, AR 72205*, German Raul Perez Bakovic, Shannon L.

Servoss, *Chemical Engineering, UA Fayetteville, Fayetteville, AR 72701.*

The lack of neuronal tissue regeneration as a result of acute damage leads to loss of feeling or, in some cases, paralysis. Our emphasis is on the use of carbon nano-onions as an extracellular matrix to promote regeneration. Nano-onions are concentric shells of carbon atoms that are globular in shape with a high surface to volume ratio. This summer we focused on the differentiation of PC12 cells on varying nano-onion gradients on collagen. Cell growth and differentiation was monitored over seven days and compared to appropriate controls. Results and future work will be reported.

5A. Examining the Interaction of the SWR Complex (SWR-C) with Sgo1 in Chromosome Segregation. Jacob Allen Ginter, Ines Pinto, *Biology, UA Fayetteville, Fayetteville, AR 72701.*

The baker's yeast *Saccharomyces cerevisiae*, has long been used as a model organism to study basic cellular processes, and will be used in my proposed studies. In all eukaryotes, DNA organizes itself into chromosomes. DNA wraps around histones, which form nucleosomes, then further condense into chromatin, which makes up each chromosome. Each nucleosome is made up of 4 subunits, labeled H2A, H2B, H3, and H4. Two histones interact with each other to form an octamer, which is what the DNA winds itself around. Previous work in the lab has shown that haploid *S. cerevisiae* can diploidize in the presence of specific histone mutations. The protein complex SWR-C is involved in replacing regular H2A histone subunits with the variant H2A.Z subunits. It has been shown that an increase of H2A.Z subunits near the centromere of chromosomes results in rapid diploidization of haploid cells. Sgo1 proteins are responsible for detecting tension between sister chromatids and arresting the cell cycle if problems with microtubule attachment is detected. I will delete two genes associated with the SWC complex, along with deleting or overexpressing the SGO1 gene, to see how the levels of Sgo1 protein affect the increase-in-ploidy phenotype of the SWR-C mutants. Understanding why specific protein deletions display increased ploidy in *S. cerevisiae* may provide clues as to what mechanisms cause chromosome-segregation associated disorders like Down's syndrome and cancers.

5B. Development of a C57Bl6J Mouse Model for Calcific Aortic Valve Disease progression. Shelby Johns, Ishita Tandon, Kartik Balachandran, *Biomedical Engineering, UA Fayetteville, Fayetteville, AR 72701.* Calcific aortic valve disease (CAVD) is a complex disease which progresses from sclerosis to stenosis, resulting in 50% increased chances of heart failure. The standard of care is valve replacement as diagnostic and therapeutic

strategies are lacking. Current CAVD mouse models are based on either genetic modification or western diets. The goal of this project was to develop a diet based wild-type mouse model of CAVD, which is more relevant to human CAVD progression. C57BL/6J wild-type male mice were fed either a normal or pro-CAVD diet (normal diet + 75 IU/g Vitamin D + 1.5% dicalcium phosphate) for 16 weeks. Echocardiography was performed every four weeks to determine the ejection fraction of the heart. The Pro-CAVD mice showed reduced ejection fraction by twelve weeks. Histological and immunohistological analysis was performed for hallmarks of early CAVD progression. Lipid and Calcium deposition was observed near the aortic valve leaflet commissures at 16 weeks in pro-CAVD mice. Vimentin and α SMA expression patterns suggested increased activation; osteocalcin, osteopontin and Runx2 expression suggested increased osteogenesis; and Ki67 expression suggested increased proliferation near commissures in pro-CAVD mice. Overall, our data suggests we successfully created a wild type CAVD model showing hallmarks of early CAVD progression.

6A. Testing the Prospect of Essential Oils as a Homeopathic Alternative to Antibiotics. Vi Le, Jamie Fletcher, Roger Lightner, Jeff Shaver, *Chemistry, Biology, UA Fort Smith, Fort Smith, AR 72904.*

With certain treatments, like penicillin, becoming less effective due to an increase in antibiotic resistance, alternative methods of treatment need to be tested. For our research project, essential oils (EOs) were tested on different strains of gram-positive rods/cocci and gram-negative rod-shaped bacteria to measure their growth inhibition. Previous research has shown that EOs can inhibit the growth of bacteria. We hypothesized that if a variety of essential oils are screened for activity against fourteen different bacteria, some EOs will inhibit the growth of specific types of bacteria, because of their unique antibacterial properties. Cultured bacteria were exposed to six different EOs and the inhibition zones were measured. Based on our results, in general, gram-negative rods were more prone to inhibition by the selected EOs than gram-positive cocci/rods, with some exceptions. This was not expected, however, as it contradicts the general findings of gram-negative bacteria being more resistant to antibiotics than gram-positive bacteria, because gram-negative bacteria have an outer membrane, LPS core, and a greater ability to mutate and acquire genetic material than gram-positive bacteria. Cinnamon, Tea Tree, and Peppermint exhibited significant bacteria growth inhibition, particularly for gram-negative bacteria, but Lemon was ineffective for all bacteria tested. These findings suggest that further research on the effectiveness of EOs as antibiotics is worth pursuing and may contribute to the development of new alternative treatments. In addition, our current research also focuses on the testing, using both

antibiotic disks and EOs, of isolated and cultured bacteria from environmental samples.

6B. Analysis of *Pseudomonas aeruginosa* Virulence in Wild-Type *Dictyostelium discoideum* Strains. Asher Parvu, *Biology, UA Fort Smith, Fort Smith, AR 72904*, Jeff Shaver, *Biology, UA Fayetteville, Fayetteville, AR 72701*,

Dictyostelium discoideum is an ideal organism to test the pathogenicity of *Pseudomonas aeruginosa*, since it is a unicellular, bacterivorous, haploid eukaryote and its genes share sequence homology with human genes. *P. aeruginosa* is a free living pathogenic bacteria that causes nosocomial infections in immunocompromised patients. The goal of this project is to study the interactions between a wild-type strain of *D. discoideum* and *P. aeruginosa*. Interactions between axenic strains of *Dictyostelium* and *P. aeruginosa* have revealed conserved virulence pathways in *P. aeruginosa*. We hypothesize that the wild-type *D. discoideum* would be resistant to *P. aeruginosa* because wild-type *D. discoideum* have environmentally induced adaptive mechanisms to cope with pathogenic bacteria. Wild-type strains of *D. discoideum* will be isolated from Massard Prairie soil and its interactions with *P. aeruginosa* will be studied and compared to interactions between axenic strain of *D. discoideum* and *P. aeruginosa*.

7A. Timing of Exosome Production Controls Neuron Differentiation in PC12 Cells. Justin McGee, Nathan Reyna, *Biology, Ouachita Baptist University, Arkadelphia, AR 71998*.

Exosomes are extracellular vesicles ranging in size from 40 to 100nm used in cell to cell communication. Research in our lab has shown exosomes isolated from differentiating cells can cause neurite differentiation. However, this initial experiment only used exosomes isolated from fully differentiated cells. To determine the timing of exosome production in relation to differentiation, exosome were isolated from cells prior to and after differentiation. Preliminary analysis reveals that exosomes isolated 6 days after NGF treatment induced more rapid cell differentiation than day 2 exosomes, indicating exosome contents vary with the cell type and development stage.

7B. Effects of Gravity and Varying Wavelengths of Light on Phototaxis in *Dictyostelium discoideum*. Madison Morrison, Jonathan Rankin, Jim Taylor, *Biology, Ouachita Baptist University, Arkadelphia, AR 71998*.

Dictyostelium discoideum is well-known as a model organism due to its atypical life cycle. *D. discoideum* lives as a single celled amoeba until it experiences a lack of resources, at which point the slime mold transitions into a multicellular "slug" stage. This slug senses

changes in its environment and moves toward an optimal position for its survival, at which point it forms a fruiting body and reproduces. It is thought that movement of *D. discoideum* is largely due to cAMP waves which are themselves initiated in response to irradiation by some light source. The effects of red and blue light in association with antigravity conditions (produced by clinostat) were studied for phototaxis and subsequent location of fruiting bodies. Preliminary results indicate that red-blue light has the most significant effect on slug movement, followed by blue light, and finally red light. Results also indicate that gravity does indeed have an effect on slug motility, as slugs in clinostats showed considerably less/more random movement than controls which were stationary in normal gravitational conditions.

8A. It's all in the gill: Functional characterization of gill Na⁺/K⁺-ATPase in freshwater and seawater acclimated rainbow trout. Lane Justus, Christian Tipsmark, Laura Ellis, *Biology, UA Fayetteville, Fayetteville, AR 72701*.

In the gills of rainbow trout, a1a- and a1b-paralogs of Na⁺/K⁺-ATPase are expressed reciprocally during salinity acclimation. The a1a paralog is important in Na⁺ uptake in fresh water (FW) while a1b is involved in salt secretion in seawater (SW), but the functional difference is not clear. This study compared Na⁺/K⁺-ATPase maximal activity (V_{max}) and apparent affinity for Na⁺ and K⁺ (K_m), and the specific inhibitor ouabain in gill of FW and SW rainbow trout (*Oncorhynchus mykiss*). Trout acclimated for two weeks to SW experienced an 8-fold decrease in a1a and a 2-fold increase in a1b when compared to FW control. A coupled Na⁺/K⁺-ATPase enzymatic assay was used and apparent affinity for K⁺ established by varying concentrations of K⁺ while keeping Na⁺ concentration constant and vice versa for apparent K_m for Na⁺. This was followed by Michaelis-Menten curve-fitting and V_{max} and K_m analysis. V_{max} was higher in SW than FW acclimated trout likely due to increased protein abundance. The present study demonstrated no significant difference in apparent affinity for Na⁺ or K⁺ with salinity change suggesting that the functional significance of paralog shift could relate to other kinetic parameters or distinct physiological regulation. Protein expression and apparent ouabain affinity data collected presently will be presented.

8B. Generation of Lipin 5xS/T>A Mutant using CRISPR/Cas9 Methodology. Heidi O'Dell, Michael Lehmann, *Biology, UA Fayetteville, Fayetteville, AR 72701*.

Lipins are proteins required for normal fat storage and fat tissue development in animals, from *Drosophila* (fruit fly) to humans and other mammals. Both *Drosophila* Lipin and mouse lipin1 are highly phosphorylated proteins. Phosphorylation controls

various functions and intracellular localization of the proteins. By targeting specific phosphorylation sites, the functional importance of these sites can be better understood. In this project, a group of sites immediately downstream of the highly conserved N-terminal (NLIP) domain of *Drosophila* Lipin will be targeted. Induced mutations will replace five phosphorylatable serines and threonines with alanines, rendering them non-phosphorylatable (Lipin 5xS/T>A). Included in those phosphorylation sites is a predicted site for the insulin-dependent protein kinase Akt. To create a fruit fly mutant carrying these mutations, CRISPR/Cas9 technology is being employed. Generation and characterization of the Lipin 5xS/T>A mutant will allow us to detect roles that these phosphorylation sites have in regulating Lipin in the fruit fly. The mutant will thus help with the identification of similar roles of the corresponding sites in human lipins.

9A. Human T-Cell Lymphomas Treated with Retinoids. Chris Mizell, Brenda Rosales, Lance Bridges, *Biology, UA Fort Smith, Fort Smith, AR 72904.*

Retinoids, natural and synthetic derivatives of vitamin A, have been used to treat cutaneous T-cell lymphoma (CTCL) for over three decades. Unfortunately, the full clinical potential of retinoids is unrealized due to common adverse side effects associated with use. Multiple human T-lymphoma cell lines were cultured with retinoids at various times and concentrations. Cell growth and viability was assessed with a Trypan blue exclusion assay to determine which treatment conditions maximized the desired outcomes of suppressed growth and cellular death. As the natural role of retinoids in immunity is to target immune cells to the gut by inducing the expression of the integrin $\beta 7$ receptor, the relative expression of this marker was analyzed to determine if its expression correlated with cell death. This approach will optimize conditions to produce desired clinical endpoints and refine retinoid regimens to curtail the unwanted side effects that have limited retinoid use. Future studies will determine if retinoid-induced $\beta 7$ expression is associated with apoptotic death. This work could provide insight into the potential mechanism of retinoids which are a proven beneficial therapy of CTCL.

9B. Soil bacteria resistance to 6 common antibiotics. Evan Merritt, Jeff Shaver, *Biological Sciences, UA Fort Smith, Fort Smith, AR 72904.*

With an increase in the use of antibiotics, antibiotic resistance has become more prevalent in all aspects of biology. Resistance occurring in soil dwelling bacteria is a topic of interest particularly given that many antibiotics are becoming increasingly less effective and creating barriers to agriculture and medicine. Given that bacteria from this area are commonly encountered,

data on the resistance presented by these bacteria can be of great importance. Currently my research focuses on bacteria isolated from soil and exposed to 6 different antibiotics. I hypothesize that these bacteria will show increased resistance to beta lactam antibiotics such as penicillin and amoxicillin while continuing to show susceptibility to non-beta lactam antibiotics. Six pure cultured bacteria were exposed to six differing antibiotics two of which were beta lactam antibiotics. Gram staining was performed on all six cultures of the six four were gram negative bacilli (two appeared spore forming), one a gram negative bacilli, and one gram positive cocci. Gram positive cocci appeared to have the greatest resistance to all antibiotics, and showed no inhibition with beta lactam antibiotics. The two suspected spore forming gram positive bacilli also showed resistance to the beta lactam antibiotics. The remaining isolates did not show resistance to beta lactam antibiotics. The data suggests that further research is required for definitive conclusions given that only half of the isolates experienced resistance to the beta lactam antibiotics. However, the six isolates showed varying resistances to all six antibiotics. This leads to the conclusion that soil bacteria show a wide range of differing resistances depending on the antibiotics used and not necessarily a significantly larger resistance to beta lactams. Future research will focus on identification of the presence of the beta lactamase gene through PCR, and further sampling to increase the significance of the data.

10A. Do nanodiamonds show antibacterial properties toward pathogenic bacteria. Tristen C. Unruh-Cone, Bailey McMullen, Janaki K. Iyer, *Biology, Northeast State University, Tahlequah, OK 74464.*

With the number of antibiotic-resistant strains of bacteria increasing, it has become vital that feasible alternatives to antibiotics are discovered. Diamond nanoparticles (DNPs) have provoked the interest of microbiologists and other scientists due to their small size, inert chemical nature and the ability to modify their surface with different functional groups. DNPs have been shown to be nontoxic towards eukaryotic mammalian cells, however our experiment focused on the antibacterial activity of DNPs against prokaryotic cells. The hypothesis of this study was that DNPs would have an antimicrobial effect on bacterial growth. The prokaryotic model bacteria tested in this study was *Escherichia coli* strain C15 that was isolated from a patient suffering from pyelonephritis (kidney infection). We treated suspensions of *E. coli* strain C15 with different concentrations of DNPs. After the incubation period, the bacteria were diluted and spread onto sterile L-agar plates. The colony forming units (CFU) were enumerated and compared with the untreated sample. The results showed that treatment of *E. coli* strain C15 with DNPs yielded a statistically significant ($P < 0.05$) decrease in CFUs compared to the untreated samples. These findings indicate that the DNPs indeed

exhibit antimicrobial properties. Thus, DNPs are good candidates for antibacterial applications.

10B. Characterizing the role of Mcm10 in coordinating genome replication and checkpoint signaling pathways.

Brandy Fultz, Casey Eddington, Sapna Das-Bradoo, *Natural Sciences, Northeastern State University, Tahlequah, OK 74464.*

Minichromosome maintenance protein 10 (Mcm10) is an essential replication protein that is upregulated in cervical cancer and glioblastomas; in fact, the expression of Mcm10 correlates with the stages of cancer progression, arguing that it might contribute to tumor aggressiveness. These studies are consistent with the notion that Mcm10 contributes to genetic changes associated with genome instability, as seen in cancer cells. We hypothesize that Mcm10 functions during replication and checkpoint activation pathways to maintain genome stability. Yeast two hybrid (Y2H) results from our lab show a robust interaction between Mcm10 and Pol2, the catalytic subunit of Polymerase epsilon (Polε). Moreover, Mcm10 interacts with the C-terminus domain of Pol2, an essential domain that participates in S phase checkpoint activation. In addition, we have mapped the interaction of Mcm10 to a 200 amino acid range within the checkpoint domain of Pol2 and used site-directed mutagenesis to further narrow the site of interaction. To substantiate the Y2H, we have confirmed the physical interaction of Mcm10 and Pol2 through co-immunoprecipitation (Co-IP). Currently, we are conducting arrest and release experiments to conclude if the interaction of Mcm10 and Pol2 is essential for normal replication. Our data sheds new light on the function of Mcm10 in DNA replication and S phase checkpoint pathways. Overall, understanding Mcm10 and its functions will help us understand how it supports genome integrity, a lack of which leads to genetic changes with tumorigenic consequences.

11A. Functional Characterization of Putative MAP Kinase Phosphorylation Sites of the Metabolic Regulator Lipin.

Hannah D. Davis, Stephanie Hood, Josephine Gottsponer, Michael Lehmann, *Biology, UA Fayetteville, Fayetteville, AR 72701.*

Lipin proteins play central roles in the control of lipid metabolism. As enzymes, lipins convert phosphatidic acid into diacylglycerol, which is used either for the synthesis of neutral fats (triacylglycerols, TAGs), or the synthesis of membrane phospholipids. As transcriptional co-regulators, they control genes involved in energy metabolism. Functions of both mouse lipin 1 and *Drosophila* Lipin are controlled by phosphorylation. In both species, nuclear translocation, which is required for execution of the transcriptional co-regulator function, is controlled by the insulin-sensitive protein kinase Target of Rapamycin (TOR). Interestingly,

both mouse lipin 1 and *Drosophila* Lipin also contain putative phosphorylation sites for mitogen-activated protein (MAP) kinases. MAP kinases have so far not been implicated with controlling lipin functions. To examine the functional importance of these sites, we are in the process of generating and characterizing a *Drosophila* Lipin mutant in which the MAP kinase sites have been rendered non-phosphorylatable. With the use of CRISPR/Cas9 technology, a group of eleven serine and threonine residues predicted to be MAP kinase target sites are converted to alanine residues, generating a Lipin 11xS/T>A mutant. Characterization of the mutant flies will involve examination of viability, developmental timing, fat storage, and intracellular localization of the mutant Lipin protein.

11B. Anthropogenic Influence of Increasing Phosphorus and Light on Freshwater Gastropods.

Anabel Jones, Brooke Howard-Parker, Michelle Evans-White, *Political Science and Biology, UA Fayetteville, Fayetteville, AR 72701.*

Freshwater systems provide services to humans (e.g. drinking water, food, recreation, etc.) and animals (e.g. water, food, habitat, etc.), as well as performing ecologically important services such as carbon (C) and nutrient cycling. These systems are at risk due to expanding urbanization and agriculture and the pressure to meet human needs. Inputs to streams from human activities can reduce overall health and functionality of these systems including their ability to continue providing ecosystem services. Human inputs can influence energy and nutrient transfer across trophic levels, affecting biodiversity, and large-scale biogeochemical cycling, which relates to climate change. Part of the goal of ecological research is to find a balance between meeting human needs while maintaining the integrity of natural systems and macroinvertebrates are commonly studied for assessing freshwater system health in the face of growing pressure from human activities. We used freshwater snails (family: Physidae) as our study organism because 1) they are important top-down controls on microbial biofilms and serve as stream nutrient recyclers and 2) they were sufficiently abundant to provide us with the greatest statistical power through replication. We performed a 23-day feeding experiment using leaf litter discs that were pre-conditioned in a full-factorial, 2x3 (two light levels [ambient=100%/full light, shade=19% of full light] and three phosphorus [P] levels [low=10ug/L, moderate=100ug/L, high=500ug/L]) layout, resulting in six unique feeding treatments with 10 replicates per treatment (n=10; N=60). We hypothesized that snail shell length, shell width, and soft body dry mass would increase with increasing P treatments, especially under shaded conditions. Light had a significant main effect (p=0.0184) on snail shell width where increases were greater under shaded conditions, but P level was not

important ($p=0.0538$) and no interaction occurred ($p=0.4790$). There were no significant main effects (light $p=0.1338$; P $p=0.0538$) or treatment interaction ($p=0.4790$) affecting snail shell length, but increases along the P gradient were observed, especially under shaded conditions. There were no significant main effects (light $p=0.897$; P $p=0.904$) or treatment interaction ($p=0.419$) affecting snail soft body dry mass and no clear patterns emerged, but decreases were seen in all cases except for under ambient-moderate P and shaded-high P conditions. Trends in shell changes were generally supportive of our hypothesis, but soft body mass results could indicate snails may be diverting C energy towards metabolic adjustment to stressful environmental factors rather than laying down biomass.

12A. Mapping Neurodegenerative Diseases. Mark Spradlin, Brandy Ree, Jeff Shaver, Prescilla Devora, Debbie Robertson, *Biology, UA Fort Smith, Fort Smith, AR 72904.*

Huntington's, Parkinson's, and Alzheimer's are all neurodegenerative diseases commonly associated with improper functioning NMDA receptors. NMDA receptors are essential neurotransmitter receptors found in many species, including mammals and *Drosophila melanogaster*, and function in memory and learning formation. The NMDA receptor is regulated via protein-tyrosine phosphorylation (ptpmeg). Ptpmeg is a highly expressed protein in the central nervous system of *Drosophila*, where it is responsible for the proper formation and maintenance of axonal projections in the mushroom body. The mushroom body is the center for olfactory learning and memory. Ptpmeg has two vertebrate homologs, PTPN3 and PTPN4 that are expressed in the nervous system of mammals. Studies have shown that PTPN4 physically associates with the NR2B subunit of the mammalian NMDA receptor. Preliminary data suggests that Ptpmeg binds directly to the dNR1 subunit of the NMDA receptor in *Drosophila* brains. This study will test the hypothesis that Ptpmeg acts to reduce dNR1 phosphorylation in *Drosophila* neurons, based upon the function of phosphatases in removing phosphate groups from proteins. This hypothesis will be tested by analyzing the effect of mutant Ptpmeg compared to wild type Ptpmeg on phosphorylation levels of dNR1 in *Drosophila*. Clarification of the functional impact of Ptpmeg: dNR1 interaction could better aid us in the understanding of the role this interaction plays in development of disease. Thus, opening the door to new pathways to understanding and treating neurodegenerative diseases in humans.

12B. Monitoring Water Temperatures in Massard Creek with Digital Loggers. Josie Nuñez, Dave Mayo, Jeff Shaver, Jay Randolph, *Biology, Earth Science, UA Fort Smith, Fort Smith, AR 72904.*

South Fort Smith was once part of Massard Prairie, a vast tallgrass ecosystem that has largely been lost to development. Now only about 2% of the 10,000-acre prairie remain as isolated patches in Ben Geren Park and the Fort Smith Regional Airport. Jay Randolph, horticulturist and Certified Golf Course Superintendent at Ben Geren Golf Course is leading an effort to restore several acres of tallgrass vegetation using seeds harvested from remnant patches of native prairie. UAFS STEM faculty and students are partnering with Randolph to monitor the environmental impact of the restoration on the Massard Creek watershed. Recognizing that temperature is a crucial component of water quality, a digital temperature logger was deployed in Massard Creek adjacent to the restoration area. A second logger was deployed nearby to record air temperature. The loggers record water and ambient air temperature once every 15 minutes. Once a week, stored data is downloaded using a cellphone app and relayed to a desktop computer at UA Fort Smith. The nearly continuous record of water temperature changes will be used along with other data to test the hypothesis that tallgrass restoration is beneficial to water quality in Massard Creek watershed.

13A. Examining the Expression Profile of PD-1/PD-L1 in EGFR-Positive Glioblastoma Multiforme. Kelsey O'Brien, Sheldon McCown, Alyson Cole, Nick Kowalkowski, Mary Beth Jones, Kaitlyn Thomas, Blake P. Johnson, *Biological Sciences, Ouachita Baptist University, Arkadelphia, AR 71998.*

Glioblastoma (GBM) is a highly aggressive and lethal form of primary brain tumor with an extremely poor prognosis. Systemic suppression of the immune system, specifically T-cell impairment, significantly contributes to GBM development and progression. Recent advances in cancer immunotherapies have shown great promise in alleviating such tumor-associated immunosuppression, namely programmed cell death 1 (PD-1)/programmed death ligand 1 (PD-L1) checkpoint inhibitors. Regrettably, early clinical studies evaluating the efficacy of PD-1 inhibition in recurrent GBM have rendered only modest improvements in overall survival rates; the clinical effects of PD-L1 inhibition, however, remain poorly understood. Here, we show that EGFR dysregulation correlates with PD-L1 expression in GBM. Furthermore, PD-L1 is highly upregulated in EGFRΔIII-positive relative to U87-vector. Collectively, these findings indicate that EGFR signaling influences PD-L1 expression levels, inclusive of various cancer cell lines, therefore highlighting the potential of PD-L1 inhibition in EGFR-positive tumor types.

13B. The Effects of Light Intensity on the Cultivation of *Arthrospira platensis*. Jonathan Rankin, Madison

Morrison, James Taylor, *Biology, Ouachita Baptist University, Arkadelphia, AR 71998.*

Arthrospira platensis, more commonly named spirulina, is a filamentous cyanobacteria which grows naturally in warm, alkaline lakes located in Africa as well as Central and South America. This cyanobacteria is a known superfood supplement due to its high protein, vitamin, and mineral content. In this experiment, four containers filled with spirulina in solution were placed into chambers containing white light, but differed in light intensities. Chamber A contained an intensity of 18 $\mu\text{mol}/\text{m}^2/\text{s}$, while chamber B contained an intensity of 10 $\mu\text{mol}/\text{m}^2/\text{s}$. Each experiment was allowed to run for a total of 48 hours with cell counts and oxygen production examined every 24 hours. Chamber A resulted in a total average of 2.4 mL after 24 hours and 3.7 mL after 48 hours, while chamber B produced an average of 1.5 mL after 24 hours and 2.0 mL after 48 hours. The cell counts increased over the 48 hour periods. Chamber A resulted in an average increase in cell growth of 16,847 cells/mL after 24 hours and 18,590 cells/mL after 48 hours, while chamber B resulted in an average increase in cell growth of 18,416 cells/mL after 24 hours and 25,257 cells/mL after 48 hours. Therefore, it can be concluded that a higher intensity light will result in greater oxygen production, while a lower intensity light appeared to result in a higher rate of population growth.

14A. Mechanistic basis of death receptor 5 regulation by a natural product in breast cancer cells. Andre Figueroa, *Biomedical Engineering, UA Fayetteville, Fayetteville, AR 72701*, Harsh Patel, M. Saeed Sheikh, *Pharmacology, SUNY Upstate Medical University, Syracuse, NY, 13210.*

From all cancer types in females, breast cancer has the highest projection for new cases and the second highest projection of deaths in the United States in 2018. This creates the necessity of new treatment methods to be developed constantly. It has been previously shown that plant based compounds are a very effective source of pharmaceutical drugs, including many that fight cancer. QA, a natural derived compound, is a potential novel anticancer agent previously studied in the laboratory, which has been seen to mediate anticancer effects in human breast cancer cells. QA, at least in part, upregulates death receptor 5 (DR5) and consequently induces apoptosis in in vitro human breast cancer cell lines. However, because QA's mechanism of action is still unknown, this study aimed to examine protein stability as a possible mechanism of DR5 upregulation by QA. In this study, MCF-7 human breast cancer cell lines were treated with QA or dimethyl sulfoxide as a control for approximately 24 hours. Cycloheximide (CHX) was then used to inhibit total protein synthesis, including DR5. This allowed a study of DR5 protein

stability independent from synthesis. Then, samples underwent CHX treatment, and harvested 1, 2, 3, and 4 hours after. From this process, cell lysates were prepared for Western blot analysis to determine DR5 levels. Main results of this study show that in the first 4 hours of CHX treatment there are no major differences in stability between QA-treated and control groups and that shorter time points could provide more insight into this mechanism.

14B. Determining the effect of alpha-synuclein on differential susceptibility in Parkinson's disease.

Manasa Veluvolu, Tara Stuecker, Ben Fahey, Jeffrey Lewis, *Chemistry, Biology, UA Fayetteville, Fayetteville, AR 72701.*

Parkinson's disease is a disorder that results in symptoms such as increase in muscular rigidity and tremors as well as changes in posture, walking, and/or speech. It is a progressive disease that can significantly decrease quality of life over time. A characteristic of PD is the degradation of dopaminergic cells, but also the accumulation of Lewy bodies, within the brain. A main component of these bodies is the protein alpha-synuclein. All individuals have this protein, but the mechanism by which they turn into deadly aggregates that kill dopaminergic cells is still unknown. The purpose of this study is to determine how α -syn is increasing in toxicity to cause PD by studying the protein and its expression in the model eukaryotic organism, *Saccharomyces cerevisiae*. Our lab has discovered that compared to the usual strain of yeast used to experiment for PD studies, other wild yeast strains can have increased or decreased susceptibility to this protein. We hope that by understanding differential gene expression with which genes are being under- or over-expressed as a result of α -syn production and its toxicity, we can better understand what genes are linked to this disease. By performing RNA-seq to determine how the transcriptional response differs between the various strains, we can help further our understanding of the pathways that can be targeted to decrease PD prevalence. This can be highly beneficial for precision medicine in the future in diagnosing and treating PD.

15A. Using a molecular-genetic approach to investigate the interactions between rice and nitrogen-fixing bacteria, *Azospirillum brasilense*.

Randall Rainwater, Jacklyn Thomas, Grant Wiggins, Qinqing Yang, Yasir Rahmatallah, Galina Glazko, Arijit Mukherjee, *Biology, University of Central Arkansas, Conway, AR 72035.*

Nitrogen availability is limiting to plant growth and has long been overcome through applications of nitrogen-rich fertilizer. While this has revolutionized crop yield worldwide, it has come at substantial economic, environmental, and health cost. Excess nitrogen from

fertilizer run-offs in drinking water can be linked to serious health problems. Biological Nitrogen Fixation (BNF) is increasingly viewed as a viable alternative to fertilizers for supplying nitrogen to plants. Several reports have shown that the BNF in cereals (e.g., rice, corn, wheat, etc.) comes from nitrogen-fixing bacteria. For instance, major cereal crops can form beneficial associations with nitrogen-fixing bacteria like *Azospirillum*. Our current understanding of the molecular aspects and signaling that occur between important crops like rice and these nitrogen-fixing bacteria is limited. In this study, we used an experimental system where the bacteria could colonize the plant roots and promote plant growth in wild type rice and symbiotic mutants (*dmi3* and *pollux*) in rice. Our data suggest that plant growth promotion and root penetration is not dependent on these plant genes. We then used this colonization model to identify regulation of gene expression at two different time points during this interaction: at 1day post inoculation (dpi), we identified 1622 differentially expressed genes (DEGs) in rice roots and at 14dpi, we identified 1995 DEGs. We performed a comprehensive data mining to classify the DEGs into the categories of transcription factors (TFs), protein kinases (PKs), and transporters (TRs). Several of these DEGs encode proteins that are involved in the flavonoid biosynthetic pathway, defense and hormone signaling pathways. We also identified genes that are involved in nitrate and sugar transport and other genes that are implicated to play a role in other plant-microbe interactions. Overall, findings from this study will serve as an excellent resource to characterize the host genetic pathway controlling the interactions between non-legumes and beneficial bacteria. The use and improvement of such a promising agricultural tool could provide enormous economic, environmental, and health benefits.

15B. Characterization of Cooking Smoke and Related Health Effects in Kanembwe, Rwanda. Mason Rostollan, Leah Horton, *Biology, University of Central Arkansas, Conway, AR 72035*.

Globally, emissions from traditional cooking methods produce large amounts of smoke that lead to increased particle inhalation by individuals cooking. Due to existing gender roles, those affected are primarily women and children. A potential partial solution to this problem may lie in an alternative cooking method: a rocket stove. Previous work has shown rocket stoves reduce the amount of wood needed compared to traditional three-stone fires and that the rocket stoves burn the wood more completely. In this study, set in Kanembwe, Rwanda, we characterize smoke particles abundance produced by each cooking method (rocket stoves and three-stone fires) via scanning electron microscopy (SEM). We further characterized the smoke particle composition by energy dispersive x-ray

spectroscopy (EDS). To paint the study into context, semi-structured interviews were conducted among research participants to gain a better understanding of their perception of personal health and the perceived changes that rocket stoves had on the user's health. We further measured the peak expiratory flow rate (PEFR) of each participant as an indicator of lung health to quantify an effect of the rocket stove intervention on participants' lung health. The data suggest a higher abundance of all particle sizes in the three-stone fire except for fine particles which were in higher abundance in the rocket stove. Cooking method had no effect on lung health with respect to PEFR values. However, oral responses suggest less visible and inhaled smoke from participants using the rocket stoves and that the participants can spend less time near the smoke when cooking.

16A. Evaluating the Effect of Mutant EGFR on GPIT Subunit Expression in Glioblastoma Multiforme. Sheldon McCown, Kelsey O'Brien, Blake P. Johnson, *Biology, Ouachita Baptist University, Arkadelphia, AR 71998*.

The glycosylphosphatidylinositol (GPI) anchor is a lipid and glycan modification added to the C-terminus of substrate proteins in the endoplasmic reticulum via the multi-subunit GPI transamidase, or GPIT. Several subunits of GPIT, namely GPAA1, have previously been characterized as oncogenes across a variety of tumor types, specifically breast cancer where it contributes to enhanced cellular invasion. Using a *C. septicum* alpha toxin enrichment strategy, we have previously documented significantly elevated plasma levels of GPI anchored proteins occurring in glioma patients relative to non-malignant controls. Furthermore, we have previously uncovered significant increases in GPIT subunit levels, notably GPAA1, occurring in GBM relative to normal human astrocyte controls, which corresponded with increases in GPI anchored protein content. Interestingly, GPAA1 overexpression has previously been linked to physical association with EGFR in multiple epithelial tumor types, leading to increased GPIT activation via PIG-T and PIG-U phosphorylation. In this study, we aimed to evaluate the expression profile of the GPI biosynthesis pathway in the context of amplified, overexpressed, and/or mutant EGFR-GBM. Collectively, these studies will better our understanding of the oncogenic relationship between GPIT and EGFR and the therapeutic potential for GPIT inhibition in EGFR-positive GBM.

16B. Antibiotic Susceptibility of *Staphylococcus aureus*. Lindsey DeSoto, Ruth Plymale, *Biology, Ouachita Baptist University, Arkadelphia, AR 71998*.

Methicillin-resistant *Staphylococcus aureus* (MRSA) is an

antibiotic-resistant pathogen that causes many health problems, and can be fatal when it infects major organs. The CDC approximates that nearly 94,400 patients in the United States suffer from MRSA each year. The goal of this project is to find antibiotics that may increase the number of therapeutic options for Staphylococcus aureus infections. Seventy nutrient-limited, antibiotic-producing soil bacteria have been previously tested using a collard seed germination assay in order to determine the toxicity of their antibiotics. Twenty-eight of these bacteria allowed collards seed germination rates of 90% or higher, showing that the antibiotics produced were of low toxicity. These twenty-eight bacteria were then grown up on tryptic soy agar plates, and colonies from each bacterium were grown up in two different types of media—peptone starved or glucose starved. Each bacterium was grown on the starvation media in a shaking incubator for five days. An acetonitrile: water: acetic acid solvent was then added in order to extract the antibiotics produced by the starving bacteria. The acetonitrile solvent was then evaporated off the antibiotics and the antibiotics were resuspended in water and filter sterilized. The effect of the sterile antibiotics on S. aureus NRRL B-767 were then tested in a cellular respiration assay using 2,3,5-triphenyl tetrazolium chloride (TTC). The results from these tests will be presented.

17A. It takes guts to be a killifish: Investigating molecular mechanisms of solute and water transport in fish intestine. Saxyam Gautam, Julie A. Stanley, Christian K. Tipsmark, *Chemistry, Biology, UA Fayetteville, Fayetteville, AR 72701*.

The Atlantic killifish (*Fundulus heteroclitus*) is a hardy euryhaline teleost which thrives in both fresh water and seawater by regulating the uptake and excretion of water and solutes. In fresh water, the main role of the intestine is digestion with some ionoregulatory retention of ions from the diet. In seawater, killifish actively drink seawater to regulate blood volume; their intestine then prevents dehydration via solute-linked osmosis. The present study investigates expression of genes thought to be critical to solute and water handling by intestinal epithelia. Specifically we studied the Na,K,2Cl cotransporter that is instrumental in secondary active solute transport, aquaporins being the conduit for water movement and finally tight junction claudin proteins that define the paracellular barrier between cells. Tissue distribution analysis confirmed that the analyzed genes are highly expressed in killifish intestine when compared to other tissues. Real-time qPCR analysis showed that intestinal mRNA expression of Na,K,2Cl cotransporter and aquaporin paralogs were elevated after seawater acclimation. One claudin paralog was specifically expressed in posterior intestine of freshwater fish, suggesting that this gene product has a distinct function in this intestinal segment allowing

killifish to ionoregulate in fresh water. Protein expression analysis by Western blotting and fluorescence microscopy is underway and this data will be presented.

17B. IoT Bluetooth Tracking and a Digital Eye: Alternatives to Ocular Prosthetics. Carter Buckner, Ian Harris, *Computer Science, UA Fayetteville, Fayetteville, AR 72701*.

Ocular Prosthesis is a common route taken after any procedure to remove a deformed or malevolent human eye (i.e. atrophy, injury, or infection). An ocular prosthetic is typically split into two parts: the ocular implant and the scleral prosthetic. The retention of muscles tissues can allow, in some cases, for the tissues to fuse together with the ocular implant (dependent on implant type) and allow for limited control of the prosthetic (i.e. eye tracking). The project tests hardware possibilities (and limitations) of small hardware (i.e. a TinyScreen and Raspberry Pi) and explores the possibilities of creating an ocular prosthetic that tracks to a user's real eye. This research project aims to improve eye tracking in ocular prosthetics by:

- Testing the extent of the TinyDuino processor, Bluetooth, and TinyScreen shield at producing a realistic image of an eye that tracks eye movement from the user's native eye.
- Communicative Bluetooth capabilities of the Raspberry Pi B+ and Bluetooth Low Energy TinyShield.

18A. Glucose Availability Impacts Proteotoxic Stress. Landon Gatrell, Mindy Farris, Whitney Wilkens, Priya Rana, *Biology, University of Central Arkansas, Conway, AR 72035*.

Alterations in protein folding may lead to aggregation of misfolded proteins, ultimately leading to toxicity and cell death. Protein aggregation has been shown as a normal consequence of aging, but it is largely associated with age-related disease, particularly neurodegenerative diseases like Alzheimer Disease (AD) and Huntington Disease (HD). Under normal circumstances, glucose enrichment shortens the lifespan of the model organism *Caenorhabditis elegans*; however, recent research suggests that glucose enrichment actually provides some protection against cell stress, including proteotoxicity. Huntington Disease is a useful model for neurodegenerative research, as it is strictly genetic and caused by mutation of a single gene. We are investigating glucose-mediated neuroprotection against Huntington Disease models of the nematode *Caenorhabditis elegans*. Using multiple strains of *C. elegans*, we investigated glucose-mediated neuroprotection against polyglutamine phenotypes. We found that glucose enrichment negatively impacted lifespan consistently across strains, though the only additive effect of polyglutamine and glucose occurred when polyglutamine was expressed in body-wall

muscles. Motility of worms was only affected by polyglutamine or glucose on Day 1. Reproduction of worms was negatively impacted by both polyglutamine and glucose, and this effect was additive. Our results suggest that there may be a difference in the mechanisms of proteotoxicity based on the cell type in which it occurs. Additionally, it appears that the lifespan-shortening effect of glucose overshadows the neuroprotective effect; this possibly occurs by preserving short-term function of neurons through energy availability increase while leaving the aging effect intact. Neurodegenerative diseases represent a significant threat to national health and healthcare expenses. By understanding the mechanisms behind glucose-mediated neuroprotection, we can begin to understand the underlying toxic factors present in HD, which are currently unknown, and potentially isolate target areas for treatment of HD.

18B. Butanone Association Learning and Short-term Memory in Wild-type and Poly-Q Caenorhabditis elegans. Priya Rana, Whitney Wilkins, Mindy Farris, Landon Gatrell, *Biology, University of Central Arkansas, Conway, AR 72035/*

Butanone Association Learning and Short-term Memory in Wild-type and Poly-Q Caenorhabditis elegans By Whitney Wilkins, Priya Rana, Dr. Mindy Farris, Landon Gatrell Abstract This experiment investigates C.elegans capability of changing their behavior in response to a conditioned stimulus paired with an unconditioned stimulus. Strains of wildtype (N2) and poly-glutamine (poly-Q) model AM101-Q40 were used for learning association to ten percent butanone. In previous studies, N2 has demonstrated a positive association to butanone after exposure to it in the presence of food. AM101-Q40 has not yet been examined. This strain serves as a model for Huntington disease, as polyglutamine expansion in the neurons causes increased proteotoxicity with age. Common symptomology within Huntington disease patients is a decrease in cognitive functioning before motor dysfunction occurs, primarily in the prodromal phase. AM101-Q40 individuals are to be observed for a similar pattern of early cognitive deficiencies in learning and short-term memory. Methodology was adapted from the C. elegans Positive Butanone Learning, Short-term, and Long-term Associative Memory Assays protocol (Kauffman et al. 2011). Chemotaxis assays were conducted on NGM plates vacant of OP50 Escherichia coli with ten percent butanone and ninety-five percent ethanol spotting over 0.4M sodium azide, locations separated from one another and the deposition origin. A compilation of L4 and young adult populations were used for each assay. Thus far, two naive assays and two zero time point assays after one-hour long exposure to ten percent butanone with OP50 E. coli were conducted. Results suggest that N2 are capable of

butanone association after butanone inoculation, and AM101 are less so by a Learning Index of 0.637. The ages in which assays were conducted were before typical neuronal degradation occurs in AM101-Q40, suggesting the mechanism(s) for learning are severely inhibited before full proteotoxicity of the neurons. Further experimentation is currently being conducted, extending time points post butanone inoculation for analysis of short-term memory References Brignull, H. R., Morley, J.F., Morimoto, R. I. (2007). The stress of misfolded proteins: C. elegans models for neurodegenerative disease and aging. *Advances in Experimental Medicine and Biology*, 549, 167-189 Kauffman, A., Parsons, L., Stein, G., Wills, A., Kaletsky, R., Murphy, C. (2011) C. elegans Positive Butanone Learning, Short-term, and Long-term Associative Memory Assays. *Journal of Visualized Experiments* (49), e2490 Paulsen, J. S. (2011) Cognitive impairment in Huntington disease: diagnosis and treatment. *Current Neurology and Neuroscience Reports*, (5), 474 Torayama, I., Ishihara, T., and Katsura, I. (2007) Caenorhabditis elegans integrates the signals of butanone and food to enhance chemotaxis to butanone. *The Journal of Neuroscience: The Official Journal of The Society For Neuroscience* 27(4), 741–750.

19A. Collagen Alters Tumorigenic Behavior of Papillary Thyroid Cancer Cells Harboring BRAFV600E Mutations. Haylee Oliver, Jonathan Jenkins, Anna Sharabura, Jordan Carl, Laura J. MacDonald, *Biology, Hendrix College, Conway, AR 72032.*

Thyroid cancer is the most common endocrine malignancy, and incidence is expected to exceed that of colon cancer by 2030. Papillary thyroid cancer is typically more aggressive and is associated with mutations in BRAF, while mutations in RAS are associated with follicular thyroid cancer. Jolly and others reported that papillary thyroid tumors derived from cells harboring activating BRAFV600E mutations and PTEN deletions are enriched with fibrillar collagen that corresponds with decreased survival. We investigated whether growth on collagen and other extracellular matrix components affected sensitivity to MEK and AKT inhibition. Cell lines derived from mouse models of papillary thyroid cancer tumors were grown in the presence and absence of thin plated collagen I, collagen IV, or fibronectin and assessed for rate of growth and sensitivity to inhibitor treatments using the GR50 metric. Growth on thin collagen contributed to a more mesenchymal morphology, increased proliferation, and decreased sensitivity to chemotherapy drugs, suggesting that collagen plays an important role in dictating tumor cell behavior that may lead to increased disease progression.

19B. MEK Inhibition Decreases Motility in Papillary Thyroid Cancer Cells Harboring BRAFV600E Mutations.

Madison Blue, Karen Morris, William Gibson, Roshaneh Ali, Laura J. MacDonald, *Biology, Hendrix College, Conway, AR 72032*.

The rate of diagnosis of thyroid cancer is increasing faster than that of any other cancer. The two most common types of thyroid cancer are papillary thyroid cancer, associated with mutations in BRAF, and follicular thyroid cancer, associated with mutations in HRAS. Both mutations occur in the MAPK signaling pathway yet display unique morphology, progression, and metastasis. In this study, cell lines derived from mouse models of papillary and follicular thyroid cancer containing either a BrafV600E or HrasG12V mutation, respectively in combination with PTEN deletion were examined through time-lapse microscopy to evaluate differences in motility. Papillary thyroid cancer cell lines and follicular thyroid cancer cell lines displayed similar overall motility, but differed when treated with a MEK inhibitor. Notably, motility of follicular thyroid cancer cell lines was unaffected by MEK inhibition, but papillary thyroid cancer motility was significantly reduced. Collectively, our results suggest the MAPK signaling pathway is critical for motility in papillary thyroid cancer cells, but not follicular thyroid cancer cells.

20A. Antibiotic Responsiveness in Mycobacterium smegmatis. Kailee Jones, Ruth Plymale, *Biology, Ouachita Baptist University, Arkadelphia, AR 71998*.

Antibiotic resistance is an area of growing concern in the medical field. Previously treatable illnesses are now not responsive to some antibiotics. This growing resistance problem leads us to a search for antibiotics that could offer new treatment options. Tuberculosis, though not a common problem in the United States, is one of the more serious illnesses among the antibiotic resistance spectrum. Antibiotic resistant strains of pathogens are generally caused by the misuse of therapeutic antibiotics. Once these resistant antibiotic strains are present in a population, they are more likely to spread and infect others. In areas where proper treatment is not available for tuberculosis, antibiotic resistant strains begin to grow out of control. Throughout this project, we are looking for alternative antibiotics that could potentially be used to control Mycobacterium tuberculosis, the bacterium that causes tuberculosis. However, because of the risks associated with using M. tuberculosis in the lab, Mycobacterium smegmatis mc2155 was used as a surrogate. M. smegmatis is similar in cell structure and size to M. tuberculosis, leading us to believe the results of the antibiotics on M. smegmatis would be comparable to those on M. tuberculosis. Antibiotics were produced from different soil bacteria grown in either peptone starved or glucose starved media, and the antibiotics were extracted using an acetonitrile:water:acetic acid solvent. The extracted antibiotics were tested against

M. smegmatis to determine their success at inhibiting cellular respiration. The effectiveness of the lab-produced antibiotics was determined using 2,3,5-triphenyltetrazolium chloride (TTC) and was compared to that of isoniazid, a commercial antibiotic commonly used in tuberculosis treatment. The results of these cellular respiration assays will be presented.

20B. Measuring the Effects of Natural Antibiotics on Candida albicans. Mallory Tabler, Ruth Plymale, *Biology, Ouachita Baptist University, Arkadelphia, AR 71998*.

The problem of antibiotic resistance has grown over the decades due to improper prescription dosages, not finishing prescriptions, and simply the evolution of pathogens. When antibiotics targeted to kill a specific pathogen start to not work, infections of the pathogen become much harder to treat and, as a result, are more dangerous. For example, fluconazole-resistant Candida is ranked as a serious threat according to the CDC, causing 3,400 infections and 220 deaths annually. We are working to address the problem of fungal antibiotic resistance by isolating antibiotic-producing soil microbes and screening the antibiotic compounds against Candida albicans. Specifically, isolated antibiotic-producing bacteria were grown in starvation conditions and antibiotic extracts were prepared using an acetonitrile:water:acetic acid solvent. These antibiotic mixtures were screened in a cell viability assay using susceptible C. albicans (NRRL Y-12983) and resazurin dye. The results of these viability assays will be presented.

21A. Using a molecular-genetic approach to investigate the interactions between rice and nitrogen-fixing bacteria, Azospirillum brasilense. Grant Wiggins, Quinqing Yang, Randall Rainwater, Charles Wilson, Allee Haynes, Arifit Mukherjee. *Biology, University of Central Arkansas, Conway, AR 72035*.

Nitrogen availability is limiting to plant growth and has long been overcome through applications of nitrogen-rich fertilizer. While this has revolutionized crop yield worldwide, it has come at substantial economic, environmental, and health cost. Excess nitrogen from fertilizer run-offs in drinking water can be linked to severe health problems. Biological Nitrogen Fixation (BNF) is increasingly viewed as a viable alternative to fertilizers for supplying nitrogen to plants. Several reports have shown that the BNF in cereals (e.g., rice, corn, wheat, etc.) comes from nitrogen-fixing bacteria. For instance, major cereal crops can form beneficial associations with nitrogen-fixing bacteria like Azospirillum. Our current understanding of the molecular aspects and signaling that occur between important crops like rice and these nitrogen-fixing bacteria is limited. In this study, we used an experimental system where the bacteria could colonize

the plant roots and promote plant growth in wild-type rice and symbiotic mutants (*dmi3* and *pollux*) in rice. Our data suggest that plant growth promotion and root penetration is not dependent on these plant genes. We are currently studying the growth promotion effect and root colonization in other plant mutants. Next using this experimental model, we are interested in identifying the transcriptomic responses in the host plant roots and bacteria. We have already completed the dual RNA-seq experiment and are waiting for the data to be analyzed. We are also interested in identifying the bacterial genes required for interactions with plant using genome-wide Tn-seq. We are currently optimizing the protocol to generate a bacterial mutant library for this experiment. Overall, findings from this study will serve as an excellent resource to characterize the host genetic pathway controlling the interactions between non-legumes and beneficial bacteria. The use and improvement of such a promising agricultural tool could provide enormous economic, environmental, and health benefits.

21B. Characterizing the Social Amoeba Microbiome.

Phong Nguyen, Eleni Sallinger, Robert Miller, Laurel Woods, Alexandra Melton, Tammy Haselkorn. *Biology, University of Central Arkansas, Conway, AR 72035.*

Symbiosis is the interaction between two organisms either in close physical proximity or within each other. Symbioses vary in the mechanisms for achieving and maintaining the associations, in the role of the microbe in the host biology, in the evolutionary history of the relationship, and in the genomic features of the microorganism. We are using the social amoeba, *Dictyostelium discoideum*, which naturally eat bacteria, as a model to study symbiosis. *D. discoideum* can form stable associations with bacteria that can resist amoeba digestion, such as *Burkholderia* bacteria. *Burkholderia*, and other bacterial partners of *D. discoideum* have been identified only after they have been cultured on a plate in the lab. However, ~99% of the bacterial diversity cannot be cultured using traditional microbiological laboratory methods. To investigate the natural diversity of bacterial symbionts in amoebae, we will be collecting and analyzing the social amoebae microbiome using direct DNA 16S rRNA sequencing. By using such culture independent methods, we hypothesize that more species of bacteria will be detected compared to using culture dependent methods. Collection of soil samples will be gathered locally, and DNA extraction, PCR, transformation into *E. coli* bacteria, and DNA sequencing will be performed for four different species of social amoeba: *P. palladium*, *D. violaceum*, *D. purpureum*, and *D. giganteum*. We predict that each species will have its own unique microbiome. Preliminary data suggests a variety of previously undetected bacterial and fungal species may be symbiotic associates. As we observe these amoeba-

bacteria interactions as they happen in nature, by identifying the complete microbiome and starting to identify the factors that shape it, we will be closer to understanding the evolutionary and biological significance of this symbiosis.

22A. A Genomic Assessment of the Effects of CdSe/ZnS and InP Quantum Dots on Baker's Yeast.

Cullen Horstmann, Kyoungtae Kim. *Biology, Missouri State University, Springfield, MO 65897.*

The potential applications and uses of Nanomaterials (NMs) such as Quantum Dots (QDs) increase daily. Amazing utilizations of QDs such as medical imaging, specific tissue targeting and potential photodynamic UV therapy is made possible with extremely small semiconductor particles only a few nanometers in length (Hsu et al. 2013). However, as the incorporation of NMs increase in everyday commercial products like water resistant t-shirts, inkjet printing and diode lasers (bar code readers, laser pointers, CD, DVD, Blu-ray disc readers, etc.) research regarding their toxicity and their long-term effects on the environment fall short (Ramirez et al. 2015). The objective of this research was to analyze and investigate the possible mechanisms of toxicity of CdSe/ZnS and InP QDs on Yeast. After treating three samples with CdSe/ZnS QDs and three samples with InP QDs and comparing them to three non-treated control samples an mRNA-Seq was performed and all samples were sequenced. After further comparison of the treated and non-treated samples, data was gathered via the CLC genomic workbench software shedding light on the effects QDs have on individual genes and their expression. Furthermore, gene ontology (GO) term analysis was conducted on the highly differentially expressed genes to give further insight on miss-regulated gene functions and their effects on Yeast.

22B. Investigating Novel Protein Interactions in NLRP3.

Karina Sewell, Christopher R. Lupfer. *Biology, Missouri State University, Springfield, MO 65897.*

Investigating Novel Protein Interactions in NLRP3 Karina Sewell and Christopher R. Lupfer Abstract: NOD-Like receptors (NLRs) are intracellular proteins that play an important role in the regulation of the innate immune response to pathogens. There are 22 NLR proteins encoded in the human genome. Specifically, NLRP3 can detect the presence of pathogens by recognizing cellular damage leading to the formation of a multi-protein complex known as the inflammasome. The inflammasome is responsible for activation of the Caspase-1 protein that ultimately leads to the activation of inflammatory cytokines IL-1 β and IL-18. Mutations to the NLRP3 gene lead to autoinflammatory diseases. Even though we know the function of NLRP3, how it is activated and the proteins that it interacts with are still unknown. By creating a yeast two-hybrid system, we

can discover novel proteins that interact with NLRP3. Determining these novel proteins will allow us to learn more about how NLRP3 is regulated and how the immune system works to fight off infection.

23A. Dual Inhibition of SHIP1 and SHIP2 in the Treatment of Diet Induced Obesity in Mice. Shamara Lawrence, Sandra S. Fernandes, William G. Kerr. *Biology, UA Pine Bluff, Pine Bluff, AR 71601.*

Chronic low-grade inflammation in the visceral adipose tissue promotes the onset of obesity. Recent therapeutic approaches have revealed that specific targeting of the inflammatory pathway involved in the immune response in adipose tissue could oppose the effect of inflammatory stressors. Srivastava et al. show that inhibition of the phosphatase SHIP1 (SH2-containing inositol polyphosphate 5-phosphatase) using a small-molecule inhibitor (K118) increases the anti-inflammatory response of immunoregulatory cells, which promotes a lean-body state. Because K118 targets both SHIP1 and its paralog SHIP2, we would like to determine if specific targeting of both SHIP1 and SHIP2 permits control of diet-induced obesity (DIO). Here we examined the effect of dual inhibition of SHIP1 and SHIP2 DIO in mice, by treating them with specific target inhibitor, namely 3AC (SHIP1) and As1949490 (SHIP2) for 4 weeks. We hypothesize that the inhibitors will increase the proliferation of the immunoregulatory cells in adipose tissue, which would promote lean body physiology. We found that treated mice had reduced body weight and fat content. Therefore, the findings suggest that blocking both SHIP1 and SHIP2 tampers the inflammatory pathway that perpetuates obesity, causing the mice to lose body fat.

23B. Anti-Methamphetamine Antibody Gene Therapy Prevents Against Some METH-Induced Blood Brain Barrier Dysfunction. Kennede McLeroy-Charles, Chris Bolden, Charles E. Hay, *Chemistry and Physics, UA Pine Bluff, Pine Bluff, AR 71601*, Paris Margaritis, Eric C. Peterson, *Pharmacology and Toxicology, UAMS, Little Rock, AR 72205.*

Methamphetamine (METH) is one of the largest substance abuse problems with over 25 million users worldwide, with no FDA approved pharmacological treatment. METH abuse is associated with many adverse physiological effects, including leakage of the Blood Brain Barrier (BBB) and hyperthermia. The BBB is a semipermeable barrier that maintains brain homeostasis by limiting paracellular transport, intercellular signaling, and excluding xenobiotics from the brain. METH has the ability to directly interfere with homeostasis by disrupting expression of proteins that maintain tight junctions (TJ) in specialized vascular endothelial cells. The goal of this research was to determine if AAV-7F9-Fc, a novel antibody-gene therapy, is able to mitigate METH-induced detrimental

BBB effects and associated neuroinflammation. Balb/C mice were assigned into one of the following treatment groups: Saline+Saline, Saline+METH (10 mg/kg), AAV-7F9-Fc+METH, AAV-7F9-Fc+Saline, and Empty Vector+Saline. Mice were administered a single 1x10¹¹ dose of AAV-7F9-Fc 21 days before studies were begun. On study day, temperatures were recorded 1 hour before and after METH or saline administration and mice were sacrificed 2 hours after. Expression of important BBB TJ proteins (claudin-5, occludin, and zonula occludin-1) were measured via Western Blot, and temperatures were recorded throughout. Our results indicated that mice administered METH showed an increase in core body temperature by 4-5°C, and that AAV-7F9-Fc prevented this increase in core body temperature. In the Frontal Cortex of Saline+METH mice, there was an observed decrease in expression levels of the TJ proteins claudin-5 and occludin, and this decrease was mitigated in AAV-7F9-Fc+METH mice. This data suggests that the antibody gene therapy AAV-7F9-Fc could possess some neuroprotective potential in mitigating METH-induced hyperthermia and resulting BBB dysfunction.

24A. Correlation between body size and activity levels in Red-eared sliders (*Trachemys scripta-elegans*). Angel Castro, Calin O. Marian, *Biology, University of Central Arkansas, Conway, AR 72035.*

Physical activity levels are often good measures of health and wellness in living systems. In the Red-eared slider (*Trachemys scripta elegans*), activity levels might change as the turtle grows and ages. Therefore, our goal in this study is to identify a possible correlation between body size and activity levels of the Red-eared sliders. Here we present a time-lapse image analysis of turtles observed over a period of time. Through the use of specialized software, we constructed a track of the movements of each turtle over time and measured the distance traversed as determined by the length of each track. Preliminary results show that even amongst turtles of similar body size, there are differences in activity levels as measured by distance moved over time. A strong (or lack of) correlation between activity levels and body size may later be used to establish the relative fitness levels in this species.

24B. Host Specificity of *Burkholderia symbiont of D. discoideum*. Haley Hensley, Haley Goodwin, Julia Roberson, Anthony Barkdull, Ashleigh Batte, Alexandra Melton, Tammy Haselkorn, *Biology, University of Central Arkansas, Conway, AR 72035.*

Symbiosis can be defined as the interaction between different organisms living together. Symbiotic relationships can be anywhere in a range from beneficial to detrimental for one or both symbionts. *Dictyostelium discoideum* will make a good model system to study eukaryote-bacterial symbiosis because

it is a single celled eukaryote that houses a naturally occurring bacterial symbiont in the Burkholderia genus. Burkholderia infection permits other food bacteria to reside in D. discoideum spores, which allows the amoeba to take a food source along with it in the dispersal process and farm the bacteria in its new location. This is beneficial when D. discoideum spores land in a food poor location, however, there is a cost to infection when there is a food source available. While 25% of D. discoideum in nature are infected with three different species of Burkholderia symbiont, it has not yet been detected in any other amoeba species, and its potential to infect different hosts is unknown. When pathogens infect a new host, theory predicts that they will have a greater fitness cost initially, particularly when that host is distantly-related to the original host. We are testing the host range of these Burkholderia symbionts by growing different species of social amoeba, D. giganteum, D. purpureum, and P. palladium on mixtures of each of the different Burkholderia species and food bacteria. We are measuring their capability to infect, fitness (spore production), and persistence through a multitude of assays. We predict that the more distantly related the amoeba from D. discoideum, the less persistent it will be in maintaining the infection, and the higher the fitness costs will be. This will allow us to explore the mechanisms of a novel symbiont infection and better understand how Burkholderia can be costly in some situations, yet beneficial in others.

25A. Sex Differences in Humoral Response of Mice to Plasmodium yoelii. Tyler Appell, *Biology, Harding University, Searcy, AR 72143*, Jason Stumhofer, *Microbiology and Immunology, UAMS, Little Rock, AR 72205*.

Malaria is an infectious disease caused by an obligate intracellular protozoan parasite of the genus Plasmodium. While a number of Plasmodium species cause disease in humans Plasmodium falciparum, which is found throughout Africa, Asia, and South America causes the most severe disease. P. falciparum is transmitted from person to person by the bite of female Anopheles mosquitoes. Every year P. falciparum causes 225 million cases of malaria and nearly one million deaths, most of which are young children and pregnant women. One variable that influences the development of disease and immunity against malaria is sex. Sex is a biological variable that affects immune responses to both self and foreign antigens. Generally, adult females mount stronger innate and adaptive immune responses than adult males, and this results in more severe clinical disease in women while men tend to have higher pathogen loads. These dynamic differences in the immune response between males and females occur in the case of malaria and may impact vaccine induced protective immunity against this disease. As the adaptive immune response, particularly the production

of parasite specific Abs, is essential for the control of blood stage parasite growth, we were interested in determining if the absence of surface proteins involved in the activation of B and T cells results in differences in controlling Plasmodium infection between male and female mice. Utilizing a rodent model of malaria, male and female mice deficient in CD19, a B cell coreceptor, CD28, a T cell co-stimulatory molecule, or both CD19 and CD28 were infected with P. yoelii and the course of the infection was monitored and compared to that of wild-type (WT) mice.

25B. The Effects of Caffeine on Motor Cognition. Bradley Marschall, Juan Priety Malave, Kelsea Hall, Lance Gibson, *Biomedical Engineering, Harding University, Searcy, AR 72143*.

The effect of caffeine on motor cognition was tested by instructing the subjects of this experiment to sort a bag of M&M's by color before and after drinking either Yerba Mate (an Argentine herbal tea with a high caffeine concentration), coffee, or water (as a control). Overall the results showed that all of the tested beverages had a very insignificant effect on blood oxygen levels. However, there was an increase in heart rate for the coffee drinkers, whereas the Yerba Mate subject's heart rate marginally increased. The beverage that yielded the best average sorting time after consumption overall was Yerba Mate with coffee close behind. In conclusion, Yerba Mate provided its drinkers with better motor cognition skills and lower heart rates compared to the coffee drinkers, and would be a more efficient source of caffeine for those in need of more energy and mental alertness.

26A. De Novo Biosynthesis of Resveratrol in Metabolically Engineered Synechocystis sp. PCC 6803. Tyler Maxwell, Qingfang He, *Biology, UA Little Rock, Little Rock, AR 72204*.

Resveratrol, a plant-derived polyphenol, is a component of grape skins that is widely studied due to its demonstrated anti-inflammatory, antioxidant, and anti-carcinogenic properties. Demand for resveratrol for clinical and food use has been steadily increasing, and currently the main source of the compound is the Japanese knotweed Polygonum cuspidatum, which is an invasive species whose root system can damage building foundations, roads, and flood alleviation structures. Therefore, a more eco-friendly mode of synthesis is necessary. Microorganisms present an ideal mechanism for large-scale production of resveratrol due to the potentially high yield and low cost. To date, the efforts to synthesize resveratrol in microbial systems have largely relied upon the supplementation of other compounds involved in the biosynthetic pathway, such as p-coumaric acid and L-tyrosine. The purpose of this project is to achieve the de novo synthesis (free of large amounts of supplementation) of resveratrol by

enhancing the expression of three key enzymes involved in the tyrosine-initiated pathway: tyrosine ammonia-lyase (TAL), 4-coumaroyl-CoA ligase (4CL), and stilbene synthase (STS). To do this requires the optimization of the codons of the genes encoding TAL (from *Saccharothrix espanaensis*), 4CL (from *Nicotiana tabacum*) and STS (from *Vitis vinifera*). The genes for these three enzymes will be assembled into an expression plasmid pACYCDuet-1 before being transformed into *E. coli* BL21 DE3. The recombinant strain was cultivated in a 2xYT-rich culture medium without the addition of other phenylpropanoids. Genomic DNA was extracted from the resulting strand and transformed into *Synechocystis* sp. PCC6803. Presence of resveratrol will subsequently be detected via high performance liquid chromatography (HPLC) and liquid chromatography/mass spectrometry (LC/MS).

26B. The Impact of TMEM165 in N-linked Glycosylation with respect to Breast Cancer. Humam Shahare, Pavitra Murali, *Biology, UA Little Rock, Little Rock, AR 72204*, Karen Abbott, Richard R. Drake, *Winthrop P. Rockefeller Cancer Institute, UAMS, Little Rock, AR 72205*.

The progression of Ductal Carcinoma in Situ (DCIS) to Invasive Ductal Carcinoma (IDC) is currently unpredictably dangerous due to the lack of biomarkers able to indicate migration and growth in early stages (1 and 2) of breast cancer. This unpredictability results in unavoidable potential risks to patients, commonly resulting in avertible and unnecessary surgeries. In response, the gene TMEM165 was studied for its viability as a biomarker of IDC. Identified in a previous glycoproteomic study, TMEM165 encodes for a transmembrane protein found to be heavily expressed in invasive breast cancer, however not expressed in normal breast tissues. A CRISPR/Cas9 mediated knockout of the TMEM165 gene in the breast cancer cell line MDA MB231 was conducted resulting in significant reduction in cell migration. TMEM165 is suspected to play a role modifying the glycosylation of cell surface proteins, influencing tumor cell properties such as intracellular signaling, cell motility, and the ability to metastasize. In this study, we analyzed the kidney cell line (HEK293) and cervical cancer cell line (HeLa) to compare the glycosylation changes observed in the control and gene knockout MDA MB231 cell lines. We also analyzed the differential expression of glycosyltransferases enzymes active during glycosylation via qRT-PCR. This study provided an objective evaluation of the effect of TMEM165 on glycans, glycoproteins, and transferases enzymes that participate in the progress of IDC Breast Cancer.

27A. Effect of aspartame and glucose on the lifespan and stress resistance of *C. elegans*. Lauren Smith, Stefani Hall, Mindy Farris, *College of Natural Sciences and Mathematics, University of Central Arkansas, Conway, AR 72035*.

Caenorhabditis elegans share many biological characteristics with complex organisms, such as humans. This similarity is useful when studying mutations in conserved pathways and how they affect lifespan when stressed. Glucose has been shown to shorten the lifespan of *C. elegans*. This occurs through the inhibition of several transcription factors that extend lifespan such as DAF-16 and HSF-1. Its effects on stress resistance, however, are complex. We found that glucose conferred resistance to heat stress, but only early in life (day 1 adults). Glucose has negative effects on resistance to heat stress for day 7 adults. DAF-2, the only insulin receptor in *C. elegans*, has been shown to regulate the lifespan of many organisms. *daf-2* worms have a mutation in the DAF-2 receptor and have an extended lifespan to almost double that of the wildtype (N2) worms. These mutants are also more resistant to extrinsic stressors, such as heat, when compared to the wildtype worms. The effect of added glucose on the stress response of *daf-2* is unknown. We hypothesized that, when heat stressed, the addition of glucose would negate the life-extending qualities of the *daf-2* worms, making them less resilient to stress. Our results show that the presence of glucose increases *daf-2* stress resistance even further, but as with N2, only early in life. Exposure to heat stress later in life diminishes the advantageous effects glucose has on stress resistance, as seen in trials when worms are heat stressed at mid- and late- adulthood (day 7 and day 13 adults). Aspartame, an artificial sweetener that is used as a substitute for sugar, is very popular and often preferred as a more healthy option. Studies using *C. elegans* as a model organism support the idea that aspartame has less negative effects on lifespan than glucose. We expect worms on aspartame to have a reduced lifespan compared to that of the control (wildtype) group. However, we predict that the lifespan of the aspartame worms will be longer than the worms feeding on glucose, as studies have shown that aspartame causes *C. elegans* to have an extended healthspan.

27B. Interactions between semantic and perceptual information in visual search: insights from eye movements. Savannah Bell, Taylor Dague, Kenith Sobel, Christian Hopkins, Amrita Puri, *Biology, University of Central Arkansas, Conway, AR 72035*.

Visual search tasks are used to investigate how visual attention enhances processing of selected items within the visual field and can provide insight into neurodiversity in perceptual processing. Recent research has shown that semantic information can play a role in visual search for letters and digits, and can interfere with processing of perceptual information. For example, in the size congruity effect (SCE), participants view two numbers that have different physical and numerical sizes, and are asked to identify the physically (or numerically) larger (or smaller) number. Reaction times (RTs) are faster when the target's physical and

numerical size are congruent, implying that the processing of numerical (semantic) and physical (perceptual) size interact. Although this effect has been replicated in numerous studies, there is still debate about the stage of processing at which the interaction between the two types of information occurs. Here, we investigated the stage at which semantic (numerical size) and perceptual (physical size) information interact in neurotypical individuals by tracking eye movements. Participants searched for a target digit among distractors (e.g. a 2 or a 3 surrounded by 8's or 9's) in circular displays containing 5, 7, or 9 digits. Targets were either congruent (e.g., a physically large 9 among physically small 2s and 3s) or incongruent (e.g., a physically large 2 among physically small 8s and 9s). We recorded the participants' eye movements and measured the time it took participants to initially fixate on the target, the duration of fixation on the target, and the total number of fixations. Participants took longer to initially fixate incongruent compared to congruent targets, suggesting that semantic and perceptual information may be processed together early rather than interacting at a later decision stage. Early interference between perceptual and semantic information could lead to a longer processing time of individual items in the visual search display and therefore delayed initial fixation of incongruent targets. This pattern is somewhat surprising because of recent studies consistent with the idea that physical and numerical size are processed independently until the decision stage. Additional experiments will address whether fixation patterns remain consistent with the early interaction view when displays are modified to encourage participants to make eye movements on a greater proportion of trials. Future studies will address whether the stage of processing at which semantic and perceptual information interact to influence the efficiency of visual search differs between neurotypical participants and individuals with neurodevelopmental conditions such as autism.

28A. Maternal Commensal Bacteria Inhibits Intrauterine ZIKV Infection and Fetal Growth Restriction in a Mouse Model. Julio Molina-Pineda, *Math and Science Division, University of the Ozarks, Clarksville, AR, 72830*, Maxim Seferovic, Gregory Valentine, Kjersti Aagaard, *Obstetrics and Gynecology, Baylor College of Medicine, Houston, TX 77030*.

ZIKV has been associated with congenital infection, microcephaly, and pregnancy loss as a result of viral mutations that facilitate maternal to fetal viral spread. Commensal bacterial microbes have been demonstrated to modulate host immunology and even viral infection. We therefore hypothesized that commensal bacteria would influence maternal to fetal transmission of ZIKA virus. Employing a mouse model of Zika infection, we compared ZIKV transmission rate and pup infectivity between normal conventional (C) and germ free (GF)

gnotobiotic mice. Timed, pregnant Swiss-Webster mice were given four doses of 1×10^4 PFU of a contemporaneous first passage Zika strain (ZIKV) or a mock injection (M) on embryonic days 4 through 7. Conventionalized (GF exposed to bacteria at weaning) or immune inhibiting anti-IFN1 antibody were negative and positive controls, respectfully. Tissues were recovered at e18.5 just prior to delivery and TRIzol extracted for genomic viral RNA. TaqMan based qPCR was performed from cDNA and quantified against ZIKV standard curves. For ZIKA infected pregnancies placentas were positive in 82% of demised fetus compared to 52% of live pups ($p=0.04$). No virus was found in either maternal or fetal brains, however, virus was recovered from maternal spleen and uterus, and was highest by an order of magnitude in fetal placental tissue overall ($p<0.001$). Maternal spleens of GF Zika infected mice had greater viral infection (2.1×10^4 vs 8.7×10^3 RNA copies/g $p=0.055$) compared to conventional mice, and uteruses of GF Zika infected had greater viral infection (1.0×10^4 vs 6.1×10^2 RNA copies/g, $p=0.04$). Only 25% of conventional uterus were infected compared to 78% of GF (ChiSquared, $p=0.03$). The findings demonstrate that growth restriction and fetal demise, the two principle manifestations of ZIKA vertical transmission in mice, are mitigated by the commensal bacteria. We speculate that commensal microflora interact with the host immunity to mediate maternal resistance and thereby mitigate vertical transmission of the congenital pathogen.

28B. Use of an in vivo closed-head weight-drop model to investigate the effects of multiple mild and moderate traumatic brain injuries on cellular and vasogenic edema. Sara Venier, *Biology, Celeste Dunn, Naysa Sturdivant, Jeffrey Wolchok, Kartik Balachandran, Biomedical Engineering, UA Fayetteville, Fayetteville, AR 72701*.

Mild traumatic brain injury has long been coined a "silent epidemic" due to subtle initial symptoms, which cause people to avoid seeking medical treatment. As a result, the consequences of repeated injuries have long been underestimated and underreported [1]. Repeated mild TBIs occurring over an extended period can result in cumulative and cognitive defects, with an elevated risk of neurodegenerative diseases [2]. In this study, we investigated the effects single and multiple, mild or moderate TBIs have on cellular and vasogenic edema. Both cerebral and vasogenic edema have been known to increase the deterioration of brain function in the days following a TBI [3]. By using a closed-head traumatic brain injury in vivo model, we induced both mild and moderate TBIs on mice. Mice were placed on a foam pad, and a weight was dropped directly onto their heads from two different heights to administer the impact of a mild and moderate TBI. The mice were sacrificed after receiving either one or two TBIs, and had

their brains removed, sectioned, and stained using hematoxylin and eosin—in order to image and observe edema. Cellular edema is a fluid imbalance within cells, which typically causes swelling—in brain tissue, it can be observed by the widening of intracellular space around nuclei [3]. Our imaging depicted large intracellular spaces in both mild and moderate TBI conditions, which indicate that our closed-model system caused cellular edema. Vasogenic edema can be seen when the blood-brain barrier ruptures, allowing fluids to accumulate around the leak [4]. This was also seen in our model through deposits of blood products, which is indicative of hemorrhage. Although prior studies have given rise to similar results, these past studies used a stereotaxic device and/or performed a craniotomy prior to administering a TBI, which may elicit other injuries. We feel the closed-head model allows for a more accurate assessment of the effects of mild and moderate TBI because it demonstrates what is more likely to happen outside of a simulated environment, which is beneficial to better understanding brain activity and response post-injury. Using a closed-head model, we were able to find that even when impact is not administered post-craniotomy, it will still create observable edema and hemorrhage. [1] M. e. al., "Lifelong behavioral and neuropathological consequences of repetitive mild traumatic brain injury," *Annals of Clinical and Translational Neurology*, vol. 5, no. 1, pp. 64-80, 2018. [2] National Center for Injury Prevention and Control, "Traumatic Brain Injury & Concussion," Centers for Disease Control and Prevention, 14 June 2017. [Online]. Available: <http://www.cdc.gov/traumaticbraininjury/outcomes.html>. [Accessed 8 May 2018]. [3] D. E. Kimbler, J. Shields, N. Yanasak, J. R. Vendor and K. Dhandapani, "Activation of P2X7 Promotes Cerebral Edema and Neurological Injury after Traumatic Brain Injury in Mice," *PLoS One*, vol. 7, no. 7, p. e41229, 2012. [4] J.-Q. Chen, C.-C. Zhang, S.-N. Jiang, H. Lu and W. Wang, "Effects of Aquaporin 4 Knockdown on Brain Edema and the Uninjured Side after Traumatic Brain Injury in Rats," *Medical Science Monitor*, vol. 22, pp. 4809-4819, 2016.

29A. Population genetic survey of a foundation prairie plant, big bluestem (*Andropogon gerardii*) following a prairie sod transplant in Northwest Arkansas. Katie Matthews, Scott Woolbright, *Biology, UA Little Rock, Little Rock, AR 72204*.

Efforts to save or restore remaining North American tallgrass prairies rely on foundation grasses like *Andropogon gerardii* (big bluestem/BBS). Because foundation species genes are strongly linked to community and ecosystem patterns and processes, restoration success is likely to be influenced by the preservation of foundation genetic variation. Here, we exploit unanticipated consequences of a sod transfer experiment to better understand how BBS variation alters or is altered by below-ground interactions in ways

that affect restoration success. Sod cut from a northwest Arkansas prairie remnant (Site 1) threatened by development was moved to a heavily disturbed agriculture site within another nearby prairie remnant (Site 2). The transfer (Site 3) was monitored for regeneration and changes in species richness and abundance. Observed changes in BBS cover prompted us to initiate a population genetic study to characterize standing-level genetic variation among the native sites (Sites 1 & 2) and to document changes in Site 3. BBS abundance was low at Site 1, accounting for ~10% cover. However, following sod transfer, abundance increased to ~50% cover at Site 3, apparently at the expense of other species. We are currently extracting and analyzing DNA samples from all three sites in order to determine how the extent to which Sites 1 & 2 differ genetically, as well as the extent of sexual vs. asexual reproduction is altering genetic variation of Site 3. The transfer of a thin layer of prairie to a site with decades of intense disturbance almost certainly influenced the shift in BBS abundance. If so, we have a unique opportunity to look for links between foundation species genetics and interactions with soil communities that have apparently favored BBS, and, potentially, specific BBS genotypes. Our project could therefore prove useful for understanding how below-ground disturbances influence conservation or restoration efforts involving foundation plants.

29B. Identification of Factors that Impact the Efficiency of Plasmid Transfer among Enteric Bacteria such as *Salmonella enterica* and *Escherichia coli*. Ashlyn Carlton, *Agriculture, UA Pine Bluff, Pine Bluff, AR 71601*, Steven Foley, Jing Han, Yasser Sanad, *Division of Microbiology, National Center for Toxicological Research, Jefferson, AR 72079*.

It is believed that factors such as the exposure to antimicrobial agents or other environment stresses have the ability to impact the capacity of plasmids to be transferred among different enteric bacteria, such as in *Salmonella enterica* and *Escherichia coli*. In order to assess the influence of antimicrobial exposure on the conjugation efficiency of such plasmids, this study will quantify the rates of plasmid transfer under multiple exposure conditions and will apply RNA sequencing to determine genes that may be differently expressed during drug exposure and conjugal transfer. The objective will be to classify the fundamental genetic mechanisms that impact the differences in conjugation. As a means to achieve these goals, conjugation assays will be subject to various selective pressures (different antibiotics with numerous concentrations) to identify the influence of the exposure to different antibiotic concentrations on the efficiency of conjugation. Following the exposure, these assays will be evaluated based on the number of transconjugants recovered in comparison to non-antimicrobial exposed controls. Thereafter, mRNA will be isolated in selective samples

where the conjugation efficiency is considerably different in contrast to non-exposed controls. These isolations will be made in order to evaluate the distinctions in gene expressions on, using RNA sequencing-based methods on the Miseq. Ongoing studies will likely supply innovative knowledge regarding the role of genetic influences on the conjugation efficiency under multiple selective pressures.

30A. Develop Retina Imagine. Zeqing Dong, Olufisayo Ayodele, Recep Emre Hacisofoaoglu, Mahmut Karakaya, *Dept. of Computer Science, University of Central Arkansas, Conway, AR 72035.*

Purpose: The increasing number of people with diabetes has led to an increase in diabetic retinopathy (DR), a major causes for blindness. Since DR is caused by damage to the small blood vessels in the retina, it may signal no symptoms before reasoning significant consequences. Early detection with annual eye exams is the key to prevent the blindness at diabetic people. This study is to evaluate affordable and convenient smartphone-based portable retinal imaging systems available on the market for diabetic retinopathy detection. The evaluation is performed with data collection from synthetic retinal images. **Methods and Materials:** We attached the D-EYE and Peek Retina devices to an iPhone 6 to collect data from synthetic retinal images. We changed the data collection variables including image lighting, camera application, and other factors that might affect image quality. We tested different combinations of variables to find the best image quality. Then, we evaluated the quality of the images, also, the data availability. **Results:** The D-EYE and Peek Retina devices were able to capture satisfactory images that were viable for analysis to determine the presence of retinal diseases. **Conclusion:** These smartphone-based portable retinal imaging systems can be used as an alternative to the direct ophthalmoscope. Since they are small, portable, and affordable for the patients, it is convenient and valuable for DR screening during a general health screening in urban areas and even by individuals at their own homes.

30B. Butanone Association Learning and Short-term Memory in Wild-type and Poly-Q Caenorhabditis elegans. Whitney Wilkins, Priya Rana, Landon Gatrell, Mindy Farris, *Biology, University of Central Arkansas, Conway, AR 72035.*

This experiment investigates C.elegans capability of changing their behavior in response to a conditioned stimulus paired with an unconditioned stimulus. Strains of wildtype (N2) and poly-glutamine (poly-Q) model AM101-Q40 were used for learning association to ten percent butanone. In previous studies, N2 has demonstrated a positive association to butanone after exposure to it in the presence of food. AM101-Q40 has not yet been examined. This strain serves as a model for

Huntington disease, as polyglutamine expansion in the neurons causes increased proteotoxicity with age. Common symptomology within Huntington disease patients is a decrease in cognitive functioning before motor dysfunction occurs, primarily in the prodromal phase. AM101-Q40 individuals are to be observed for a similar pattern of early cognitive deficiencies in learning and short-term memory. Methodology was adapted from the C. elegans Positive Butanone Learning, Short-term, and Long-term Associative Memory Assays protocol (Kauffman et al. 2011). Chemotaxis assays were conducted on NGM plates vacant of OP50 Escherichia coli with ten percent butanone and ninety-five percent ethanol spotting over 0.4M sodium azide, locations separated from one another and the deposition origin. A compilation of L4 and young adult populations were used for each assay. Thus far, two naive assays and two zero time point assays after one-hour long exposure to ten percent butanone with OP50 E. coli were conducted. Results suggest that N2 are capable of butanone association after butanone inoculation, and AM101 are less so by a Learning Index of 0.637. The ages in which assays were conducted were before typical neuronal degradation occurs in AM101-Q40, suggesting the mechanism(s) for learning are severely inhibited before full proteotoxicity of the neurons. Further experimentation is currently being conducted, extending time points post butanone inoculation for analysis of short-term memory. **References** Brignull, H. R., Morley, J.F., Morimoto, R. I. (2007). The stress of misfolded proteins: C. elegans models for neurodegenerative disease and aging. *Advances in Experimental Medicine and Biology*, 549, 167-189 Kauffman, A., Parsons, L., Stein, G., Wills, A., Kaletsky, R., Murphy, C. (2011) C. elegans Positive Butanone Learning, Short-term, and Long-term Associative Memory Assays. *Journal of Visualized Experiments* (49), e2490 Paulsen, J. S. (2011) Cognitive impairment in Huntington disease: diagnosis and treatment. *Current Neurology and Neuroscience Reports*, (5), 474 Torayama, I., Ishihara, T., and Katsura, I. (2007) Caenorhabditis elegans integrates the signals of butanone and food to enhance chemotaxis to butanone. *The Journal of Neuroscience: The Official Journal Of The Society For Neuroscience* 27(4), 741–750

31A. The Walking Dead: Bestowing Catalytic Activity to a Noncatalytic Protease. Sykes Martin, *Natural Sciences, Ouachita Baptist University, Arkadelphia, AR 71998, JA Hoggard, AS Martin, B Sarcar, LC Bridges, Biochemistry, Molecular, and Cell Sciences, Arkansas College of Osteopathic Medicine, Fort Smith, AR 72916.*

ADAMs (a disintegrin and metalloprotease) are well established sheddases that transform latent, cell surface molecules into biologically active, soluble derivatives. The sheddase role of ADAMs in processing biologically decisive molecules such as amyloid precursor protein (APP), GPCR activators, cytokines such as TNF-a, and

growth factors, has established that dysregulation of ADAM function is detrimental to normal cell function and promotes disease. However, of the 21 human ADAMs, nearly half (8/21) inexplicably lack the consensus site required for catalysis. Despite their prevalence, the biological role of ADAMs lacking hallmark shedase activity remains unknown. Through mutagenesis we provide the first evidence that a noncatalytic "dead" ADAM can be bestowed with catalytic activity and specificity in a manner similar to active ADAMs. Human ADAM7 lacks only the glutamate within the active consensus site of HEXHXXGXXH. Introduction of this single amino acid produced protease activity that exhibit specificity like that previously reported for human ADAM28. Our findings suggest that noncatalytic ADAMs may have emerged from catalytically active ADAMs, and we posit they may serve as an ancillary level of enzyme regulation to fine tune ADAM protease activity.

31B. Global Demethylation Attenuates Glutaminase and Nerve Growth Factor in TNBS-Induced Colitis.

Christy Eslinger, *Micro-Cell & Molecular Biology, Tulsa Community College, Tulsa, OK 74119*, Kenneth Miller, Subhas Das, *Anatomy & Cell Biology, Oklahoma State University, Stillwater, OK, 74078*.

One-third of all Americans suffer from inflammatory bowel disease (IBD) leading to inflammatory pain. Many studies have reported the involvement of epigenetic factors in persistent pain. Adults who were exposed to childhood abuse are approximately twice as likely to have ulcerative colitis. In an effort to combat the inflammatory pain and predisposition for IBD, different epigenetic factors need to be investigated. Cytosine methylation and its binding partner, MeCP2 can act together as either a transcriptional activator or a repressor. Our lab has shown two proteins, glutaminase (GLS) and nerve growth factor (NGF) at the center of inflammatory pain. This project was undertaken to determine if these two proteins and their gene expression are modulated by epigenetic factors. Methods: Female SD rats were used to induce colitis through intracolonic infusion of 2.5% TNBS in 25% ethanol and pretreated and co-treated with azacytidine (Aza, 50nM). Twenty-four hrs post-treatment, rats were sacrificed and their colon and associated sensory ganglia (L6/S1) were extracted. Genomic DNA, RNA and proteins extracted were used for bisulfite conversion, methylation specific PCR, PCR and WB. Results: Our data suggest that Aza decreased the TNBS-induced inflammation seen in gross examination. TNBS-induced colitis increased the DNA methylation of GLS and NGF genes. Global demethylation by Aza treatment decreased TNBS-induced GLS and NGF gene expression. Aza also decreased MeCP2 protein expression suggesting reduced interaction of MeCP2 with these gene promoters. Therefore, Aza-induced demethylation can be targeted for therapeutic use to treat

inflammatory pain. Conclusion: Aza can be used to block TNBS-induced methylation and inflammation-induced GLS and NGF alterations. Funding: INBRE-SURP, HR16-003

32A. A heterodimeric thiosulfate dehydrogenase from *Halothiobacillus neapolitanus*. Maria Marasco, *Biology, Davi Proffitt, Ilerioluwa O. Sowande, Newton P. Hilliard Jr., Physical Sciences, Arkansas Tech University, Russellville, AR 72801*.

Halothiobacillus neapolitanus is a sulfur-oxidizing microbe unique in its use of both an incomplete S4 pathway and a sox pathway during oxidation of thiosulfate. In addition, the S4 pathway is comprised of a heterodimeric thiosulfate dehydrogenase, which is not seen in other chemolithotrophic species and genes for the sox pathway are not located in a single operon. GeLC-MS proteomics of cultures grown at pH 7, on thiosulfate containing media, indicates an approximately 20-fold higher expression of sox pathway proteins soxAX and soxYZ over the S4 pathway proteins tsdAB. Cultures grown at pH 5.3 show little or no change in expression of sox pathway proteins. Expression of thiosulfate dehydrogenase may show a slight increase of ~2.5 fold at the lower pH however, it's overall lower expression level makes this assignment difficult. Proteins involved in oxidation of other substrates such as elemental sulfur and sulfide demonstrate much clearer pH dependent expression with 2 to 5 fold change. Proteins involved in sulfide oxidation are particularly interesting with a 5-fold increase of *sqrF* at low pH compared to >2-fold decrease for *sqrD* and *sqrE*. In the absence of traditional operon structure as is found in other sulfur oxidizing chemolithoautotrophs, determination of regulatory mechanisms for these pathways has been limited.

32B. Relative Gene Expression Study on *Centruroides vittatus* Investigating Sodium Toxin Gene Activity.

Chloe Fitzgerald, Aimee Bowman, Taylor Bishop, Ashlyn Tedder, Alyssa Kool, Cody Chivers, Tsunemi Yamashita, *Biology, Arkansas Tech University, Russellville, AR 72801*.

Scorpions release venom when capturing prey or fighting off predators, and a large portion of this venom consists of neurotoxins. The area in the tail where the venom is produced and housed is called the telson gland. The neurotoxins produced are mostly composed of a combination of different sodium toxins which alter the kinetics of sodium channel gating in the nervous system cells where they have been injected. This exploratory study on the sodium β toxin gene activity for the striped bark scorpion, *Centruroides vittatus*, specifically focused on gathering relative quantification data for six neurotoxin variants in particular: Na668, Na667, Na1210, CsBeta, CvAlpha, and Na3066. This was accomplished by quantitative real-time polymerase

chain reaction, or qRT-PCR. Preliminary experiments have been conducted on both male and female organisms by which threshold values yielded from these have been statistically analyzed within biological replicates as well as computationally analyzed through the $\Delta\Delta C_t$ method, which has gathered a tentative ratio of activity for these gene variants. The goal of this study was to determine the level of expression for the different sodium β toxin genes in the telson gland relative to body tissue in male and female scorpions of the eastern population. This information may one day be used to help develop anti-toxins for medical use.

33A. Papillary and Follicular Thyroid Cancer Cell Lines Display Distinct Transcriptional Programs Despite Having Mutations in the Same Signaling Pathway.

Emma Reynolds, Brianna LeBoeuf, Laura J. MacDonald, *Biology, Hendrix College, Conway, AR 72032.*

Thyroid cancer is one of the most prevalent endocrine cancers and incidence is expected to surpass colon cancer by 2030. Treatment options are limited for those diagnosed with advanced forms of thyroid cancer, highlighting a need for research into mechanisms of dedifferentiation and progression. The most common subtypes of thyroid cancer are papillary thyroid cancer and follicular thyroid cancer. Papillary thyroid cancer is associated with mutations in BRAF, while follicular thyroid cancer is associated with mutations in HRAS. Both subtypes are associated with mutations in the MAPK signaling pathway, but the two cancers display distinct pathology and metastasize to different areas of the body. While papillary thyroid cancer metastasizes to the local lymph nodes, follicular thyroid cancer progresses to the lungs and bones. We evaluated cell lines derived from mouse models of papillary and follicular thyroid cancer to determine how their associated mutations altered gene transcription. Next generation sequencing libraries were generated from papillary and follicular thyroid cancer cell lines lacking PTEN and harboring either a BrafV600E mutation or an HrasG12V mutation, respectively. Following sequencing, differential gene expression was evaluated using DESeq and gene ontologies were developed to determine relevant functional groupings. Overall, our study identified hundreds of differentially expressed genes between papillary and follicular thyroid cancer cell lines and illuminated distinct differences in genetic profiles between the two subtypes. Notably, genes associated with signaling through the extracellular matrix were upregulated in papillary thyroid cancer, while genes associated with immune signaling were upregulated in follicular thyroid cancer.

33B. From Molecular to Behavioral: A Study of *C. elegans*. Portia Renee, Brenda Houck, *Biology, Hendrix College, Conway, AR 72032.*

Movement is an essential function for any organism's survival. In *C. elegans*, glial-like cells known as GLR cells form connections with neurons thought to support head movement, but their function remains unknown. These connections, called gap junctions, are analogous to those of vertebrates and are composed of innexin proteins. 25 innexin proteins exist in *C. elegans*, 11 of which are localized to GLR cells. Research has shown that vertebrate gap junctions support coordinated movement. We hypothesize that gap junctions of GLR cells in *C. elegans* contribute to coordinated head movement. In previous experiments, our lab found mutant worm strains lacking innexin proteins localized to GLR cells have significantly different head movements when tested in behavioral assays. To further test the role of GLR cells and their connections in head movement, we aim to ablate these cells and examine the subsequent movement behavior. We have worked toward generating a transgenic worm containing a phototoxic species capable of inducing GLR cell death when exposed to light through development of a plasmid to be injected into the gonads of *C. elegans*. Additional experiments using RNA interference have allowed us to test the effects of suppressing specific innexin protein expression on *C. elegans* head movement and support our previous findings.

34A. The Spider Microbiome. How did It Get There? Is it Dangerous? The Role of the Environment in Forming the Spider Microbiome. Ethan Compton, Brandon A. Hogland, Amber G. Hug, *Biology, Harding University, Searcy, AR 72143.*

The national microbiome initiative has been enacted to encourage all researchers to study organisms relative to human health. Many arthropods are known to carry microorganisms important to human health, yet not all groups have been focused on. Previous studies on arthropods highlighted the presence of a bacterial microbiome responsible for disease transmission to humans. However microbiome data on spiders is lacking. *Rabidosia rabida* is a common terrestrial wolf spider found in many parts of Eastern North America. We hypothesized that *R. rabida* would have a microbiome consisting of common microbes found in soil and on the surface of plants due to its natural habitat of fields and low grasses. We also hypothesized that *R. rabida* could potentially have microorganisms living in and on its surface that could be pathogenic to humans. In addition, we hypothesized that there would be no difference in the colony count of bacterial isolates from plants when compared to the colony count of bacteria isolated from soil. We isolated 126 different bacterial from spiders, the soil and plants. 16s rRNA sequencing and BLASTn analysis were performed. Our analysis indicated that spiders carry bacteria on and within them that include only a few microbes from the environment and an assortment of bacteria not found on soil and plants. Several opportunistic pathogens

were isolated from the spiders, indicating their importance as potential vectors of disease.

34B. Dissecting potential roles for FAK and Abl kinases in mediating CAP1 regulation of ERK and breast cancer cell functions. Lauren Calhoun, Joshua Gray, Rokib Hasan, Faith Allen, Thomas Kelly, Guolei Zhou, *Biology, Arkansas State University, Jonesboro, AR 72401.*

We previously reported that knockdown of the actin-regulating protein CAP1 (Cyclase-Associated Protein 1) causes activation of ERK (External kinase-Regulated Kinase) in the metastatic breast cancer cells, as well as enhanced invasiveness and proliferation derived from the altered ERK activity. However, CAP1 as a cytoskeletal protein is unlikely to regulate ERK directly, and another signaling molecule is believed to mediate CAP1 regulation of ERK and the breast cancer cell functions. Our previous findings and relevant literature suggest adhesion molecule FAK (Focal Adhesion Kinase) and tyrosine kinase Abl as candidate signaling molecules that may link CAP1 to ERK, and the cancer cell functions. Both FAK and Abl have been reported to interact with CAP, and have functional connections with CAP. Moreover, both kinases have been documented to regulate ERK and are also implicated in cancerous transformation and metastatic progression. To determine potential roles for FAK and Abl, we use a combination of approaches including RNAi silencing and chemical inhibition of FAK and Abl kinase activities, to determine if they suppress the elevated ERK activity and enhanced proliferation and invasiveness derived from CAP1 depletion. Our preliminary results support that FAK likely links CAP1 to ERK, and potentially the cancer cell functions.

35A. Morphological and genetic variance in *Rhizobium leguminosarum*. Iris Aquino Pineda, Sonia Leonardo, LaShall Bates, Gary Bates, *Biology, Northwest Arkansas Community College, Bentonville, AR 72712.*

Rhizobium leguminosarum is one of the microbes that cause nodulation to occur in legumes. One of the first steps of nodulation involves the bacteria infecting the host. This infection process is very specific and demonstrates single gene interactions between the host and the pathogen. This relationship has caused many different biovars and strains of biovars of this species to be identified based on the host plant or selected differential plants. Commercially available specimens are a mixture of multiple strains of *R. leguminosarum* to enable some type of an interaction to occur. Various *R. leguminosarum* were collected, analyzed, and categorized for morphological and genetic variance. This investigation was looking for a strain that could survive and infect under low oxygen conditions.

35B. Investigating the effects of GPX1 under environmental stress. Ashley Prella, Bowman Fedosky,

Victoria Smith, Brandon Jatho, Gary Bates, LaShall Bates, *Biology, Northwest Arkansas Community College, Bentonville, AR 72712.*

Glutathione Peroxidase 1 (GPX1) protects cells from oxidative damage by catalyzing the reduction of hydrogen peroxide by glutathione. Several alternatively spliced transcript variants have been found for this gene. Plasmids were designed using biobricks that contain differing promoters and the GPX1 construct. The purpose of this research is to produce a transgenic organism containing GPX1 to examine the effects of various environmental stress factors. Different transformation methodologies were compared to determine what method was best suitable for the production of this synthetic plasmid.

36A. Uncovering A Cancer Defense Mechanism By Investigating MCM10:MRC1 Interaction. Batuel Okda, C. Longden, B. Wright, C. Hillman, S. Das-Bradoo, *Department of Natural Sciences, Northeastern State University, Tahlequah, OK 74464.*

Cancer is the leading cause of death around the world. Cancer results from a variety of reasons, but it ultimately leads to a similar outcome – unstable genome. In a normal cell, genome stability is maintained by a multitude of proteins involved in DNA replication and repair pathways. In our lab, we have observed interaction between DNA replication protein, Minichromosome maintenance protein 10 (Mcm10) and DNA damage repair protein, Mediator of Replication Checkpoint 1 (Mrc1). Both of these proteins are guardians of our genome and mutations in any one of them leads to cancer. To observe Mcm10 and Mrc1 (full length and truncations) interaction, yeast two-hybrid assays were performed. Plasmids coding for individual protein fused to either activation or binding domains were transformed into yeast and interaction was studied in terms of reporter gene (LacZ) activation. Interaction was observed qualitatively by plating on X-gal plates and quantitatively by measuring β -galactosidase activity in the cell lysates. We observed a strong interaction between Mcm10 and Mrc1 by yeast two-hybrid assay. Interestingly, this interaction was specific to the conserved region on Mrc1 (about 500 amino acids). Furthermore, systematic deletion of the conserved Mrc1 region indicated a potential binding site for Mcm10. Our data suggests that Mcm10 binds strongly to Mrc1 and this interaction is specific to the conserved region on Mrc1. Further mutational analysis will reveal the molecular mechanisms that underline this interaction which is crucial for understanding cancer development and progression.

36B. Using CRISPR-Cas9 to understand the function of Polymerase epsilon in budding yeast. Sarah Woller, Batuel Okda, Brandy Fultz, Casey Eddington, Sapna Das-

Bradoo, *Natural Science, Northeastern State University, Tahlequah, OK 74464.*

DNA polymerase ϵ (Pole) maintains genome stability by assisting in DNA replication and DNA damage checkpoint activation pathways. Pol2 is the catalytic essential subunit of Pole. The N-terminus domain of Pol2 functions in DNA replication but surprisingly it is the C-terminus region that is essential and functions in DNA damage checkpoint activation. Our laboratory is interested in investigating the C-terminus region of Pol2 that remains a mystery in terms of structure and function. Methods: Based on multiple sequence alignment algorithms, we have identified 12 highly conserved amino acids in the C-terminus region of Pol2. Next, we harnessed CRISPR-Cas9 technology to introduce these Pol2 mutations on the genomic loci via DNA double strand break induction and repair. Currently, we are studying the mutants for their growth phenotype and cell cycle progression under normal and DNA damaging conditions. Results: We were successful in constructing Cas9 plasmids carrying different guide RNA (gRNA) sequences that target specific regions on Pol2. We have now integrated all the Pol2 mutations (single and double) on the yeast genome. Conclusion: We have successfully created a plethora of Pol2 C-terminus mutations on the genome that will help to decipher the function of this essential domain in DNA damage checkpoint. Grant support: Research supported in this publication was supported by the National Institute of General Medical Sciences of the National Institutes of Health under award number P20GM103447.

37A. Design and Usage of a 3-D Printed Raspberry Pi powered Electronic Image Capture Device. Brandon Jatho, Cordell Templeton, Jonathan Patrick, Gary Bates, LaShall Bates, *Biology, Northwest Arkansas Community College, Bentonville, AR 72712.*

The ability to capture quality images, store and display results is often lost at small institutions based on their difficulty in obtaining the latest research technology. To this end, an Electronic Image Capture Device which can be used for both Petri dishes and electrophoretic gels was designed, programmed, and 3-D printed. This device incorporated a Raspberry Pi, a small single board computer, a neopixel LED ring, a camera, and a 3-D printed housing. This device has the ability to receive input from the user to alter the color of the lights. This allows photos of petri dishes or gels to be taken under various light conditions which is vital for visualizing different types of reporter genes. The device can either store the output or send it to central data hub.

Chemistry and Biochemistry

Friday Oral Platform Session

ORAL – 3:20. Squaramide-based anti-parasitic drugs toward the discovery of novel treatments for American trypanosomiasis. Emily N. H. Tran, Gregory R. Naumiec, *Chemistry, University of Central Arkansas, Conway, AR 72035.*

American trypanosomiasis, or Chagas disease, is a neglected tropical disease caused by the parasite *Trypanosoma cruzi*. This illness is known to affect over one sixth of the world's population, most prevalently in Central and South America. The two current treatments for Chagas disease utilize the drugs Nifurtimox and Benznidazole, potent anti-parasitic medications that eliminate *T. cruzi*. Though effective drugs, their side effects are extremely harsh. Some of these effects include difficulty eating, passing stool, and cardiac complications which could result in sudden death. Our research project focuses on the production of a library of drug candidates that are inexpensive yet innocuous to treat Chagas disease. Squaramide-based drug derivatives synthesized from 3,4-dihydroxycyclobut-3-ene-1,2-dione (squaric acid) have shown to have anti-parasitic properties against *T. cruzi*. Our target compounds are synthesized in three short synthetic steps. Squaric acid is first converted to the squaric ester diethyl squarate via condensation with ethanol. Diethyl squarate is subsequently converted to the targeted squaramides when reacted with a variety of amines. This class of compounds have demonstrated low toxicity in humans and high affinity for the *T. cruzi* parasite. Through a series of condensation reactions, potential drugs are being created from alkyl and aryl amines. The availability of these compounds will enhance the chances of discovering a novel and safer remedy for Chagas disease. Currently, significant progress has been made in the synthesis of a diverse drug library. Future research involves testing the potency of these drug candidates and synthesizing a new generation of drug derivatives.

ORAL – 3:35. The Effects of Proton Abstraction on the Binding Selectivity of Ligands in the Phenylalanine Hydroxylase Active Site. Madison Perchik, Rachel Giampapa, Larryn Peterson, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112.*

There are many molecules that act on dopamine and dopamine-like binding sites in enzymes and transport proteins. Some effects of these proteins are beneficial while others are detrimental. We are designing inhibitors for this group of proteins. Phenylalanine hydroxylase (PheOH) is a tetradhydrobiopterin-

dependent monooxygenase that influences the rate determining step of converting phenylalanine into tyrosine by hydroxylating phenylalanine. Both phenylalanine and tyrosine are important components in the anabolism of dopamine. A deficiency of PheOH can cause hyperphenylalaninemia, which gives rise to phenylketonuria (PKU), a severe disease that can cause mental retardation if one's diet isn't strictly monitored. A suite of dopaminergic derivatives has been developed as potential inhibitors of the PheOH enzyme. The inhibitory effectiveness of these dopaminergic derivatives has been measured via in silico models in which the strength of interaction between each substrate and the enzymatic active site was analyzed. A crystal-structure of the PheOH active site, with bound thienylalanine, was isolated from the Protein Data Bank (PDB ID: 1KW0). The positions of novel dopaminergic derivatives were optimized in the active site using M062X/6-31G with implicit solvation and with flexible amino acid side-chains. Interaction energies between the ligands and the protein were calculated using M062X and MP2 with the 6-311+G* basis set. From recent studies, there are promising novel catechols that do not inhibit this enzyme. Results show trends where certain molecules lose a proton, strongly effecting their binding strength.

ORAL – 3:50. Identification of Oxidative Enzymes in the Metabolism of Synthetic Cannabinoid 5F-AKB-48. Anna Pinson, *Biochemistry, Harding University, Searcy, AR 72143*, Azure Yarbrough, Ryoichi Fujiwara, Anna Radominska-Pandya, *Biochemistry, UAMS, Little Rock, AR 72205*.

Synthetic cannabinoids (SCBs) have been the cause of many hospitalizations and deaths in the recent past. Abuse of these dangerous compounds is on the rise as users mistake them for the natural cannabinoid, tetrahydrocannabinol, in Cannabis sativa. To protect the human body, harmful compounds of exogenous and endogenous origin are metabolized by cytochrome P450s (P450s) and other drug-metabolizing enzymes. In some cases, SCBs remain in the body for extended periods of time, resulting in toxicities. In order for doctors to properly treat these toxicities, the modes of metabolism for these compounds must be further investigated. This study focuses specifically on a third generation SCB, 5F-AKB-48, and its oxidation via P450s. 5F-AKB-48 was incubated with human liver microsomes (HLMs) and recombinant P450s to identify potential metabolites, which were analyzed by UPLC and MS. The results indicated the biosynthesis of mono-, di-, and trihydroxy metabolites during the oxidative reactions with HLMs. Several recombinant enzymes were assessed 5F-AKB-48, and CYP3A4 and CYP3A5 were identified as the most active isoforms. The dihydroxy metabolite was the major product that was produced from the conversion of the original monohydroxylated

derivative after one hour of incubation. Interestingly, CYP2J2, the isoform mainly expressed in the cardiovascular system, was also active in the oxidation; however, the monohydroxylated derivative was the major product. Additionally, specific inhibitors of the P450s were used in the incubations with HLMs to confirm the presence of these isoforms in the human liver. Because CYP3A4 and CYP3A5 are inseparable in their recombinant forms, further incubations were carried out with genotyped HLMs that contained high and low activity CYP3A5. These results differentiated between the roles of CYP3A4/5 in the oxidation of the SCB. This preliminary data showed that CYP3A4 is the major hepatic isoform involved in the metabolism of 5F-AKB-48, while CYP2J2 is involved in the biotransformation of SCBs from the heart tissues. Our studies are the first investigations to identify the specific P450 isoforms involved in the metabolism of 5F-AKB-48. We also hypothesize that altered metabolism by these P450s can be caused by genetic mutations. These studies were funded by the Arkansas IDeA Network of Biomedical Research Excellence [INBRE 117-100609 AP] and [(NIH/NIDA DA039143 to ARP and PLP].

ORAL – 4:05. Chemical Approaches for Investigating Cancer Growth Inhibition and Male Contraception by DEC-TEC and PROTAC. Fernanda Hernandez Sanchez, *Math and Science Division, University of the Ozarks, Clarksville, AR 72830*, Zhunag Jin, Martin M. Matzuk, *Center for Drug Discovery, Baylor College of Medicine, Houston, TX 77030*.

Among the Bromodomain and Extraterminal family of proteins (BET), the bromodomain protein 4 (BRD4) and bromodomain testis-specific protein (BRDT) are attractive and promising therapeutic targets for cancer and male contraception respectively. In this work, a series of dual small molecule inhibitors for BRD4 and BRDT proteins were designed and synthesized based on DNA-Encoded Chemistry Technology (DEC-TEC) and proteolysis targeting chimera (PROTAC). In vitro activities of the small molecule inhibitors on the bromodomain 1 (BD1) and the bromodomain 2 (BD2) of the two protein targets (BRD4 and BRDT) were determined by alphascreen assay demonstrating auspicious results, as well as in inhibitory activity on MV4;11 cells growth.

ORAL – 4:20. Human Glioblastoma Multiforme Growth Retardation by Inhibition of Cystine Transport. Benjamin D. Justice, Mariusz P. Fajewski, *Physical Sciences, Arkansas Tech University, Russellville, AR 72801*.

Gliomas, or tumors with origins in glial cells make up approximately 80% of all malignant brain cancers. These tumors are associated with significantly low survival rates. Glia express an obligate exchange transport

protein, Xc-, which among numerous functions, is responsible for providing the cells with cystine (cysteine dimer), a precursor for glutathione, an antioxidant. Cancerous glia overexpress Xc- protein to ensure abundant supply of glutathione, necessary for their rapid metabolism, growth and division. This project focused on investigation of novel inhibitors of the Xc- protein and their influence on glioma cell functioning. The new molecules were hypothesized to impair production of glutathione in glioma, which produced oxidative stress conditions. The hypothesis was tested by assays of human gliomas treated with the inhibitors at different concentrations for different number of days. The results obtained from this project lay grounds for optimization of the inhibitors (selectivity, potency) by SAR studies and possible extension of the idea to treatment of other types of cancer.

ORAL – 4:35. Fighting Drug Resistant Mycobacterium tuberculosis Using Modified Rifamycins. Jordan Trant, Natalie Milligan, Amanda Ford, Irosha Nawarathne, *Chemistry, Lyon College, Batesville, AR 72503.*

Tuberculosis, which is caused by the bacteria *Mycobacterium tuberculosis*, is a lung disease which kills roughly 1.5 million people a year. The most common family of antibiotics for this disease are rifamycins, which were developed 40 years ago. Rifamycins work by binding to the RNA polymerase (RNAP) and inhibiting RNA synthesis. The bacteria has since mutated in multiple ways leading to the low effectiveness of rifamycins. Among rifamycin resistant (RifR) strains of MTB due to single mutations, mutant S450L accounts for about 43% of the all the RifR strains. As an attempt to change the structure of rifamycin to make it effectively bind to the mutated MTB RNAP, we hypothesized to modify the hydroxy on the C-8 position through chemical various chemical reactions. The resultant rifamycins were tested with mutated RNAP in an in vitro transcription assay that was developed in our lab. Some of these modified rifamycins demonstrate the potential to be developed as an imaging agent to facilitate diagnosis through TB screening, thus promoting prevention and/or early treatment of the disease. In this presentation, these factors will be discussed in detail. This project was supported by the Arkansas INBRE program and the Research Technology Core of the Arkansas INBRE program with a grant the National Institute of General Medical Sciences, (NIGMS), P20 GM103429 from the National Institutes of Health.

Chemistry/Biochemistry

A – Saturday 8:00 – 9:00 Posters

B – Saturday 9:15 – 10:15 Posters

(Posters designated “U” will be judged.)

101A. Synthesis and in vivo antimicrobial studies of potent pyrazole-derived hydrazones. Jedidiah Whitt, C. Duke, D. Gilmore, M.A. Alam, *Chemistry and Physics, Arkansas State University, Jonesboro, AR 72401.*

The Centers for Disease Control and Prevention recently stated that the number of antibiotic-resistant infections has increased to more than two million per year, and these infections are responsible for 23,000 deaths in the United States annually. The ESKAPE pathogens (*Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa*, and *Enterobacter* spp.) are responsible for 80% of nosocomial infections. Traditional antibiotics have failed to treat many of these infections, as new bacterial machinery have evolved to combat the functional mechanisms of standard drugs. Additionally, due to the complex nature of bacterial cell walls and outer membranes, drug design is limited to molecules that can easily accumulate within the bacterial cell. The pyrazole scaffold has been observed in a variety of drugs that are effective analgesic, anti-inflammatory, antidepressant, anti-mycobacterial, anti-tumor, antiviral, as well as antimicrobial agents. Halogenated compounds possess notable therapeutic properties for infection or cancer treatment. Based on this information, we have designed many novel halogenated pyrazole derived compounds to be tested with five of the ESKAPE pathogens, as well as *Bacillus subtilis* and Methicillin Resistant *S. aureus*. These novel structures were synthesized in our lab, and contained a reactive aldehyde group for subsequent attachment of hydrazine or amine substituents. The compounds were screened for activity against our bacterial strains and MIC values were recorded. Our most potent compounds were chosen for in vivo activity assessment following injection into *Galleria mellonella* that had previously been inoculated with a lethal concentration of bacteria. Cytotoxicity studies of our active compounds were performed using HEK293 cells treated with two concentrations of our compound.

101B. Near Infrared Emitting Fluorophores for Selective Detection of Human Serum Albumin. Siddhi Patel, Rajib Choudhury, Anindya Ghosh, *Physical Science, Arkansas Tech University, Russellville, AR 72801.*

Human Serum Albumin (HSA) is the most abundant protein in human blood plasma. However, the concentration of 20 mg/L or higher in urine is an indication of kidney or cardiovascular disease. Also, the

low amount of HSA indicates liver cirrhosis which is the condition results in scarring in liver tissue and liver damage. Therefore, it is vital to have reliable method for detection of HSA concentration with high accuracy in clinical diagnosis. Although there are well-known methods available for determination of HSA concentration in medical diagnosis, they are time-intensive and expensive methods. In this project, we aim to develop small molecule based fluorophores for selective and quantitative detection of HSA in biological samples. We have synthesized two long-wavelength emitting (near infrared region) small molecule fluorophores in two easy step reaction. We have studied photophysical properties in different environment to compare their structure-optical properties. They both showed positive solvatochromism and displayed viscosity dependent fluorescence. Both fluorophores were water soluble at experimental conditions. They had negligible emission in phosphate buffer. However, addition of HSA greatly increased the emission of the fluorophores which led to detection of nano-molar amount of HSA protein in spiked synthetic urine samples. Through binding assay and displacement analysis, it was indicated the binding of the fluorophores into the protein's II-A subdomain which led to quantitative and selective detection of HSA in synthetic urine samples.

102A. Identification of Fat Mobilizing Substance (FMS) and Comparison of Lipolytic Activity in Urine of Fasting and Non-Fasting Humans via HPLC. Jake Garner, Cindy White, *Chemistry and Biochemistry, Harding University, Searcy, AR 72143.*

A Fat-Mobilizing Substance (FMS) has been identified in the urine of individuals with lipodystrophy or who have fasted for 36 hours. If identified, isolated, and sequenced; this protein or hormone could be studied further to reduce the effects of lipodystrophy. Furthermore, being able to sequence a protein that helps in the breakdown of body fat, without disrupting the body's protein composition, could be a big step in fighting the obesity epidemic that America is facing today.

102B. Photocatalytic Activity of TiO₂ in a Closed Circuit: Eliminating Organic Contaminants in Water using Methyl Orange as a Model Compound. Rebecca Sain, McKenzie DiLeo, Dennis Province, *Chemistry and Biochemistry, Harding University, Searcy, AR 72143.*

This research focused on the disinfecting ability of photocatalysis using UV rays and a TiO₂ nanoparticle surface. The purpose was to build a closed system that would rely on photocatalysis to eliminate organic contaminants in water with the intent of recycling it for drinkable reuse. A simple circuit was constructed using UV LEDs, and the degradation of methyl orange as a

model compound was observed. Optimal parameters such as voltage, currents, resistance, and luminosity for maximum results were determined so that the most efficient system could be constructed. Mass Spectrometry and UV-Vis Spectroscopy were used to determine the rate of photocatalysis breakdown by measuring the absorbance of methyl orange at 365 nm. Due to photocatalytic efficiency, low power and mass, a system such as this would potentially be beneficial in space craft water usage and recycling for extended missions.

103A. Metal Bis-dithiophene Complexes for Hydrogen Production. Mary Neil Hodl, William Eckenhoff, *Chemistry, Rhodes College, Memphis, TN 38112.*

Hydrogen gas produced by artificial photosynthesis is a promising future solar fuel that could potentially become the dominant energy source on earth. Dithiolenes have shown to be an active class of ligands with several metal ion-based catalysts for hydrogen production. However, complexes with dithiophene ligands have not yet been investigated for hydrogen production. We have synthesized both Co and Ni bis(2,3-dihydro-5,6-thiophenedithiolate) and evaluated them for their capacity to serve as hydrogen evolving catalysts. Electrocatalysis with acetic acid showed a catalytic wave at -1.73 V vs Fc/Fc⁺. Light-driven hydrogen production with [Ru(bpy)₃]Cl₂ and ascorbic acid yielded preliminary turnover numbers as high as 700. These preliminary numbers are encouraging for further studies with these complexes.

103B. Design, Modeling, and Synthesis of Potential Inhibitors of LpxC. Carter P. Embry, Rebeca J. Roldan, Andrea O. Pajarillo, Mauricio Cafiero, Larynn W. Peterson, *Chemistry, Rhodes College, Memphis, TN 38112.*

Gram-negative bacteria are becoming increasingly resistant against known antibiotic treatments, prompting the need to discover new treatment mechanisms. The LpxC enzyme catalyzes the first committed step in the biosynthesis of lipid A, a component of the outer membranes of Gram-negative bacteria, making its inhibition a promising target for the development of new treatments. Using known characteristics of the LpxC active site, potential inhibitors were designed to optimally bind to and inhibit the enzyme. Nucleoside containing and non-nucleoside analogues of the natural substrate were chosen to probe the interaction with the zinc ion and hydrophobic region. In silico, the analogues were positioned in the LpxC active site, and their structures were optimized using a two-layer DFT/PM6 ONIOM model. Selected compounds were synthesized and characterized for subsequent in vitro study of their antibacterial activity.

104A. Analysis of protein data bank deposited GPCR conformations. Mohammad Ali, Daitlin E. Scott, Bayazit Karaman, *Computer Science, Hendrix College, Conway, AR 72032.*

G protein-coupled receptors (GPCRs) are proteins that span the cellular membrane and detect molecules outside the cell and activate internal transformation (I don't know what you mean by this). GPCRs are vital drug targets which makes them extremely beneficial. Approximately 34% of all Food and Drug Administration (FDA) approved drugs target this protein family. Drug-design targeting GPCRs, however, is especially difficult because they are very dynamic proteins that can take on a variety of conformations, and it is unknown which conformation the drugs bind to. Our ultimate goal is to learn how GPCR conformations transform during activation and if there are common traits that are applicable to all GPCRs. We searched the Protein Data Bank (RCSB) to identify 92 and 13 of crystallized inactive and active GPCRs. We identified the single protein chains in each structure. We aligned the proteins according to their sequences and accepted those which met our threshold of 25%. We extracted the alpha-carbons in the protein back bone and accepted 89 single chained proteins that met our 25 % conservation threshold which is indicative of structural similarities for GPCR's. To find the major structural motions of the protein during activation, we will analyze the GPCR structures with principle component analysis (PCA). PCA is a reductionist method to identify statistically significant changes based on root-mean square deviation of the proteins' backbone coordinates. By understanding these conformational changes upon activation, we can construct more accurate models of activated GPCRs and design drugs to interact with these specific conformations.

104B. Spectroscopic Determination of Divalent Metal Ions to DNA Hairpin s. Harrison Russell, Kyle O'Connor, Jjulie Gunderson, Bill Gunderson, *Chemistry, Hendrix College, Conway, AR 72032.*

Slipped-strand DNA structures can form when complementary repeating sequences on a single-strand pair up to form thermodynamically stable hairpins. The formation of these hairpin structures is believed to contribute to the expansion of nucleotide repeat tracts, which are mutations associated with the development of many hereditary and anticipative neurodegenerative diseases in humans. Mg²⁺ is a divalent cation that is known to play important structural roles within DNA molecules, but the number of Mg²⁺ binding sites and the affinity of Mg²⁺ to slipped strand DNA structures are not known. The objectives of this study are to determine the stoichiometry of interaction and the dissociation constant (KD) for Mg²⁺/hairpin DNA binding. Mg²⁺ is spectroscopically silent and cannot be

observed directly. To determine the binding characteristics of Mg²⁺ to DNA hairpins, competitive titrations with Mn²⁺ were performed. Concentrations of Mn²⁺ were determined using electron paramagnetic resonance (EPR) spectroscopy, and the number of Mg²⁺ binding sites and the KD for Mg²⁺ were calculated using a binding isotherm. The results show that DNA hairpins bind Mn²⁺ with a significantly higher affinity than Mg²⁺.

105A. Implicit and explicit solvation studies of urea and anions in water. Eliza Henson, Jill Ellenbarger, *Chemistry, John Brown University, Siloam Springs, AR 72761.*

Water contamination by various anions can cause adverse, long-term health effects. Due to the global prevalence and severity of these health effects, the current research project stimulates the development of inexpensive, urea-based detectors of anionic water contamination. Urea is of particular interest because it forms multiple hydrogen-bonding interactions with anions and water molecules, making it ideal for supramolecular chemistry. To determine practicality, this project seeks to understand how urea behaves in solution, aided by the use of implicit and explicit solvation models. The solvation energies of several urea-based compounds and anions were calculated using a series of implicit solvation models (SMD, CPCM, PCM, and IEFPCM) which all proved to be precise but inaccurate up to 14 kcal/mol when compared to experimental values. The SMD model was particularly precise, inspiring further research into exactly how the continuum model differs from the experimental energies, but also prompting the shift towards using explicit solvation models. The importance of initial interaction distance of urea-chloride complexes in implicit solvent models was explored by placing the anion at a range of distances and optimizing the structure. The resulting complexes showed that the anion could end up at a variable and often inaccurate distance from urea, further supporting the move away from continuum solvation models. The solvation of urea-based compounds and a series of anions was additionally modeled explicitly within GROMACS to evaluate interaction distances and solvation favorability. The current research also supports a concurrent project investigating the potential applications of urea as a biological transport molecule by modeling the solvation of various tripodal structures.

105B. Investigating Anion Interactions with Tripodal Urea-Based Anion Transporters. Natalie Lowry, Jell Ellenbarger, *Chemistry, John Brown University, Siloam Springs, AR 72761.*

Cystic Fibrosis is a lethal autosomal recessive disease caused by the absence or malfunction of the cystic

fibrosis transmembrane conductance regulator (CFTR) protein which functions as an ion channel that transports chloride out of cells. Over the last decade, chemists have been interested in developing synthetic anion transporters that would fulfill the role of the CFTR protein. This study is focused on urea-based tripodal anion transporters. The interaction energies between chloride and tris-urea, tris-thiourea, and tris-selenourea receptors were calculated using density functional methods. The strength of the receptor-chloride interaction energies increase from tripodal tris-urea, to tris-thiourea, and then tris-selenourea. The interaction energies between these tripodal transporters and nitrate, along with other biologically relevant anions, were also studied. All three tripodal transporters are more selective to chloride compared to the other biologically relevant anions. The influence of the addition of biological fragments, such as amino acids, to the tripodal transporters are also being studied.

106A. DFT Study of the Selectivity of Monoamine Oxidase B (MAOB). Audrey Woody, Samantha Jelinek, Larry W. Peterson, Maruicio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112*.

MAOB is an enzyme located on the outer mitochondria that is responsible for degrading penylethylamine, benzylamine, and dopamine. MAOB inhibitors are generally used as a treatment for Parkinson's disease, because they stop the breakdown of dopamine. By selectively designing an inhibitor for the MAOB enzyme, the breakdown of dopamine can be reduced, thus leading to an increase of the neurotransmitter. A suite of dopaminergic derivatives have been developed as potential inhibitors of the MAOB enzyme. The inhibitory effectiveness of these dopaminergic derivatives has been measured via silico models in which the strength of interaction between each substrate and the enzymatic active site were analyzed. A crystal-structure of the MAOB active site, docked with the widely employed diabetes drug pioglitazone, was isolated from the Protein Data Bank (PDB ID: 4A79). The positions of novel dopaminergic derivatives were optimized in the active site using M062X/6-31G with implicit solvation and with flexible amino acid side-chains. Interaction energies between the ligands and the protein were calculated using M062X and MP2 with the 6-311+G* basis set. Mutations of glutamine to histidine and glutamine to glutamic acid are being tested in order to present new information about active site behavior.

106B. DFT study of the binding of ligands in SULT1A3 active site. Kayla Puzdrakiewicz, Larry Peterson, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112*.

Sulfotransferase 1A3 (SULT1A3) aids in the regulation of various endogenous and exogenous substrates in the

body via sulfation. Specifically, this enzyme catalyzes the reaction that selectively sulfates dopamine and acetaminophen. In order to distinguish the selectivity of SULT1A3, the electronic interaction energies between the active site of this enzyme and a suite of molecules known to inhibit enzymes in the dopamine pathway have been calculated using M062X with the 6-311+G* basis set. The SULT1A3 active site was isolated from the crystal structure with dopamine bound (PDB ID:2A3R). Optimized structures for eleven ligands bound in the active site were obtained by M062X/6-31G with implicit solvation by water and relaxed amino acid side chains. At least one of the ligands currently studied would bind to SULT1A3 more strongly than dopamine and some previously studied ligands (D.J. Bigler et al. / *Computational and Theoretical Chemistry* 1051 (2015) 79–92).

107A. A Drug Repositioning and Diversification Strategy for Discovery of Compounds with Anti-Cancer Activity. Matthew Chapa, Daniel Gibson, Terry Bateman, *Chemistry, Henderson State University, Arkadelphia, AR 71999*.

Finding new uses for, and improving existing drugs offers greater likelihood of success in developing viable therapeutics while reducing the risk in investing in development. Our research is involved in developing simple analogs of the prescription drug Tramadol via a simple three-step synthesis that can easily be modified to produce a large number of compounds. These compound libraries will be screened for bioactivity through via a number of bioassays. The results of the initial screens will be used to improve the analog diversification strategy.

107B. Use of cytosine-based tautomericly ambiguous nucleosides for induction of viral mutagenesis. Rachel King, Vincent Dunlap, *Chemistry, Henderson State University, Arkadelphia, AR 71999*.

Human Immunodeficiency Virus (HIV) is an incurable disease that uses the replication mechanisms of the host against itself. It is hypothesized that if a tautomer of a nucleotide is corrupted and inserted into the host, then the HIV molecule will be overloaded and fall apart. To do this, 2'-deoxycytidine will be tautomerized into a form that is unfamiliar with the HIV molecule. Using silica gel chromatography, the cytosine was tested for change. Mutagenesis has been successful in the lab, on a 100 mg scale, however incorporation of the mutated nucleotide into HIV has not been attempted.

108A. Utilization of Click Chemistry to Modify Hydroxynaphthoquinone Scaffolds to Develop Efficacious Drug Leads. Emerson Smith, Thomas Maloney, Michael Humphrey, Caleb Ray, Irosha

Nawarathne, *Chemistry, Lyon College, Batesville, AR 72503.*

Naturally occurring and synthetically derived hydroxynaphthoquinones (juglone, lawsone, phthiocol, plumbagin, laphachol) have a wide range of pharmacological uses such as anti-bacterial, anti-fungal, anti-viral, anti-parasitic, anti-inflammatory, anti-proliferative, anti-cancer, and anti-tubercular. The naphthoquinone scaffold is present in the core structure of many drugs already. Taking advantage of Michael Addition reactions, we plan to add various groups with amino functional moiety to the hydroxynaphthoquinone to create multitudes of biologically significant 1,4-naphthoquinones with modifications and test them for their various antimicrobial and anticancer properties. This research is funded by FutureFuel Chemicals LLC in Batesville and Lyon College.

108B. Photocatalysis as a Means of Disinfecting Water During Space Flight. Shelby Roberts, Jade Toth, Elizabeth Reed, Dennis Province, Cindy White, *Chemistry and Biochemistry, Harding University, Searcy, AR 72143.*

Human presence in space necessitates that all biospheres in which astronauts work and live be self-contained, including recycled air and water systems. To this end, a low power and green solution to water purification is desired. Photocatalysis is a promising solution to this issue. Titanium Dioxide nanoparticles can be photocatalytically activated using UVLED light at a wavelength of 365 nm to create reactive oxygen species (ROS) that break down organic impurities and pathogenic organisms. In this project, concentrations of a variety of bacterial species before and after treatment with TiO₂ and light were analyzed in order to determine the efficiency of disinfection parameters established in previous experiments.

109A. Single versus Double Ringed Ligands as Inhibitors for ALDH. Caroline Magee, Larryn W. Peterson, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112.*

L-DOPA is commonly used as a xenobiotic for patients with conditions such as Parkinson's disease. L-DOPA is transformed into dopamine by DOPA-decarboxylase. Dopamine derived from L-DOPA is deactivated via metabolism by a series of enzymes including Aldehyde dehydrogenases (ALDH). The targeted inhibition of the ALDH enzyme may help to prolong the effectiveness of L-DOPA, resulting in a net increase in pharmacological efficiency. By selectively designing an inhibitor for ALDH, the effectiveness of the L-DOPA can be extended by regulating the metabolism of dopamine derived from L-DOPA. The effectiveness of a series of potential inhibitors has been measured via in silico models in which the strength of interaction between each substrate and the enzymatic active site was analyzed. A

crystal-structure of the ALDH enzyme with an inhibitor bound in its active site (PDB ID: 4WP7) was used to create a model of the active site. Novel dopaminergic derivatives were optimized in the active site using M062X/6-31G with implicit solvation and with relaxed amino acid side-chains. Ligands can fit into the active site in a number of ways; this work examines single molecule orientations and double molecule orientations. Interaction energies between the ligands and the protein were calculated using M062X with the 6-311+G* basis set. Some potential inhibitors show promising results such as the MP and CM series. Mutant enzymes were also studied for their affinity for the ligands.

109B. Evaluation of hybrid and pure DFT methods for the binding of novel ligands in the tyrosine hydroxylase enzyme. Rebecca Evans, Larryn Peterson, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112.*

The Minnesota 2006 density functional methods include both pure and hybrid models, each of which benefitting different aspects of various systems. The Tyrosine Hydroxylase (TyrH) enzyme contains a Fe²⁺ in the center of the active site. M06-2X, M06-L, and M06 have all been used to evaluate the binding strength of novel ligands in the TyrH active site. TyrH is the rate determining enzyme in the synthesis of the catecholamine, dopamine. TyrH converts tyrosine to L-DOPA, which is administered in the treatment of Parkinson's patients, as dopamine cannot cross the blood brain barrier. The inhibition of TyrH reduces dopamine in the brain to undetectable levels. A crystal structure of the active site of Tyrosine Hydroxylase with a known inhibitor bound was obtained from the protein data bank (PDB ID: 2TOH). In this work, dopaminergic derivatives were inserted into the enzymatic active site in silico in order to test the strength of the interactions between the substrate and active site, to determine if any of these derivatives could be effective inhibitors. M06-2X is a hybrid functional, while M06-L and M06 are both pure; all of these functionals were used to optimize structures and to analyze interaction energies. While all the methods are suited for large complexes, such as the active site of an enzyme, M06-2X is stated to be best for interaction energies, M06-L best when a transition metal is present, and M06 as an intermediate between the two (Yan Zhao, Donald G. Truhlar, *Chem Phys Lett.* 502, 2011, 1-13). The novel dopaminergic derivatives were optimized with implicit solvent with either M06-2X, M06-L, or M06 and 6-31G with relaxed amino acid side-chains. Interaction energies between the ligands and protein were determined using the same DFT methods as mentioned above with the 6-311+G* basis set. M06-2X and M06 are hybrid functionals, while M06-L is pure; all of these functionals were used to optimize structures and to analyze interaction energies. Preliminary results show significant

differences between the methods within the same complex, as well as potential in determining a well-suited derivative, that has seeded other promising ligands.

110A. Drug Repositioning and Diversification Strategy for Discovery of Compounds with Anti-Cancer Activity.

Daniel Gibson, Mathew Chapa, David T. Bateman, *Chemistry, Henderson State University, Arkadelphia, AR 71999.*

Drug repositioning is a low risk, high reward drug development strategy that reduces the cost and time needed for drug and target discovery by repurposing existing drugs. Tramadol is a prescription drug for pain-relief and depression but has shown to possess off-label uses as an antipyretic, antibacterial, and antifungal. The purpose of our research is to reposition Tramadol as an anticancer drug. A library of analogs of Tramadol containing diversified functional groups will be synthesized with a simple three-step process, tested for bioactivity, and screened for anticancer activity.

110B. Synthesis of imidazolylbenzamides as possible antimalarial candidates.

Emily Williford, Martin Campbell, *Chemistry, Henderson State University, Arkadelphia, AR 71999.*

With nearly 215 million new cases in 2015, resulting in over 400,000 deaths, malaria continues as the scourge of the tropics, especially Africa and Southeast Asia. Despite the success of artemisinin-based combination therapies, the parasite continues to develop drug resistance. Therefore, there is need for new artemisinin codrugs as well as new classes of anti-malarials. Recently, GlaxoSmithKline and other organizations have published a variety of vetted structural motifs that are potential candidates for the next line of antimalarials. Currently, we are investigating the synthesis of a series of tertiary cyanobenzamides based on one such a structural motif. We report progress to date on a convergent synthesis route to a variety of these benzamides bearing substituted imidazole groups as well as a small alkyl group.

111A. Comparison of FFT-Infrared and Raman spectral methods for analysis of xylenes.

Drake Jackson, Edmond Wilson, *Chemistry and Biochemistry, Harding University, Searcy, AR 72143.*

With Raman spectrometers becoming more common in the laboratory, the question arises if analytical methods utilizing a Raman spectrometer is more efficient and accurate than methods using a Fast Fourier Transform Infrared Spectrometer (FFT-IR). Advantages of Raman spectral methods include use of glass or quartz sample cells instead of salt cells, Raman is sample path length independent; instrumentation is less complicated with

no moving parts. Results of an analysis of a commercial xylene sample containing ortho-, meta-, and para-xylenes, using both Raman and FFT-IR instruments, are given.

111B. Melanin Concentrating Hormone Receptor 1 (MCH1R) Antagonists for Treating Addiction.

Britny Kirkpatrick, James Tarrant, Dennis Province, *Biochemistry, Harding University, Searcy, AR 72143.*

Melanin Concentrating Hormone (MCH) is a 19-amino acid neuropeptide, predominantly expressed in the lateral hypothalamic area and zona incerta and MCH-producing neurons project throughout the brain. The MCH receptor is a G-coupled protein receptor and is involved in the regulation of feeding behavior and energy homeostasis, maintenance of REM sleep, depression, anxiety and is associated with emotional reactivity and reward behaviors connected to certain addictions. Of the two known MCH receptors, MCHR1 is widely distributed in the brain, including the hypothalamus, thalamus, olfactory cortex, amygdala, striatum, and hippocampus, in all vertebrates. We intend to prepare a series of fluorinated octahydro-2H-pyrido[1,2-a]pyrazine analogs and test their anti-addiction properties in an ethanol self-administration model in rodents. Further, these fluorinated analogs may prove useful as ¹⁹F probes in NMR that will allow us to study these anti-addiction properties in the brains of animals and possibly in humans.

112A. DFT analysis of water clusters, dopaminergic derivatives, and their desolvation energies.

Emily Sanders, Mallory Morris, Larryn Peterson, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112.*

Our current research explores the synthesis, metabolism, and excretion of novel catecholamines which could serve as drugs in the dopaminergic pathway. By studying all of the enzymes involved in the dopaminergic pathway, we can paint a comprehensive picture of how these catecholamines will behave in our bodies which will help us find novel drugs that could treat conditions such as Parkinson's disease. Computational models of dopaminergic analogs were used to examine the substrates' binding in the enzymatic active site. The binding of a ligand to an enzyme not only involves the interaction between the ligand and the enzyme but also the energy lost or gained by desolvation of the ligand. Desolvation of dopaminergic derivatives was examined using a series of hydration shells that increase in size and many different suites of ligands. The desolvation energies were calculated using M062X with the aug-cc-pvdz, cc-pvdz, and cc-pvtz basis sets. Ligands with amine group in the sixth position of the ring exhibited the least favorable energies, whereas neutral ligands exhibited the most favorable desolvation energies in the explicit water

model. This information will be combined with prior research done on ligand/enzyme interaction in order to get a more comprehensive understanding of ligand binding in this system.

112B. Measuring the Desolvation Energy for the Active Site of Enzymes within the Dopaminergic Metabolic Pathway. Connor Frost, Laryn Peterson, Mauricio Cafiero, *Neuroscience and Chemistry, Rhodes College, Memphis, TN 38112.*

Currently, there are two potential treatments for Parkinson's disease: L-Dopa and a stimtrod inserted into the Globus Pallidus or subthalamic nuclei (Weaver FM, Follett K, Stern M, et al. *JAMA*. 2009;301(1):63–73.). L-Dopa is by far the most common treatment for Parkinson's as it is noninvasive and many Parkinson's patients are older and unfit for invasive surgery, (Weaver FM, Follett K, Stern M, et al. *JAMA*. 2009;301(1):63–73.). In order to improve the effectiveness of L-Dopa as a treatment our current research is aimed at designing an inhibitor to both inhibit selectively the enzymes that may break down L-Dopa before it reaches the Blood Brain Barrier, while safely bypassing the enzymes that are involved in the biosynthesis of dopamine. In order to determine the binding of this potential inhibitor to these enzymes, we must determine (among other things) the desolvation energy required to strip the waters from the active site and bind the inhibitor. To do this various enzymes related to the dopamine metabolism pathway such as ALDH and tyrosine hydroxylase were optimized in pm6 and m062x/3-21G with various numbers of water pairs in order to determine a trend in the desolvation energies. While large enzymes showed inconsistent results in pm6; m062x/3-21G showed more consistent results revealing a general 'logarithmic' trend in desolvation energy the more waters that were present in the active site.

113A. Changes in Interaction Energies of Bis(phenyl(thio)urea)-chloride Complexes due to Substituent Effects. Wesley Shorey, Jill Ellenbarger, *Chemistry, John Brown University, Siloam Springs, AR 72761.*

Contamination of water sources demands attention across the globe, most notably in rural or underdeveloped areas. Urea can be used to build frameworks of selective and accessible chemosensors to detect anionic contaminants, due to the strong hydrogen-bonding donors on urea that make it excellent at interacting with anions. The strength of the bis(phenyl(thio)urea)-chloride interactions, and therefore the hydrogen-bonding distance, is altered by placing substituents on the phenyl groups, and this interaction was examined using Density Functional Methods (DFT). Electron-withdrawing moieties (fluoro,

nitro, and trifluoromethyl groups) result in significantly stronger interactions than their electron-donating counterparts (methyl and amine groups). Additionally, bis(phenylurea)-chloride and bis(phenylthiourea)-chloride interaction energies display a direct, linear relationship. Thiourea analogues create interactions with anions that are stronger by approximately 3 kcal/mol. Combining the substituent effects and the urea/thiourea relationship, interaction energies of similar bis(phenyl(thio)urea)-chloride complexes can be predicted.

113B. Cellulase Activity in Oklahoma Grown Mushrooms. Madison Thomas, Ratnaker Deole, *Natural Science, Northeastern State University, Tahlequah, OK, 74464.*

There is a great need to find alternative sources for energy due to the negative effects of fossil fuels on the environment and the finite amount of the source. Biofuels are a renewable and environmentally-friendly source of energy that are derived from biomass. One of the processes used to produce biofuel involves the breakdown of cellulose into glucose and then by way of fermentation, produce ethanol. A family of enzymes called cellulases are required to catalyze the breakdown of cellulose. Fungi are one of the most prolific producers of cellulase, as well as being an inexpensive source of this enzyme; thus, making mushrooms that harbor these fungi, a viable option for biofuel production. This research looks at cellulase activity found in Oklahoma grown mushrooms. The purpose of this study is to optimize use of cellobiase, a type of cellulase, by determining the conditions in which the most product (glucose) is produced. Enzyme assays were conducted at pH levels ranging between pH 5 to pH 8.6 and temperatures ranging between 0°C and 100°C.

114A. Design of novel inhibitors for the catechol-O-methyltransferase enzyme. Emma Cook, Katherine Hatstat, Laryn Peterson, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112.*

Parkinson's disease is characterized by a decrease of dopamine levels within the brain. L-Dopa is commonly used in the clinical treatment of Parkinson's disease, as it is able to cross the blood brain barrier when dopamine cannot. DOPA-decarboxylase transforms L-DOPA into dopamine. Dopamine derived from L-DOPA is deactivated via metabolism by the COMT enzyme. Catechol-O-methyltransferase is an enzyme that degrades catecholamines such as dopamine, epinephrine, and norepinephrine. L-DOPA is a precursor of catecholamines and is therefore an important substrate of COMT. This targeted inhibition of the COMT enzyme prolongs the effectiveness of L-DOPA, resulting in a net increase in pharmacological efficiency. By selectively designing an inhibitor for the COMT enzyme,

the effectiveness of L-DOPA can be extended through regulating the metabolism of dopamine derived from L-DOPA. The effectiveness of these dopaminergic derivatives has been measured via in silico models in which the strength of interaction between each substrate and the enzymatic active site was analyzed. A crystal-structure of the COMT enzyme active site, docked with a known COMT inhibitor, BIA 8-176, was isolated from the Protein Data Bank (PDB ID:2CL5). Novel dopaminergic derivatives were optimized using M062X/6-31G in vacuum and in implicit solvation with rigid amino acid side-chains. Interaction energies between ligands and the protein were then calculated using MO6L and the 6-311+G* basis set. A recently developed set of molecules that are more selective for increasing dopamine has been tested.

114B. Substituent Effects on Solvatochromism of [Cp2Co][Mo(bpy)Cl4]. Keren Lee, William Eckenhoff, *Chemistry, Rhodes College, Memphis, TN 38112.*

Solvatochromism is an interesting effect caused by variation in solvent polarity, as evinced by differently colored solutions depending on the solvent used. We recently discovered that [Mo(bpy)Cl4]- (bpy = 2,2'-bipyridine) is solvatochromic, shifting over 100 nm in different solvents. We sought to better understand the nature of this solvatochromism by exploring the effect of various electron donating and withdrawing groups, specifically 4,4'-dimethyl-2,2'-dipyridine and 2,2'-bipyridyl-4,4'-dicarboxylic acid.

115A. Determination of Fatty Acid Concentrations in Algae. Tye Brown, Austin Metcalf, Kendall Wells, Jordan Kane, Andrew Williams, *Chemistry, UA Monticello, Monticello, AR 71655.*

Algae are of scientific and commercial interest due to their ease of culture and high fatty acid content. It is reasonable to assume that different strains of algae contain different types and concentrations of fatty acids. Of interest is the fatty acid content contained within various algal strains in the class Eustigmatophyceae. The extracted fatty acids may be of potential use for phylogenetic classification of new algal species, in addition to human consumption and producing next-generation biofuels. Algal strains were collected and isolated from Lake Chicot in Arkansas, Tower Pond and Lake Itasca at Itasca State Park in Minnesota, and Thayer Lake in the upper peninsula of Michigan. The strains collected were subjected to a 5-step process for lipid preparation: lyophilization, lipid extraction, filtration, esterification, and methyl ester extraction. The fatty acid extracts were analyzed using GC-MS. After qualitative determination of fatty acids by mass spectrometry, relative quantities of the fatty acids were determined by peak integration, and tricosanoic acid (C23:0) was used as a standard to determine

absolute quantities. Preliminary results show differences between algal strains via relative fatty acid concentration.

115B. Fingerprint Analysis of Fatty Acids found in Algae. Hayden Jumper, Victoria Fox, *Math and Natural Sciences, UA Monticello, Monticello, AR 71655.*

Using FAME data, statistical analysis was performed on algae samples gathered from nine locations in Southern Arkansas. The analysis of the FAME data for the samples shows a potential relationship between the fatty-acid distribution patterns in a sample and the location from where the sample was gathered.

116A. Synthesis of Metal Chalcogenide Aerogels. Kennedy Smith, *Chemistry, UA Pine Bluff, Pine Bluff, AR 71601*, Alicia Blanton, Bobby Portis, Muhammad Islam, *Chemistry, Jackson State University, Jackson, MS 39217.*

The goal of this study was to create new aerogels to be used for other applications. Aerogels have had a large impact in medical and environmental industries, and there has become a great need for such materials. These are highly porous gels in which the liquid component has been replaced with gas. Metal Chalcogenide Aerogels are prepared from transition metals, as well as group 16 elements on the periodic table of elements, excluding Oxygen. Currently, many studies focus on the replication of known aerogels, but the purpose of this research is to synthesize and characterize new materials. The synthesis of these gels must consistently evolve to increase production as well as efficacy. There were three chalcogels successfully prepared, KS008: Sn(II)Ac + (NH4)2MoS4 + PS4 → Sn(MoS4)PS4; KS012: Sn(II)Ac + K2Sx → Sn(MoS4)K2Sx; and KS004: Sn(II)Ac + (NH4)2MoS4 + (NH4)2MoO4 → Sn(MoS4)MoO4, at standard temperature and pressure, that have shown promise for future application. In general, the synthesis of an aerogel encompasses three steps: sol-gel process, aging, and supercritical drying. Once the gel has solidified with its porous structure still intact, it is analyzed by a scanning electron microscope, (SEM), for Energy-Dispersive X-Ray Spectroscopy, (EDS), as well as an elemental analysis.

116B. Crystallization of Col-H Targeting Domain, PKD1-PKD2-CBD, from *Hathewayia histolytica* and Purification of Bovine Complement 1q. Huddoy Walters, *Chemistry and Physics, UA Pine Bluff, Pine Bluff, AR 71601*, Joshua Sakon, *Chemistry, UA Fayetteville, Fayetteville, AR 72701.*

Crystallization of Col-H Targeting Domain, PKD1-PKD2-CBD, from *Hathewayia histolytica* and Purification of Bovine Complement 1q The Protein complex known as the Complement system, found in the blood plasma, plays significant roles in the defense against pathogenic

materials in animals. The complement system activates when antigen-antibody aggregates stimulate a component of the protein complex known as C1. C1q is one of three proteins that form the structure of C1. During pregnancy, C1q levels directly affect the health and development of the fetus. Also, C1q is an influential factor in nervous system development and it even possesses anti-cancerous properties (Kouser et al. 2015). Due to its structural similarity to collagen and its bundle-like quaternary structure C1q could be a useful model to study trans-collagen binding. Bacterial collagenases can contain a variable number of collagen binding domains. When infecting host tissue, collagenases with multiple domains may be able to anchor to separate collagen molecules, thus trans, and then begin collagenolysis. To understand the binding mechanism of collagenase-H, a three-dimensional structure of its domains and a collagen model are needed. My research incorporates different experimental procedures to isolate and purify C1q from bovine blood and crystallize the PKD-PKD-CBD domains in collagenase-H (col-H). The triple helical domain of C1q would pose as a suitable model for collagen. Diffraction of the crystallized domain of col-H can provide its innate structure. This structure can be used to study its binding mechanism. Bovine blood was clotted and converted into the serum. The protein complex containing C1q was precipitated using Euglobulin Precipitation. Centrifugations and dialysis were used along with certain buffer solutions to purify and maintain ideal conditions for C1q extraction. Ion exchange chromatography using DEAE gel was also used as an important step in the purification of the sample. UV spectroscopy, BCA assay, SDS PAGE, and ELISA assay were used to measure protein concentrations and identify the presence of C1q. Non-reducing- SDS PAGE resulted in bands within the range of 440 kDa and reducing -SDS PAGE gels produced bands with 24-37 kDa ranges. These results are consistent with the distinctive presence of C1q. The presence of C1q was confirmed and the C1q concentrations of samples were found using an ELISA assay. The assay confirmed the effectiveness of the purification processes. The gels from SDS PAGE depicted that C1q was isolated with impurities present in the solution from the bovine sample. The crystallization of col-H domains started with a PCT test that selected 2.46ul/ml as an ideal concentration for the future nucleation of the protein. A 96 well setting drop vapor diffusion method was then used to select potentially suitable reagents and conditions for crystallization of the protein. Selected conditions were optimized using a hanging drop vapor diffusion method according to observed well results. It was found that polyethylene glycol (PEG) concentrations were the critical factor in crystallizing the domains. 19% PEG in pH4.5 acetate buffer produced best crystals.

117A. Computational Analysis of Mechanistic Pathways for Hydrogen Evolution Using a Nickel Schiff Base Catalyst. Phillips Hutchison, William Eckenhoff, *Chemistry, Rhodes College, Memphis, TN 38112.*

In producing photocatalysts capable of proton reduction, it is important to determine likely mechanistic pathways through which the reductive processes may occur. Use of computational chemistry techniques allow for the exploration of many possible mechanistic pathways and the corresponding thermodynamic favorability of each. This study makes use of Density Functional Theory (DFT) to study not only the Gibbs energy associated with different reduced species that may form from catalysis, but also seeks to determine the relevant reduction potentials and pKas. The molecules modeled are based off of confirmed crystal structures and have corresponding electrochemical data with which theoretical findings will be compared.

117B. DFT study of the selectivity of the β -1 adrenergic receptor. Megan Simons, Laryyn Peterson, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112.*

The β -2 adrenergic receptor signaling noradrenaline in the prostate region is necessary for activation of an angiogenic switch that induces exponential prostate tumor growth. Loss of ADRB2, the gene encoding the β -2 adrenergic receptor, inhibits angiogenesis. This forces the endothelial cancer cells to use their own nutrients and energy, therefore halting tumor growth. This inhibition can slow down the progression of prostate cancer, which is being researched as a potential alternative to chemotherapy for cancer treatment. The structure of the β -1 adrenergic receptor with a bound partial agonist of salbutamol was used to create a model of the β -2 binding site. Comparing structures of a β -2 adrenergic receptor (PDB ID: 5X7D) and a β -1 adrenergic receptor (PDB ID: 2Y04) showed a pattern of binding on Chain A offset by approximately 8 amino acids in its order. The adrenergic receptor with bound ligands was optimized in this derived binding site using M062X/6-31G with implicit solvation and flexible amino acid side-chains. Interaction energies between the ligands and the receptor were calculated using M062X with the 6-311+G* basis set. Some positively charged inhibitors show results of attractive negative interaction energies.

118A. NPs, svNGF and svVEGF: three protein families from snake venom with potential biomedical applications - A review. Phuc Phan, *Physical Sciences, UA Fort Smith, Fort Smith, AR 72904*, Ragupathy Kannan, Anant Deshwal, T.K.S. Kumar, *Chemistry, UA Fayetteville, Fayetteville, AR 72701.*

Snake venom has been known as a gold mine for pharmaceutical drugs for decades despite its toxicity

and lethality on a wide range of animal species. With such potentials, toxins in snake venom are used as templates to develop novel therapeutics for a myriad of diseases and disorders. This project was aimed to review and compile characteristics and applications of a few such toxins. Some demonstrate the ability to synergize with other toxins like Nerve Growth Factors (NGFs) to amplify their effects. Others like Natriuretic Peptides (NPs) show vasorelaxation effects, and Vascular Endothelial Growth Factors (sVEGFs) play important roles in the process of vasculogenesis and angiogenesis. These proteins also have other properties like inducing apoptosis, suppressing tumors, enhancing growth of blood vessels, and upregulation of other toxins. Such properties have been utilized to treat heart failure, myocardial infarction-reperfusion injury, and more. We now hope to investigate these snake venoms and their proteins further and seek answers to questions pertaining to their potential biomedical applications.

118B. Synthesis of N-Benzoyl-2-Hydroxybenzamide Analogues for the Treatment of Malaria. Allen Nguyen, Gregory Naumiec, *Chemistry, University of Central Arkansas, Conway, AR 72035*.

Malaria is a disease caused and transmitted by via several species of Plasmodium parasites including *P. vivax*, *P. ovale*, *P. malariae*, *P. knowlesi*, and *P. falciparum*. Malaria is one of many neglected tropical diseases due to its prevalence in developing nations located near the equator. It is estimated that half of the world's population is at risk of contracting malaria. Chloroquine, discovered in 1934, is one of the world's essential medicines for treating and preventing malaria; however, due to mass drug administration, strands have starting show resistance to chloroquine, especially in Africa, South America, and Southeast Asia. The second generation of drugs, mefloquine and lumefantrine, have harsh side effects, can't be used during pregnancy, and are not used to treat severe cases of malaria. On top of resistance and ineffectiveness of second generation drugs, treatment and prevention efforts in these nations are costly. Recent efforts have uncovered a lead compound based on the structure of N-hydroxybenzamides that have shown effectiveness against the *P. falciparum* parasite which is known to cause cerebral malaria. My research focuses on optimizing the synthesis of N-hydroxybenzamides as well as investigating any analogues that can increase the drug's effectiveness. The synthesis is broken into two major pathways based on the order of the reactions done: Suzuki coupling of alkyl and aryl substituents to halobenzoic acids followed by the coupling to salicylamide or coupling of halobenzoic acids to salicylamide followed by the Suzuki coupling of alkyl and aryl substituents. Currently ortho, meta, and para halobenzoic acids have protected in high yields are

currently undergoing Suzuki coupling reactions. All products were analyzed with ¹H and ¹³C NMR spectroscopy after purification by column chromatography with moderate yields.

119A. Does systemic inflammation mediate associations of the gut microbiome with estrogen profiles in postmenopausal women? A cross-sectional analysis of the Hispanic Arkansas pilot study. Clement N. Agvemang, *Chemistry, UA Pine Bluff, Pine Bluff, AR 71601*, Martin Cannon, Franck Carbonero, Letycia Nunez-Argote, Barbara J. Fuhrman, *Dept. of Epidemiology, COPH, UAMS, Little Rock, AR 72205*.

Breast cancer risk has been found to be positively associated with estrogen levels in postmenopausal women. The gut microbiome may play multiple roles in breast cancer pathogenesis, by influencing estrogen levels and/or by shaping anti-cancer immune responses. We have carried out a cross-sectional analysis to test hypotheses about the role of immune factors using stored biospecimens and available data on circulating estrogens and fecal microbial composition from a study that included 40 postmenopausal Hispanic women. We measured serum concentrations of 2 inflammation-related biomarkers. Gut microbial composition was measured as relative abundances calculated for phylum-, class-, order-, family-, and genus level-taxa. We tested for associations with 47 taxonomic categories after filtering out taxa found in less than 10% of samples and taxa representing less than 0.2% of all OTUs. General linear regression models were used to test for associations of CRP and LBP with relative abundance measures and serum estrogen concentrations. We observed that serum CRP was not associated with serum LBP. However, serum CRP was inversely associated with Lachnospiraceae, and there was a positive association between serum CRP and 17-epiestriol. We also observed no association between serum LBP and gut microbial taxa. We found out that serum LBP was inversely associated with Estradiol and Estriol. We observed many associations between microbial taxa and estrogen measures.

119B. Optical Imaging and Sensing of Escherichia coli O157: H7 using graphene quantum dots. Clement N. Agvemang, Deandre Gridley, Daoyuan Wang, *Chemistry & Physics, UA Pine Bluff, Pine Bluff, AR 71601*.

Escherichia coli O157: H7 has become a serious life-threatening problem for tens of thousands of people around the world in the past few decades. Therefore, a rapid, simple, low cost, and user-friendly biosensing label to monitor *E. coli* O157: H7 has become necessary and important. In this study, water soluble graphene quantum dots (GQDs) is synthesized via chemical/hydrothermal routes and functionalized with carboxyl groups. *E. coli* O157: H7 antibody is then

covalently conjugated to GQDs via a cross-linking reaction until an immunofluorescence probe is finally achieved. This probe can generate strong fluorescent signal and effectively recognize *E. coli* O157: H7 under a low detection limit (expecting <100 cfu/mL). This novel detection method could be as a useful tool to detect *E. coli* O157: H7 in food, water, and environment.

120A. DFT study of ligand binding in biogenic amine transporters. Abigail Polzin, Larry Peterson, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112.*

Biogenic amine transporters (BATs) are membrane proteins that are used to assist the movement of the biogenic amines (such as serotonin, dopamine, and norepinephrine) across the membrane. BATs are crucial targets for a variety of diseases. The BAT for dopamine is important in Parkinson's disease as the disease is characterized by a lack of dopamine in several areas of the brain. Understanding how a particular molecule interacts with the BAT binding site can help further refine drug development for Parkinson's disease and other disorders. In this work we examine the function of the transporter at the binding site by studying the engineered protein LeuBAT (Koldso et. al. *Front. Pharmacol.* 24 September 2015). A crystal structure of the LeuBAT active site in complex with (R)-fluoxetine was isolated from the Protein Data Bank (PDB ID: 4mm8). LeuBAT has an outward facing structure which allows drugs to not only bind inside the structure, but to also interact with the rest of the binding site surrounding the inside pocket. The structure of several ligands bound in the LeuBAT active site was optimized using MO62X/6-31G with implicit solvent and relaxed amino acid side chains. The interaction of these various ligands with the LeuBAT active site was calculated using MO62X/6-311+G*. These calculations show that LP-OH is a better inhibitor in the LeuBAT binding site than (R)-fluoxetine.

120B. Cobalt complexes with dithiothiophene ligand for the Light Driven Production of H₂. Liam Rhodes, Will Eckenhoff, *Chemistry, Rhodes College, Memphis, TN 38112.*

Over the next century, the world's population is expected to increase at a drastic rate; therefore, it is essential to consider new and more efficient sources of energy such as the use of artificial photosynthesis to generate hydrogen gas. Hence, the development of more active and robust catalysts is necessary in order to make artificial photosynthesis a viable method of hydrogen generation. Using 5,6-dihydrothieno[2,3-d]-1,3-dithiol-2-one (a-dpdt) is a promising ligand due to its electronic similarity to previously used ligands for cobalt catalyzed hydrogen production. Dithiothiophenes have not been investigated for hydrogen production. Cyclic voltammetry experiments showed reversible redox

waves at -0.66 V vs. Fc+/Fc. In the presence of acetic acid, a catalytic wave corresponding to hydrogen was observed at -2.1 V vs. Fc+/Fc. Hydrogen production was also observed under light-driven conditions with [Ru(bpy)₃]²⁺ and ascorbic acid yielding turnover numbers as high as 300.

121A. The Effect of Retinoid Receptor Agonists on K562 Cellular Proliferation. William Higgins, Melissa Kelley, *Chemistry, University of Central Arkansas, Conway, AR 72035.*

Establishment and maintenance of proper immunity requires a precise balance between cellular adhesion and proliferation. A disruption in either event culminates in a variety of pathologies encompassing immunosuppression, auto-immunity, and cancer. Retinoids, profoundly affect immune function by mediating cellular adhesion and proliferation in certain leukocytes. Retinoids, by binding to retinoid receptors (RARs or RXRs), modify the expression of a variety of signaling proteins involved in immune cell proliferation and adhesion including, integrins. Integrins are a family of transmembrane heterodimeric receptors consisting of non-covalently linked α and β subunits that are considered to be the principle receptors involved in attachment to the extracellular matrix and provide adhesive interactions that control cellular proliferation. Currently, the contributions by RARs and RXRs in immune cell adhesion and proliferation have not been examined. In this study, the effect of all-trans-retinoic acid agonists on K562 cellular proliferation was examined. Interestingly, K562 cellular proliferation levels were decreased in a time- and concentration-dependent manner when cells were treated with the RARgamma agonist. In the presence of the RARalpha or RARbeta agonists, K562 cellular proliferation was comparable to the vehicle control. Our study is the first to demonstrate that specific retinoid agonists alter cellular proliferation in K562 cells.

122A. Wet Air Oxidation of Phenol. Kayleigh Johnson, *Chemistry & Physics, UA Pine Bluff, Pine Bluff, AR 71601,* Iva Jovanovic Tews, Manuel Garcia Perez, *Biochemical Engineering, Washington State University, Pullman, WA 99164.*

Phenol is a highly toxic chemical that is very common in oil, gas, and chemical manufacturing. Due to the toxicity of phenol, any aqueous solution that is contaminated with it, has to be properly treated and disposed of. The objective of this research is to determine if wet air oxidation is an efficient way to treat waste water contaminated by phenol. Applying compressed oxygen to the phenol contaminated water in a closed batch system under pressure and high temperature contributes to the break down of phenol into components: carbon dioxide (CO₂), water (H₂O), and

other small organic acids. If complete oxidation is achieved, the aqueous waste can then be further treated with established biological methods found in most wastewater industries. Chemical Oxygen Demand (COD) will be measured in order to evaluate if the complete breakdown of phenol has occurred. High pressure liquid chromatography will also be utilized to assess the composition of the final products after oxidation. Our experimental technique uses 28 ml stainless steel batch reactors operated at a span of temperatures and residence times. The experimental matrix will help to identify the most effective process conditions for complete oxidation of the phenol solution. The temperatures span from 180-250°C in intervals of 10°C. The gases tested were nitrogen (N₂) and oxygen (O₂). The time durations included 5, 10, 15, 20, 30, and 45-minute intervals. These conditions were all tested under a pressure of 120 psi of the tested gases.

122B. Use of Biochar for Methylene Blue removal from water. Kennedi S. Weston, *Chemistry & Physics, UA Pine Bluff, Pine Bluff, AR 71601 99164*, Kamu Taulelei, Ashlie Adams, Waled Suliman *Biological Systems Engineering, Washington State University, Pullman, WA 99164*.

The goal of this study was to remove contaminants from aqueous phase solutions using the adsorption approach. We used Methylene Blue (MB) to mimic water contamination while biochar was the adsorbent. We conducted several isotherm and kinetic experiments to understand the adsorption behavior of the biochars that were used and their removal efficiency. The two biochars, SCOMC and COMBC, were made from agricultural biomass. The effect of pH, adsorbent doses, and contaminant concentrations were all studied in the batch of adsorption set ups. To measure the concentration of MB before and after biochar additions, a spectroscopy method was utilized to track MB concentration. Before that, all samples were agitated for 24hrs (max) at 200 rpm and then filtered using Whitman filter paper 42. The results showed that biochar removes MB up to 98% after only 5 minutes at pH 7. We can conclude that we can design biochar-based adsorbents for water filtration.

123A. Experimental and Computational Investigation of the Solvatochromism of [Mo(diimine)Cl₄]-Compounds. Sarah Helland, William T. Eckenhoff, *Chemistry, Rhodes College, Memphis, TN 38112*.

A solvatochromic compound is a chemical compound that changes its color based on solvent polarity. We found that the [Mo(bpy)Cl₄]-anion is highly solvatochromic over a wide range of solvents. From water to acetone, the absorbance maximum shifts over 100 nm with a corresponding color change of yellow to

blue, respectively. To expand upon this, we investigated other ligand architectures that might show similar solvatochromic behavior. Specifically, we examined 1,10-phenanthroline (phen), 2,3-bis(2-pyridyl)pyrazine (bppz), and 2,2-bipyrimidine (bpm). Monometallic complexes with these ligands showed only slight changes in their solvatochromism range, bimetallic complexes of bppz and bpm showed markedly different characteristics. In the case of [Mo₂(bppz)Cl₈]²⁻, the absorbance red-shifted ~50 nm, producing a range of green colors. The [Mo(bpy)Cl₄]-anion was computationally investigated to better understand the nature of this interesting property.

123B. DFT study of the selectivity of DOPA-decarboxylase. Peyton Antwine, Muarcio Cafiero, Laryn Peterson, *Chemistry/Neuroscience, Rhodes College, Memphis, TN 38112*.

L-DOPA is commonly used as a xenobiotic for patients with conditions such as Parkinson's disease. Clinically-administered L-DOPA is transformed into dopamine by the enzyme DOPA-decarboxylase. In order to be pharmacologically effective, L-DOPA must not be metabolized before it crosses the blood-brain barrier. Premature metabolism of L-DOPA can be prevented by inhibiting DOPA-decarboxylase in the periphery. By selectively designing an inhibitor for the DOPA-decarboxylase enzyme, a larger amount of peripheral L-DOPA can cross the blood-brain barrier. A suite of dopaminergic derivatives have been developed as potential inhibitors of the DOPA-decarboxylase enzyme. The inhibitory effectiveness of each dopaminergic derivative has been measured via in silico models in which the strength of interaction between each substrate and the enzymatic active site was analyzed. A crystal-structure of the DOPA-decarboxylase active site, docked with a known DOPA-decarboxylase inhibitor, Carbidopa, was isolated from the Protein Data Bank (PDB ID: 1JS3). The positions of novel dopaminergic derivatives were optimized in the active site using M062X/6-31G with implicit solvation and with flexible amino acid side-chains. Interaction energies between the ligands and the protein were calculated using M062X and MP2 with the 6-311+G* basis set. At present, a number of alternative competitive inhibitors of the DOPA-decarboxylase enzyme are being studied. Of the several different families of potential inhibitors being studied in our lab, several promise to be effective.

124A. Improved Synthesis of Calmodulin Antagonist TAPP for Purification and Study of Calmodulin. Josiah Johnson, Gregory R. Naumiec, Tori Dunlap, *Chemistry, University of Central Arkansas, Conway, AR 72035*.

Calmodulin (CaM) is a calcium ion sensing protein that is a major translator of calcium signaling in cells. In general, CaM binds up to four calcium ions when

cellular calcium levels rise and can then bind to and alter the function of many other proteins depending on calcium concentration, cell type, and availability of its binding target. CaM's binding of calcium is vital for multiple functions in the body, such as smooth muscle constriction, intracellular movement, metabolism, and memory. The regulation of CaM is vital. Diseases such as Down Syndrome, Parkinson's Disease, and Alzheimer's Disease are associated with inappropriate CaM regulation. Since CaM binds to multiple proteins with different binding mechanisms that are not fully understood, investigation into CaM is still underway. CaM antagonists are special form of drug that inhibits CaM. They are used to study CaM's effects on biological systems. CaM antagonists are also used to purify CaM by affinity chromatography as well. To investigate CaM's structure and function, it must be isolated from *E. coli* engineered to express CaM. The standard method for purifying CaM is a Phenyl Sepharose column. This method has a few drawbacks including the need for two consecutive columns and often-additional purification techniques such as ion exchange chromatography. Another method to purify CaM is using the CaM antagonist TAPP (2-trifluoromethyl-10-aminopropylphenothiazine) bound to Sepharose for affinity chromatography. TAPP requires only one column to purify CaM from *E. coli* with no additional purification methods. Despite the benefits of using TAPP Sepharose for CaM purification, it is not a commonly used method because of the complicated and hazardous synthesis required to make the TAPP molecule. Here we describe an efficient, safer, high yield synthesis for TAPP with subsequent coupling to Sepharose 4B and CaM purification by TAPP Sepharose.

124B. The synthesis of a fluorophore for the diagnosis of neglected tropical diseases. EmilyH. Trinh, Gregory R. Naumiec, *Chemistry, University of Central Arkansas, Conway, AR 72035.*

Our research revolves around developing a cost-efficient and accurate method of diagnosing neglected tropical diseases (NTDs) by fluorescent emissions. "Neglected" refers to the prevalence of NTDs in the more impoverished parts of the world with inadequate sanitized water supplies. NTDs are caused by parasites that are transmitted to humans by infectious vectors, such as river blindness. When a fluorophore is tethered to a NTD drug, the interactions of the drug with the disease can be observed on a molecular level. Based on these observations, current drug therapies could be improved to counteract the constant evolution of drug resistance in NTDs. The synthesis of our research is based on the naturally-occurring fluorophore chlorin, a compound found in chlorophyll which is responsible for photosynthesis via absorption of light. Chlorin displays a strong fluorescent emission in the near infrared region. When placed in the path of near infrared radiation

(NIR), the fluorophore absorbs energy for a brief moment until it reaches an excited state. As the energy relaxes back to ground state, the fluorophore releases an emission that is visible using a spectrometer. Our fluorophore, due to its permeability and low toxicity and that hemoglobin cannot absorb NIR which makes it an ideal candidate to tether to substrates for the in vivo diagnosis of NTDs. The target chlorin can be made in ten synthetic steps and partitioned into two discrete halves (eastern and western). Starting with 1H-pyrrole-2-carboxaldehyde, the western half can be synthesized in overall moderate yields across five steps. The eastern half can be synthesized in three steps starting with pyrrole and a substituted benzaldehyde. Once the synthesis is completed, the two halves will be coupled to yield the desired fluorophore and their efficacy for NIR imaging will be tested in vitro. Currently, significant progress has been made in synthesizing both halves.

125A. Surgical Therapy for Small Bowel Obstruction Decreases Readmissions and Increases Cost. Sadiq Haruna, M.B. Richardson, R.J. Reif, H. Jensen, S. Karim, W.C. Beck, J.R. Taylor, K.W. Sexton, Judy Bennett, Karl Walker, *Mathematics and Computer Science, UA Pine Bluff, Pine Bluff, AR 71601.*

Introduction: Small bowel obstruction (SBO) is common in patients hospitalized for acute abdominal pain. However, data on long-term follow-up of patients is lacking and no superior management strategy has been identified. We hypothesized that surgical management would decrease readmissions compared to medical management in the treatment of SBO. Methods: This was a retrospective study of the 2010 - 2014 National Readmissions Database. Patients diagnosed with SBO were categorized into two groups: patients that were operatively treated (surgical), and patients managed conservatively (medical). We compared the in-hospital outcomes and readmission rates between the two groups ($\alpha=0.05$). Results: Within the study period, 778,599 patients diagnosed with SBO were identified. A total of 68,400 (8.8%) patients were treated surgically, compared to 710,199 (91.2%) patients in the medical group. Overall mortality (7.7% vs 4.4%, $p<0.01$) and length of stay (15.7 vs 7.3 days, $p<0.01$) were higher in surgically treated patients. However, while 83,007 (11.7%) of the patients treated medically were readmitted, only 4,795 (7.0%) of the patients treated surgically necessitated readmission to the hospital. Cost of care was higher for surgically treated patients both during initial hospital stay (\$155,293 vs \$67,918, $p<0.01$) and at readmission (\$269,105 vs \$123,334, $p<0.01$). Conclusion: Surgical treatment of SBO was associated with higher in-hospital mortality and longer length of stay. Patients who were treated medically for SBO had significantly higher readmission rates. Despite a higher rate of readmission, conservative treatment was associated with lower cost of care both at initial hospital

admission and readmission. Non-operative management of SBO is a viable and cost-effective treatment strategy.

125B. Silver Nanoparticle Synthesis and Spectroscopy for Biosensing Applications. Nikolai Knight, Richard Walker, Seyed Amir Ghetmiri, Aboozar Mosleh, *Chemistry & Physics, UA Pine Bluff, Pine Bluff, AR 71601*.

Silver nanoparticles are important because they have a plethora of applications throughout our daily lives, ranging from pharmaceutical to industrial. These applications are due to their unique chemical and physical properties as compared to their solid bulk materials because of their high surface area and electronic characteristics. Silver nanoparticles are also extraordinarily efficient at absorbing and scattering light and have a color that depends upon the size and the shape of the particle. The silver nanoparticle would be able to sense biomaterials by agglomeration and change of spectrum due to particle size change. Different methods have been used to synthesize silver nanoparticles, many of which are very costly, yet all follow a similar chemical pathway and utilize similar functional reagents. The techniques used for the preparation of nanoparticles involved biological, physical, and chemical methods. The most common approach for synthesis of silver nanoparticles is chemical reduction by organic and inorganic reducing agents. In general, different reducing agents, such as sodium citrate and ascorbate are used for reduction of silver ions (Ag⁺) in aqueous or non-aqueous solutions to metallic silver (Ag⁰). The purpose of this research is to devise a method to successfully synthesize silver nanoparticles of different sizes (10-100 nm) at a more cost-effective yet efficient rate. The method devised for this experiment employed the use of varying concentrations of silver nitrate (AgNO₃) as the metal source and varying concentrations of glucose as the reducing agent and 0.2% wt. soluble starch as the capping ligand. These reagents are more easily accessible, especially glucose, as compared to sodium citrate which is the stronger reducing agent of the two. Herein, we report the morphology of silver nanoparticles synthesized based on the mole ratio of the metal source to reducing agent. From data acquired, an evident relationship was found between the nanoparticle size produced and the concentration ratio of the reagents. The particle sizes displayed and increase with an increase in the concentration ratio of the reagents. Characterization of nanoparticles was done by light spectroscopy analysis using a microplate reader. The data acquired was classified based on a full-width-half-maximum system. The produced nanoparticles would be functionalized with the proper aptamers for detection of biomaterials. Through further experimentation and study, these findings may lead to an increase in the industrial production of silver

nanoparticles at a cheaper and efficient rate for biosensing application.

126A. Hydrogen Production Using Thiosalen Complexes in Light Driven Systems. Cameron Tinker, John Dewer, William Eckenhoff, *Chemistry, Rhodes College, Memphis, TN 38112*.

As our global population grows, our need for innovative energy sources also grows. One new energy source can be found through the use of artificial photosynthesis to produce hydrogen gas. In our lab, we have shown the effectiveness of nickel complexes with thiosalen ligands acting as a catalyst for the artificial photosynthetic process. Three derivatives of these nickel complexes have been made [Ni(tsalen), Ni(tsalphen), and Ni(tsalto)]. Hydrogen production has been measured electro-catalytically and photo-catalytically. Hydrogen production was measured in light driven systems with [Ru(bpy)₃]²⁺ and ascorbic acid to yield turnover numbers as high as 270.

126B. DFT study of the selectivity of Tyrosinase. Elise Moix, Danielle Wilson, Laryn Peterson, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112*.

L-DOPA is commonly used as a treatment for patients with Parkinson's disease. DOPA-Decarboxylase converts L-DOPA into dopamine. Before L-DOPA can be transformed into dopamine, Tyrosinase can convert it into DOPAquinone. The targeted inhibition of Tyrosinase may lead to an increase in dopamine, resulting in a net increase in pharmacological efficiency. By creating a suite of dopaminergic derivatives specifically designed to inhibit Tyrosinase, the effectiveness of L-DOPA can be prolonged by regulating dopamine's metabolism. The interaction strength between this suite of derivatives and the enzymatic active site was analyzed in silico for effectiveness as an inhibitor of Tyrosinase. The model of the active site was created from a crystal-structure of the Tyrosinase enzyme bound with L-DOPA in its active site (PDB ID: 4P6S). New dopaminergic derivatives were optimized in the active site using M062X/6-31G with implicit solvation and relaxed amino acid side-chains. Interaction energies between the protein and the ligands were calculated using M062X with 6-311+G* basis set. Several different classes of molecules have been studied and some show promise for being competitive inhibitors.

127A. An efficient synthesis of squaramides from dibutyl squarate: Toward a treatment for Chagas disease. Assyl Arykbayeva, Gregory R. Naumiec, *Chemistry, University of Central Arkansas, Conway, AR 72035*.

Neglected tropical diseases (NTDs) generally affect low-income population in developing regions of the world

and do not receive as much attention as other infectious diseases. More than one billion people in 149 countries suffer from NTDs. NTDs are a diverse group of transmissible diseases that dominate in tropical and subtropical conditions and receive lower treatment and research funding. One of the NTDs is American trypanosomiasis or Chagas disease (CD), which is transmitted to humans by blood-sucking triatomine bugs. Infectious CD, caused by the parasite *Trypanosoma cruzi*, currently has no effective treatment. The existing drugs (nifurtimox and benznidazole) for the treatment of CD are expensive, toxic, and have severe side effects. The goal of this research project is to efficiently synthesize inexpensive and effective drug candidates for the treatment of CD by synthesizing squaramides (compounds with known anti-Chagastic properties) from dibutyl squarate in order to find a way to dramatically reduce reaction times. Squaric acid is used as starting material to synthesize dibutyl squarate, since squaric acid is relatively inexpensive and has anti-parasitic properties against NTDs such as CD. Using six different amines and dibutyl squarate, six mixed squaramide-squaric esters were successfully synthesized. These compounds are important precursors for the synthesis of drug candidates for the treatment of CD. It was observed that the reactions of amines with dibutyl squarate take much less time (30 minutes or less) than the reaction of amines with dimethyl squarate or diethyl squarate (about 24 hours), thus allowing the rapid synthesis of potential anti-Chagastic drugs.

127B. Synthesis of espintanol-based natural products for the treatment of leishmaniasis. Kayla Vinh, Gregory Naumiec, *Chemistry, University of Central Arkansas, Conway, AR 72035*.

Neglected tropical diseases (NTDs) are a group of parasitic and bacterial infections that affect developing nations near the equator. Many of these countries struggle to fight NTDs because they are hard to detect, easily communicable, and costly. One NTD of particular interest is leishmaniasis, which is caused by protozoan parasites carried by sandflies. Currently, more than twenty strains of leishmania species that cause disease in humans have been identified. 1.6 million new cases of leishmaniasis occur every year, and 350 million people are at risk for infection in Africa, Asia, and the Americas. Common treatments, such as pentavalent antimonial compounds, have harsh side effects and are not immune to resistance, thus the development of new drugs is crucial to fighting leishmaniasis where drug resistance is becoming a large concern. A class of cyclic, unsaturated hydrocarbon compounds called terpenes have shown strong anti-leishmanial capabilities across several strains. Our target molecule, espintanol, is a natural product found in the bark of the Bolivian spruce tree, *Oxandra espintana*, can be easily functionalized at

5 positions on the aromatic ring. Our research focuses on the optimization on the synthesis of terpenes as well as developing more analogs to determine their effectiveness on the parasite. We are currently one synthetic step away from the completing espintanol. All products have been purified by using column chromatography and fully characterized by ¹H and ¹³C NMR spectroscopy. Once complete, espintanol will then be functionalized with different substituents to create a library of potential anti-parasitics targeting leishmaniasis. Our proposed development of novel treatments helps combat the problem of drug resistance among the strains of leishmaniasis.

128A. Developing a New Water-Soluble Porphyrin as a Potential Photodynamic Cancer Therapy Agent.

Catherine Shirley, Joseph E. Bradshaw, *Chemistry, Ouachita Baptist University, Arkadelphia, AR 71998*.

Photodynamic cancer therapy (PDT) is a type of treatment involving the use of light in conjunction with a photosensitive agent- a chemical or series of chemicals designed for activation when exposed to light. This research project investigated the synthesis and identification of the novel photosensitive agent, H2TPP-Pro-OH. To create the water-soluble porphyrin, (S)-(+)-prolinol was added to the tetra-carboxyl porphyrin, H2TPPC, to form the final H2TPP-Pro-OH product. This compound was then purified using syringe filtration and column chromatography, and subsequently characterized using infrared (IR), nuclear magnetic resonance (NMR), and UV-vis spectroscopies. Finally, the utility of the material as a PDT agent was determined by examining the cytotoxicity of the H2TPP-Pro-OH product was determined using MTT assay on MDA-MB-231 triple negative breast cancer cells comparing dark and light exposure.

128B. Synthesis of a Novel Water-Soluble Porphyrin Derivative for use as a Potential Phototherapeutic Cancer Treatment. Travis Hankins, Joseph Bradshaw, *Chemistry, Ouachita Baptist University, Arkadelphia, AR 71988*.

Photodynamic therapy (PDT) agents are light-activated materials used for localized disease treatment. Porphyrins are classic representations of photosensitive agents. Identified by their large, planar molecular structure, porphyrins are centrally composed of four pyrrole rings. Through this project, the starting material, H2TPPC, a tetra-carboxylic acid porphyrin, was first synthesized and later modified through the addition of the amine, morpholin-2-ylmethanol. This multi-step synthesis resulted in the highly water-soluble porphyrin product H2TPP-MorphMeOH. Following this synthesis, the compound was purified using liquid chromatography, and then structurally identified and classified using infrared (IR), nuclear magnetic

resonance (NMR), and UV-Vis spectroscopies. Lastly, to determine its utility as a potential PDT agent, the cytotoxicity of H2TPP-MorphMeOH was determined using an MTT assay on MDA-MB-231 triple negative breast cancer cells comparing exposure and absence of white light.

129A. Synthesis of Dopamine and DHHCA Analogues.

Hamid A.K. Shirwany, Spencer J. Fields, C. Skyler Cochrane, Muaricio Cafiero, Larryn W. Peterson, *Chemistry, Rhodes College, Memphis, TN 38112.*

The human body contains a class of enzymes called sulfotransferases (SULTS) that are integral in the biotransformation of xenobiotics, neurotransmitters, and various other compounds. SULTS take a sulfuryl group from 3'-phosphoadenosine 5'-phosphosulfate (PAPS) and transfer the moiety to a hydroxyl group of a compound. Sulfation results in an increase in the hydrophilicity of the sulfated compound, allowing for easier transport through the blood. Of the sulfotransferases prevalent, SULT1A3 preferentially sulfates dopamine and other catecholamines. Since SULT1A3 is critical in the movement of dopamine in the body, better characterization of SULT1A3 could play a role in treatments for various diseases involving dopamine, among them being Parkinson's disease. The goals of this research include creating and analyzing analogues of dopamine to see how they interact with SULT1A3 and other related enzymes. The synthesis of cyanodopamine and carboxydopamine will be discussed, and future work will involve the synthesis of 3,4-dihydroxyhydrocinnamic acid (DHHCA) derivatives.

129B. Computational Design and Synthesis of Potential Inhibitors of LpxC Active against Gram-negative

Bacteria. Rebeca J. Roldan, Andrea Pajarillo, Carter P. Embry, Mauricio Cafiero, Larryn W. Peterson, *Chemistry, Rhodes College, Memphis, TN 38112.*

LpxC, an enzyme involved in the first committed step of the biosynthesis of lipid A, has been found to be a crucial drug target when developing new treatments for Gram-negative bacteria. The need for novel antibacterial treatments is critical, especially with the growing resistance Gram-negative bacteria is having towards already developed treatments. Through the computational analysis of the crystal structure of LpxC and its active site, novel inhibitors have been designed to mimic the natural substrate of LpxC. The computational analysis and methods to synthesize these analogues will be discussed.

Physics

Friday Oral Platform Session

ORAL – 3:20. 211. Single-Cell Investigation of the Effects of DC Electric Current on Bacteria. Ariel Rogers, *Physics, Truman State University, Kirksville, MO 63501*, Venkata Krishnamurth, Yong Wang, *Cell & Molecular Biology, University of Arkansas, Fayetteville, AR 72701.*

The long-term goal of this research is to understand the molecular mechanism of DC electric current's antibiotic effects against bacteria, which will facilitate the use of DC electric current as an alternative to commonly prescribed antibiotics to fight against resistant bacteria and to treat infections. Previous studies had shown bacteria grow significantly slower when subjected to DC electric voltages and currents. The objective of this project was to find out what is actually happening to the bacteria on the molecular level. *Escherichia coli* (*E. coli*) is used as a model system in this study and one hypothesis is that because *E. coli* has a negative charge, the proteins in the bacteria will move to either side of the bacteria and cause it to align with the electric field.

ORAL – 3:35. 212. Effects of Thickness Gradient on Magnetoresistance in a Co/Pt Multilayer. Levi Humbard, Vincent Humbert, Junseok Oh, Joseph Sklenar, Nadya Mason, *Physics, Pittsburg State University, Pittsburg, KS 66762.*

The ferromagnetic structure of cobalt platinum multilayers (Co/Pt) possess an unusual unidirectional magnetoresistance (MR) which is attributed to the presence of a thickness gradient within the material. To enhance our understanding of this effect in Co/Pt devices, several devices with varying orientations of thickness gradient were fabricated using optical photolithography and sputtering deposition. Longitudinal MR measurements were taken for these devices while an external magnetic field was rotated about them at different directions. This demonstrated a varying effect of unidirectional MR for different orientations of thickness gradient about the magnetic field rotational directions. This effect was most noticeable when the thickness gradient was along the current direction.

ORAL – 3:50. 213. The Slip-Stick Behavior of the Friction Force on a Body on an Inclined Plane. Arturo Morales Barrios, Kenneth D. Hahn, *Electrical Engineering and Physics, John Brown University, Siloam Springs, AR 72761.*

The Slip-Stick Behavior of the Friction Force on a Body on an Inclined Plane We have studied the frictional

behavior of various surfaces in contact on an inclined plane. In particular, we have surveyed what is commonly called the stick-slip phenomenon which illustrates the atomic forces between two surfaces in contact and the change from static to kinetic friction. In the stick-slip phenomenon, inter-atomic forces temporarily hold an object in static equilibrium, until those forces are briefly broken/interrupted allowing minute motion (kinetic friction) between the surfaces until equilibrium is re-established. We will show results demonstrating a gradual relaxation to equilibrium which is then followed by an abrupt shift in position and change in the static friction force. The results obtained indicate both a clear pattern of increasing relaxation times and increasing force differentiation in the slip-stick transition.

ORAL – 4:05. 214. Gas Sensing in a Microresonator System Using Non-Adiabatic Tapered Fibers. Lucas A. Blake, *Physics, Southern Arkansas University, Magnolia, AR 71753*, A.T. Rosenberger, Sreekul Raj Rajagop, *Physics, Oklahoma State University, Stillwater, OK 74078*.

Adiabatically tapered fibers have commonly been used to excite whispering gallery modes (WGMs). It has recently been shown that non-adiabatically tapered fibers can enhance refractive index sensing. The light within a non-adiabatic taper transition excites both fundamental and higher-order fiber modes, whereas an adiabatic taper transition only excites the fundamental fiber mode. The sensing enhancement comes from the interference between different fiber modes. We have theoretically shown that enhancement is also possible for absorption sensing. The enhancement can be predicted by the measured power when the modes are in and out of phase. The enhancement is proven by sending light through the adiabatic side of an asymmetrically tapered fiber. We have shown this enhancement using a setup combining the asymmetric tapered fiber and a hollow bottle resonator (HBR) with internal analyte. The light absorbed by the analyte results in changes in the dip depth of the WGM. The ratio of changes, non-adiabatic to adiabatic, shows the enhancement factor. For carbon dioxide an enhancement factor of 150 was found, in agreement with the theoretical model.

ORAL – 4:20. 215. Mechanical energy based amplifiers for probing interactions of DNA with metal ions. Jack Freeland, Prabat Khadka, Yong Wang, *Physics, UA Fayetteville, Fayetteville, AR 72701*.

DNA is one of the most investigated and talked about subjects in biology, biochemistry, and medicine as it serves as our genetic code and forms the basis of all known life. DNA itself is a very simple yet volatile substance. Along with regular cell cycle changes,

various factors such as temperature or ion concentration can alter the state of DNA and its functionality. What various factors affect DNA and their outcomes are of great interest to us for obvious reasons. Things such as repressed replication, mutations, cancer, and other diseases are a direct result of DNA changes. Having a better understanding of these factors in turn provides us a better understanding of the consequences they bring. In this project, we offer a novel and wide-reaching method to better view and understand DNA interactions. The problem with orthodox methods such as optical tweezers and atomic force microscopy, they are quite expensive and complex at times. By approaching the issue from a physics perspective, we were able to design a DNA structure that, through the exploitation of mechanical energy, allows us to observe DNA-metal ion interactions with a sensitivity not achievable through regular linear DNA in such a cost-efficient method like gel electrophoresis. DNA-metal ion interactions were chosen to be investigated due to their importance to life. On one hand, DNA-metal interactions are essential for various fundamental processes in cells: formation of secondary and higher-order structures of nucleotides, DNA repair, genomic stability, etc. On the other hand, many metal ions could be toxic, resulting in DNA damage and cell death, which can accumulate and lead to disease. Our findings revealed how unique metal ions apply unique visible effects to DNA at varying concentrations and serves as a proof of concept to our method/design. We believe many more applications such as drug screening or water purity checks are well within reach.

ORAL – 4:35. 216. Molecular Dynamic Simulations to Study Tunnel Barrier Layer Formation in Ultra-Thin Film Alumina. Christopher Klenke, Devon Romine, Daniel Fishbein, Ridwan Sakidja, *Physics, Missouri State University, Springfield, MO 65897*.

In this study, we simulated the deposition process of an ultra-thin film alumina using LAMMPS Molecular Dynamics (MD) simulation code. The chemical precursors chosen were based on the experimental set up used by our collaborators at the University of Kansas. By controlling the deposition temperature and with the use of wetting layer such as pure Aluminum, we were able to systematically define the optimal conditions to produce a denser alumina layer. We acknowledged the support from NSF through the Electronics, Photonics and Magnetic Devices (EPMD) Program program (Award No. 1809284).

Physics

A and B – Saturday 8:00 – 10:15 Posters

201A. Deep Learning Based Assessment of Physiological Measurements for Neurological Disorders: A Case Study on Gait in Parkinson's Disease. Kima Brown, Olcay Kursun, *Computer Science, University of Central Arkansas, Conway, AR 72035.*

Gait disorders are considerable cause of falls in patients with neurological diseases. Grasping these disorders allows prevention and better awareness into underlying diseases. There is recent growth in the number of news reports and public awareness on neurological disorders, specifically due to the settlement NFL deals with the retired football players. As of April 2018, the settlement administrator had received over 1,750 claims from the more than 20,000 retired players. Most of the claims paid thus far were for players with A.L.S., Parkinson's disease and chronic traumatic encephalopathy, degenerative brain disease with potential links to repeated blows to the head. It is estimated that the settlement will reach about \$1 billion. It is important to monitor and track brain health. Mobile and wearable sensor technologies can serve as affordable and practical tools to assess the severity of neurological conditions, because concussions are inescapable in traffic accidents, military combatants, in sports at our schools and professional teams, also for the children and elderly due to falls. Some are linked to these serious neurological disorders and it is important to assess the quality of motor-system control of the brain, which gait and balance analysis studies target. In this study, we analyze gait-related measurement signals on the study of Parkinson's disease (PD). The dataset is obtained from PhysioBank, a digital recording archive bank of physiologic signals related data for use by the biomedical research community. PD affects approximately 1 million Americans (estimates range between 4 to 6.5 million people worldwide) and about 1% of older adults. Solely in the US, there are 60,000 new cases diagnosed each year. PD is a chronic and progressive neurological disorder that causes tremor, rigidity, slowness, and postural instability. The database contains 93 patients with idiopathic PD and 73 healthy controls. The database includes the vertical ground reaction force records of subjects as they walked at their usual, self-selected pace for approximately 2 minutes on level ground. Underneath each foot were 8 sensors that measure force as a function of time sampled at 100 Hz. We apply deep learning techniques (LSTM, auto-encoders, transfer learning) to classify subjects as healthy or with Parkinsonism. These tools can help automate monitoring the debilitating gait symptoms of the patients with neurological diseases and thus help predict patients with severe gait

disturbances that make them prone to falls. The developed deep learning data analysis techniques can also be applied to datasets for the assessment of severity of concussion and its recovery. We also apply sensitivity analysis (feature selection) for finding the minimum set of most predictive sensors. This approach can also help us choose the most compact approach when using multi-parameter datasets (such as choosing among EEG, electrodermal activity, temperature, acceleration, heart rate, and arterial oxygen level recordings) with no loss in the classification accuracy. Minimizing the cost and the weight of the sensors to be worn makes the approach more practical for the patients.

202A. Two Photon Lithography to Fabricate Complex Structures for Stimulation and Recording of Biological System. Mahdi Salameh, *Physics, Southern Arkansas University, Magnolia, AR 71753*, Shelby Maddox, Mahyar Afshar Mohajer, Min Zou, *Mechanical Engineering, UA Fayetteville, Fayetteville, AR 72701.*

Two-photon lithography can be used to fabricate micro and nano-structures. Using the NanoScribe, micro and nano-structures such as those found on plant leaves can be replicated for the purpose of superhydrophobicity. Once replicated, hydrophobicity of the samples can be tested using a variety of experiments. Mass replication and surface chemistry of samples is also tested.

203A. Molecular Dynamic Simulations of Layered Metallic Systems. Austin Bollinger, Ridwan Sakidja, *Physics, Astronomy, and Material Science, Missouri State University, Springfield, MO 65897.*

This project studies the effects of compression on the mechanical deformation of layered metallic systems, specifically made of Ni. The study of compression mechanics can be applied to many fields of metallurgy, and in this case in the application of the mechanical modeling to elucidate how these mechanics will affect a polycrystalline system. By employing the molecular dynamics simulation, the roles of thermodynamics, compression rate, and sample size can be carefully evaluated to optimize the strength and cost efficiency of the materials under observation. The support for this project comes from the Department of Energy (NETL) Grant No. FE0031554 (Crosscutting Research Program).

204A. Design and Implementation of 3D-Printable Optomechanical Components. Ryan Bullis, Dylan Mitchell, Julie Gunderson, *Physics, Hendrix College, Conway, AR 72032.*

3D printing is an additive manufacturing modality with a range of applications that have grown drastically over the last several decades. As Fused Filament Fabrication (FFF) 3D printers have become more affordable, many

scientists and engineers have begun printing customized parts for experiments and prototypes. FFF is a 3D printing technique in which thermoplastic is extruded by a robot onto a hard, flat surface in successive layers to create an object from a Computer Aided Design (CAD) file. Because many scientific applications require parts that are expensive to purchase or manufacture, 3D printing custom parts for scientific instrumentation can save valuable (shipping and/or manufacturing) time and money and requires only one moderately priced printer. Thus, 3D printing has emerged as a viable low-cost method to produce custom scientific instruments, therefore, increasing the progress of research. Here, we present a library of 3D printable optomechanical components for use in research-grade optical systems. These components are fully compatible with commercial optomechanical components and include: posts, post holders, bases, lens mounts, kinematic mirror mounts, filter mounts, and micrometers. These components were tested for their optical stability and durability in home-built optical systems constructed entirely from 3D printable optomechanical components, and we demonstrate that these systems performed comparably to their more expensive, commercially available counterparts. Thus, we expect our library of 3D printable optomechanical components to find utility in scientific research laboratories.

205A. Designing a Passive Tracking Solar Panel System with Shape Memory Alloys and Solar Oven Technology to Power a Campus Charging Station. Emory Gregory, Hannah Brandon, Angela Douglass, *Physics, Ouachita Baptist University, Arkadelphia, AR 71998.*

Solar panels that rotate to follow the sun's position throughout the day maximize the amount of energy they can glean from the sun's rays. This experiment aims to create a passive, single axis, sun-tracking solar system that employs shape memory alloys (SMAs) as the tracking mechanism to reduce the loss of harvested energy to rotation of the panel. Sunlight directed onto cylindrical Fresnel lenses, with the help of solar oven technology, efficiently contracts the SMAs due to the sun's heat. The contraction of the SMAs rotates the solar panel so that the sunlight is incident on it normally throughout the day, resulting in the maximum absorbed energy. Experiments were conducted to determine optimal housing and attachment of the SMAs for a variety of weather conditions, and the panel setup and electronics were designed for implementation into a solar-powered charging station to be used by students on the Ouachita Baptist University campus.

206A. Synthesis of Gold Nanorods. Alexander Golden, Puskar Chapagain, *Physics, Southern Arkansas University, Magnolia, AR 71753.*

Growth of Gold Nanorods using Chemical Synthesis Method Alexander Golden and Puskar Chapagain Department of Engineering and Physics, Southern Arkansas University, Magnolia, AR-71753 Metallic nanoparticles are materials of choice because of their wide range of applications from optoelectronics to biomedicine. The study of the formation of gold nanorods, in particular have gained much importance due to its additional applications in the field of catalysis, photovoltaics, biomedical, quantum computing and sensing. Understanding the detail mechanisms of synthesis, which improves the yield, reproducibility and precise control of surface chemistry are subjects of great interest. Therefore, in this project, we employed a low cost chemical synthesis route known as seed-mediated method for nanorods formation in the hopes of streamlining the process and making it more efficient with high yield rates. To do this, we performed a series of experiments that varied the amounts of chemical precursors used including stirring rates using UV-Vis spectroscopy. Our preliminary results showed that clear signature of nanorod formation and there were in fact changes in the absorbance spectra of the nanorods suggesting that the improvements on the yield due to variation of chemicals such as CTAB, AgNO₃, and stirring rates.

207A. Design and Optimization of the Fluorino: A Low-Cost, Arduino-Controlled Fluorometer. Nancy Velazquez, Julie Gunderson, *Physics, Hendrix College, Conway, AR 72032.*

Fluorometer-based fluorescence spectroscopy is used in numerous fields including biology, chemistry, biochemistry, biophysics, biomedical engineering, and environmental science. However, since commercial-grade fluorometers are very expensive, researchers and educators at many primarily undergraduate institutions are limited in their research and educational activities. The goal of this work is to develop a low-cost, research-grade fluorometer capable of measuring intensity, wavelength, and polarization of fluorescent molecules in cuvettes. Here, we present a low-cost, education-grade fluorometer that can be used to detect fluorescence intensity dynamically. This instrument is constructed from 3D printable optomechanical components and is controlled by an Arduino Uno microcontroller. This fluorometer has the ability to detect low (~100 nM) concentrations of fluorophores at 100 ms time resolution. We compare the detection capabilities of our home-built fluorometer to the commercially available, research-grade Horiba Fluoromax-4C and the commercially available, education-grade Vernier SpectroVis+ fluorometers. We demonstrate that our home-built fluorometer entitled 'The Fluorino' is both affordable and user friendly and is thus suitable for use in undergraduate teaching

laboratories to introduce the principles of fluorescence and fluorescence spectroscopy.

208A. Partition-based Optimization model for Generative Anatomy Modeling Language. Jake Farmer, Doga Demirel, Berk Cetinsaya, Sinan Kockara, Shahryar Ahmadi, Tansel Halic, *Computer Science, University of Central Arkansas, Conway, AR 72035*.

This work presents a novel approach for Generative Anatomy Modeling Language (GAML). This approach automatically detects the geometric partitions in 3D anatomy that in turn speeds up integrated non-linear optimization model in GAML for 3D anatomy modeling with constraints. This integrated non-linear optimization model requires the exponential execution time. However, our approach effectively computes the solution for non-linear optimization model and reduces computation time from exponential to linear time. This is achieved by grouping the 3D geometric constraints into communities. Various community detection algorithms (k-means clustering, Clauset Newman Moore, and Density-Based Spatial Clustering of Applications with Noise) were used to find communities and partition the non-linear optimization problem into sub-problems. GAML was used to create a case study for 3D shoulder model to benchmark our approach with up to 5,000 constraints. Our results show that the computation time was reduced from exponential time to linear time and the error rate between the partitioned and non-partitioned approach decreases with the increasing number of constraints. For the largest constraint set (5,000 constraints), speed up was over 2,689-fold whereas error was computed as low as 2.2%.

209A. Single-Molecule Studies of Thrombin Binding to a G-Quadruplex DNA Aptamer. Hanna Detar, Julie Gunderson, *Physics, Hendrix College, Conway, AR 72032*.

Aptamers are oligonucleotides that bind to specific target molecules, and they can be synthetically selected for using a technique called systematic evolution of ligands by exponential enrichment (SELEX), which is also referred to as in vitro evolution. Previously, SELEX was used to select for a DNA aptamer that binds to thrombin, an enzyme that helps blood coagulate, and the DNA aptamer with the sequence GGTTGGTGGTTGG was shown to bind to thrombin and inhibit its enzymatic activity. Thus, the thrombin-binding aptamer is a candidate for an anti-coagulation agent. Additionally, the thrombin-binding aptamer has been shown to form an antiparallel G-quadruplex (G4) structure in the presence of KCl. The objective of this study is to characterize the binding mechanism of the thrombin/aptamer interaction and to determine how this G4 aptamer allows for efficient binding to thrombin. To characterize the thrombin/aptamer interaction,

single-molecule fluorescence resonance energy transfer (smFRET) was used to probe the conformational dynamics of a thrombin-binding DNA aptamer in the presence and absence of thrombin. The smFRET results show that formation of the G4 structure is dependent on the presence of KCl. In low (<100 mM) KCl concentrations, the aptamer interconverts between a semi-folded and fully-folded G4 structure, while the G4 structure is stabilized in KCl concentrations at or above 200 mM. The presence of thrombin traps the aptamer in the G4 configuration in low (50 mM) KCl conditions. The results of this study demonstrate that thrombin has specific affinity for the G4 structure of the aptamer. We hypothesize that upon binding to the G4 structure, thrombin induces a new conformation in the G4 aptamer through an 'induced fit' mechanism. Future studies will incorporate a new labeling scheme to detect a change in conformation of the aptamer upon binding to thrombin.

210A. Atomic Energy Calculations Using Analytical Gradients and GPU Programming. Zachary Wall, Mauricio Cafiero, *Chemistry, Rhodes College, Memphis, TN 38112*.

Calculating the wave function and energy levels of atoms and molecules is a fundamental problem in computational chemistry. In the previous work of Boys and Singer electronically correlated Gaussian functions or ECG's which contain explicit electron-electron distances demonstrated increased accuracy and efficiency. Optimizing the variational parameters contained in these ECG basis sets is the largest computational bottleneck. By calculating the analytical energy gradient with respect to these variational parameters this bottleneck is partially alleviated, but the gradient calculation is still computationally expensive. This work uses the graphics processor unit or GPU as opposed to the CPU to perform the bulk of gradient calculations. The GPU contains many more cores than a CPU and allows for faster parallel processing of simple matrix calculations. The goal of this work is to increase the efficiency of these calculations to get more accurate results on larger atomic systems.

217A. Protostellar Outflows in L1448. Jordan Rhoades, John Tobin, Nickolas Reynolds, *Physics, University of Central Arkansas, Conway, AR 72035*.

Protostars are formed from molecular clouds and are at the forefront of star formation. Outflows within the L1448 region in the Perseus molecular cloud were observed using the Sub-Millimeter Telescope. We used the data from the protostars' spectra to determine the mass, momentum, and energy of the protostars systems. This allows us to see the effects on the molecular cloud and the protostar systems at a larger scale.

218A. Investigation of Solid-State LiPON Thin Films Grown by Pulsed Laser Deposition for Application as an Electrolyte. David Beckwitt, Thomas Callaway, Nicholas Rogers, Saibal Mitra, *Physics, Astronomy, & Material Science, Missouri State University, Springfield, MO 65897.*

Lithium phosphorous oxy-nitride (LiPON) is a solid state material with good lithium ion (Li⁺) conductivity. Modern lithium batteries use liquid electrolytes as the source for Li⁺ ions. Batteries often fail due to dendritic shorts or thermal runaway reactions. One way to mitigate these problems is to switch to solid-state electrolytes such as LiPON. In this work we investigate the growth of LiPON films on pristine and copper coated soda-lime glass. LiPON thin films were grown using pulsed laser deposition (PLD). Using a target of lithium phosphate (Li₃PO₄), we deposited films while varying the nitrogen reactor pressure and substrate temperature. Two sets of films were prepared. One set was as-deposited and the other underwent post-deposition annealing. The LiPON films were studied systematically as a function of deposition parameters using x-ray diffraction (XRD), scanning electron microscopy (SEM), and energy dispersive spectroscopy (EDS). The results will be discussed.

219A. Pulsed Laser Deposition of an All Solid-State Lithium-Ion Battery. Nick Rogers, David Beckwitt, Thomas Callaway, Saibal Mitra, *Physics, Astronomy, & Material Science, Missouri State University, Springfield, MO 65897.*

Pulse laser deposition (PLD) is used to grow thin films on a variety of substrates. A high-power solid state pulsed laser beam is focused on targets of different compositions. Photons striking the target ablate the surface and eject the target material that then travels by line of sight onto the substrate. The solid-state lithium-ion battery consists of a graphite anode, a LiPON Electrolyte, a lithium cobalt oxide cathode. They are deposited onto Copper coated glass substrates. PLD is a prevalent technique that allows stoichiometric transfer of material. The deposition parameters are reactor pressures and atmospheres, number of shots, substrate temperatures, energy densities, and target to substrate distance. It has been widely used for depositions of conductors, semiconductors, ferrimagnets, and paramagnetic materials. Characterization of the produced films included XRD, SEM, and measuring conductivity. Our literature review describes the conditions when PLD is an appropriate technique. This involves factors such as film uniformity and desired film sizes that may make PLD an undesired film growth technique.

220A. Design and Development of a Preliminary Virtual Endoluminal Surgical Simulator (VESS) for Endoscopic

Submucosal Dissection (ESD) Surgery. Jake Farmer, Berk Ceninsaya, Mark A. Gromski, Sangrock Lee, Zhaohui Xia, Doga Demirel, Tansel Halic, Coskun Bayrak, Cullen Jackson, Suvranu De, Sudeep Hegde, Jonah Cohen, Mandeep Sawheny, Stavros N., *Computer Science, University of Central Arkansas, Conway, AR 72035.*

Background: ESD is an endoscopic technique for en bloc resection of gastrointestinal lesions. ESD is a widely-used in Japan and throughout Asia, but not as prevalent in Europe or the US. The procedure is technically challenging and has higher adverse events (bleeding, perforation) compared to endoscopic mucosal resection. Inadequate training platforms and lack of established training curricula have restricted its wide acceptance in the US. Thus, we aim to develop a Virtual Endoluminal Surgical Simulator (VESS) for objective ESD training and assessment. Methods: We performed a detailed colorectal ESD task analysis and identified the critical ESD steps for lesion identification, marking, injection, circumferential cutting, dissection, intraprocedural complication management, and post-procedure examination. We constructed a hierarchical task tree that elaborates the order of tasks in these steps. Furthermore, we developed quantitative ESD performance metrics. We measured task times and scores of 16 ESD surgeries performed by four different endoscopic surgeons. Then, we developed a preliminary VESS for lesion identification of colorectal ESD. Results: The average time of the marking, injection, and circumferential cutting phases are 203.4 (σ :205.46), 83.5 (σ : 49.92), 908.4 sec. (σ : 584.53) respectively. Cutting the submucosal layer takes most of the time of overall ESD procedure time with an average of 1394.7 sec. (σ : 908.43). We also performed correlation analysis (Pearson's test) among the performance scores of the tasks. There is a moderate positive correlation ($R=0.528$, $p=0.0355$) between marking scores and total scores, a strong positive correlation ($R=0.7879$, $p=0.0003$) between circumferential cutting and submucosal dissection and total scores. Similarly, we noted a strong positive correlation ($R=0.7095$, $p=0.0021$) between circumferential cutting and submucosal dissection and marking scores. Conclusions: We performed an HTA and developed a rubric for performance metrics for ESD. Based on the HTA and metrics, we carried out time and performance analysis of actual ESD videos. We presented correlations between task times and scores. We developed the preliminary VESS for lesion identification of colorectal ESD and performed a validation study at Society of American Gastrointestinal and Endoscopic Surgeons (SAGES) Annual Meeting and World Congress of Endoscopic Surgery in 2018. The study will be used to understand the lesion identification steps of surgery in regard to the skills. The findings will be incorporated into the complete VESS simulator.

221A. Modeling Atomic Layer Deposition of Alumina as an Ultra-thin Tunnel Barrier. Daniel Fishbein, Ridan Sakidja, Devon Romine, *Physics, Astronomy, & Materials Science, Missouri State University, Springfield, MO 65897.*

This reactive molecular dynamics (MD) study is trying to model the Atomic Layer Deposition (ALD) process to form an ultra-thin tunnel barrier made of alumina. We will evaluate systematic role of the precursors, namely the trimethylaluminum (TMA) and water pulse toward the chemical reactions that take place on the surface. We will then evaluate the role of temperature for the internal structure of the amorphous alumina as the final deposition product. The support of NSF (Grant No. 1809284) from the Electronics, Photonics and Magnetic Devices (EPMD) Program is gratefully acknowledged.

222A. Effects of Space conditions on Rat Leg Bones. Sidney Freyaldenhoven, H. N. Heacox, R. Mehta, B. Hill, P. Chowdhury, *Chemistry; Physics and Astronomy, University of Central Arkansas, Conway, AR 72035.*

This research analyzes rat femur and tibia bones when live rats were exposed to hind-limb suspension (HLS) (to simulate microgravity) and/or x-ray irradiation (HLS/IR) (simulate space radiation). It is hypothesized that space conditions will produce weakened bones, lower elastic moduli and abnormal concentrations of calcium and phosphorus, as compared to bones not subject to these conditions. In the experiment, approximately 8 weeks old male rats were suspended by tail for two to four weeks. The radiation was given over a 2 week period with dosage varied from 0.5 gray to 2.0 gray. The tibia and the femur bones of sacrificed rats were measured for their elasticity and cross sectioned to study the elemental changes. Elasticity measurements were done by mean of applying a known force and measuring the bending displacement using 3-point bending and also by cantilever bending method. A stress vs. strain graph allowed us to estimate the elastic modulus of a leg bone for control, HLS and HLS-IR samples. The relative percentages of elements in bone mineral of hydroxyapatite $[\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2]$ were determined using Energy Dispersive Spectroscopy (EDS) using an electron beam in a Scanning Electron Microscope (SEM). The electron beam energy ranged from 10-20 keV. The SEM images were obtained using a backscattered detector and a secondary electron detector. X-rays emitted from the sample during electron bombardment were measured using a peltier cooled SD X-ray detector with a resolution of 129 eV at 5.9 keV. $\text{K}\alpha$ - x-rays from carbon, oxygen, phosphorus and calcium formed the major peaks in the spectrum. Relative percentages of these elements were determined using a software that could also correct for ZAF factors namely Z (atomic number), A (X-ray absorption) and F (fluorescence yield). The elemental composition of femur and tibia were

analyzed and results indicated a strong relationship between the compositional ratios of calcium, phosphorus and oxygen with the location on the leg. The analysis of bone shows that there must be some change in the hydroxyl or phosphate group of the main component of the bone structure, due to hind limb suspension. The effect of radiation could be seen with dosage as low as 0.5 Gray. No statistically significant difference in elastic modulus was found between control and irradiated rats or in control and hind-limb suspended and irradiated rats; however, a significant difference was demonstrated between control and hind-limb suspended rat but for femurs only. While most p-values were not significant, trends in data sets suggest that the irradiation, hind-limb suspension, and conjoint treatment treatments produced lower elastic moduli, hence weaker femurs and tibias than such bones under normal (control) conditions. Ultimately, the results produced by this research will aid in quantifying the effects of spaceflight on the strength and composition of the human skeletal system; such research may be useful in developing a treatment, or nutritional additive to counteract such effects.

223A. Molecular Dynamics (MD) Potential Development for Carbides. Tyler McGilvry-James, Nirmal Baishnab, Ridwan Sakidja, *Physics, Astronomy and Materials Science, Missouri State University, Springfield, MO 65897.*

We utilized the methodology of MEAMfit code to optimize the many-body potentials of Embedded Atom Method (EAM) and Modified Embedded Atom Method (MEAM) to model the M23C6 intermetallic carbides where M is the transition metals. These phases are the key ingredient to strengthen the Ni-based Superalloys. By employing the code in addition to the sampling of energy and force calculations from quantum mechanics, a set of potentials can be produced and be utilized to model the mechanical properties of these carbides. Funding from DOE (NETL) Grant No. FE0031554 (Crosscutting Research Program) is gratefully acknowledged.

224A. Molecular Dynamics Simulations of Anorthite-Melt-Water Interactions. Devon T. Romine, Robert Mayanovic, *Physics, Missouri State University, Springfield, MO 65897.*

This study is a continuation of ongoing research into hydrous albite melts, which was the first attempt at creating structural data of hydrous silicate melts using MD simulation. Reaxff will be utilized to create a reaction between an Anorthite glass and water. Anorthite is an aluminosilicate with Ca incorporated into (CaAl₂Si₂O₈). Water dissolution into silicate melts like anorthite plays an important role in modifying the physical properties of the silicate melt. These

modification to the physical properties can directly impact many fields of interest, such as the eruptive power of magmas and the transfer of mass in these magmatic processes. This will also lead to a better understanding of the water cycle regarding the plate tectonics of the Earth. Using this data, we could also determine more about the tectonics of exoplanets, and even constrain habitable zones of these exoplanets. There are also potential uses for this information in the field of construction, as a lot of concrete and window mixtures use silicates in their compounds. To this extent, large simulation-cell molecular dynamic calculations are being processed to try and make a detailed quantitative structure of hydrous Anorthite melt systems. This research can be utilized in the creation of stronger and more flexible prosthetics. For example, stronger bone implants. Acknowledgements Prof. Robert Mayanovic- Advisor NASA Missouri Space Grant Consortium – Funding Extreme Science and Engineering Discovery Environment (XSEDE) computational facilities grant; XSEDE is supported by NSF grant number ACI-1053575 References 1 S. Seager, Proc. Natl. Acad. Sci. 111, 12634 (2014). 2 K.A. Milam, H.Y. McSween, J. Moersch, and P.R. Christensen, J. Geophys. Res. Planets 115, E09004 (2010). 3 A.P. Hammersley, S.O. Svensson, M. Hanfland, A.N. Fitch, and D. Hausermann, Int. J. High Press. Res. 14, 235 (1996). 4 N. Norman, Acta Crystallogr. 10, 370 (1957). 5 A.J. Anderson, H. Yan, R.A. Mayanovic, G. Solferino, and C.J. Benmore, High Press. Res. 34, 100 (2014). 6 S. Plimpton, J. Comput. Phys. 117, 1 (1995). 7 J. Du and A.N. Cormack, J. Non-Cryst. Solids 351, 2263 (2005). 8 J. Du, J. Am. Ceram. Soc. 92, 87 (2009). 9 T. Róg, K. Murzyn, K. Hinsén, and G.R. Kneller, J. Comput. Chem. 24, 657 (2003). 10 L. Martínez, R. Andrade, E.G. Birgin, and J.M. Martínez, J. Comput. Chem. 30, 2157 (2009). 11 J. Fogarty, H. Aktulga, A. Grama, A. van Duin, and S. Pandit, J. Chem. Phys. 132, 174704 (2010).

225A. Virtual Arthroscopic Tear Diagnosis and Evaluation Platform (VATDEP). Doga Demirel, *Computer Science, UA Little Rock, Little Rock, AR 72204*, Seth Cooper-Baer, Aditya Dendukuri, Jake Farmer, Mustafa Tunc, Tansel Halic, Sinan Kockara, *Computer Science University of Central Arkansas, Conway, AR 72035*, Nizamettin Kockara, *Department of Orthopedics and Traumatology, Erzincan University Medical School, Turkey*, Mark Edward Rogers, *Alabama Spine and Sprints, Birmingham, AL*, Shahryar Ahmadi, *Department of Orthopaedic Surgery, UAMS, Little Rock, AR 72205*.

Virtual Arthroscopic Tear Diagnosis and Evaluation Platform (VATDEP) Arthroscopy is a minimally invasive surgery to diagnose and treat issues, most often within a joint. Conventional arthroscopy training methods use cadavers, mannequins, or old-aged apprenticeship model. However, all these methods have limitations in realism and cost efficiency or incurring high risk.

Although the arthroscopy-based surgeries have dramatically increased over years, the efficient, risk-free and cost-effective training and assessment platform methods yet remain lacking. We therefore proposed VATDEP to develop Virtual Reality (VR) based arthroscopy simulator in collaboration with expert orthopaedic surgeons. VATDEP is designed for arthroscopic repair of crescent shaped rotator cuff tears. The simulator allows physics simulation for the surgery such as fluid flow, air bubbles, tear shaving, bleeding, tissue deformation, bone drilling and tool-tissue interactions. We incorporated haptic (tactile) interaction to provide realistic force feedback. To build an operating room setting, an adjustable frame structure has been built to mimic the operation table. A physical human torso and the arm with three portal openings are used to increase the realism for face validation. Additionally, arthroscope, shaver, burr and anchor placement instruments have been interfaced to VATDEP via the haptic devices to perform the training with actual instruments. The VATDEP simulator provides a combination of actual operating room and VR environment for surgeons to train, improve and assess their skills. We will further perform face, content, and construct validation studies with human subjects to evaluate the efficacy of the simulator. This research is supported by the Arkansas INBRE program, with an award# P20 GM103429 from the National Institutes of Health/the National Institute of General Medical Sciences (NIGMS)

226A. Virtual Fundamentals of Arthroscopic Surgery Training (VFAST). Seth Cooper-Baer, Mustafa Tunc, Jake Farmer, Kutay Macit, Tansel Halic, *Computer Science, University of Central Arkansas, Conway, AR 72035*, Doga Demirel, Berk Cetinsaya, *Computer Science, UA Little Rock, Little Rock, AR 72204*, Shahryar Ahmadi, *Orthopaedic Surgery, UAMS, Little Rock, AR 72205*.

Virtual Fundamentals of Arthroscopic Surgery Training (VFAST) Arthroscopy is a minimally invasive surgical procedure that is performed via small incisions in the patient's skin to examine, diagnose and repair the injuries inside a joint. Due to non-natural hand-eye coordination, narrow field-of-view and limited instrument control, training for arthroscopy is challenging and difficult to master. Conventional surgery education models such as cadaver, plastic mannequin, and apprenticeship training are not adequate and effective. The use of animals and cadavers is costly, unethical and mostly limited to single use. Likewise, physical bench models can be useful for arthroscope navigation and instrument handling, but they do not possess the realism to teach the surgeons the joint anatomy nor aid surgical decision-making. However, Virtual Reality (VR) based training platforms offer low-cost, repeatable and realistic practice environment for surgeons to improve their manual dexterity. Therefore,

we proposed VFAST to develop a VR training simulator based on Fundamentals of Arthroscopic Surgery Training (FAST) tasks, which is a physical box-trainer collaboratively designed and proposed by Arthroscopy Association North America (AANA), American Academy of Orthopaedic Surgeons (AAOS), and American Board of Orthopaedic Surgery (ABOS). Our aim is to develop a complete environment that will mimic all the FAST tasks for surgeons to develop their basic arthroscopy skills with supporting multiple difficulty scenarios, haptic force feedback, instant visual aid, and detailed performance report.

227A. Computational Investigations of Andalusite-Melt and Water Interactions. Weston R. Renfrow, Robert Mayanovic, *Physics, Astronomy, and Materials Science, Missouri State University, Springfield, MO 65897.*

Water directly affects magmatic processes and mass transport within the Earth's crust. By studying how water dissolves in a silicate melt and modifies its structural and physical properties, we can gain a better understanding of Earth's volcanic and tectonic processes. In addition, our studies may ultimately allow us to better delineate the habitable zone of rocky exoplanets. Currently there are no studies on hydrous (i.e., with soluble water) silicate melts with sufficient data on the structure of such systems. Andalusite is a nesosilicate having the chemical formula Al_2SiO_5 . Molecular dynamics (MD) simulations are performed on large-scale computational cells containing slabs of andalusite melt that is initially surrounded by water molecules. ReaxFF force fields are utilized to realistically model the chemical reactions between the andalusite melt and water molecules, hydroxide and hydrogen species. We will discuss the results from the MD simulations that are used to make a quantitative structural analysis of the hydrous andalusite melt.

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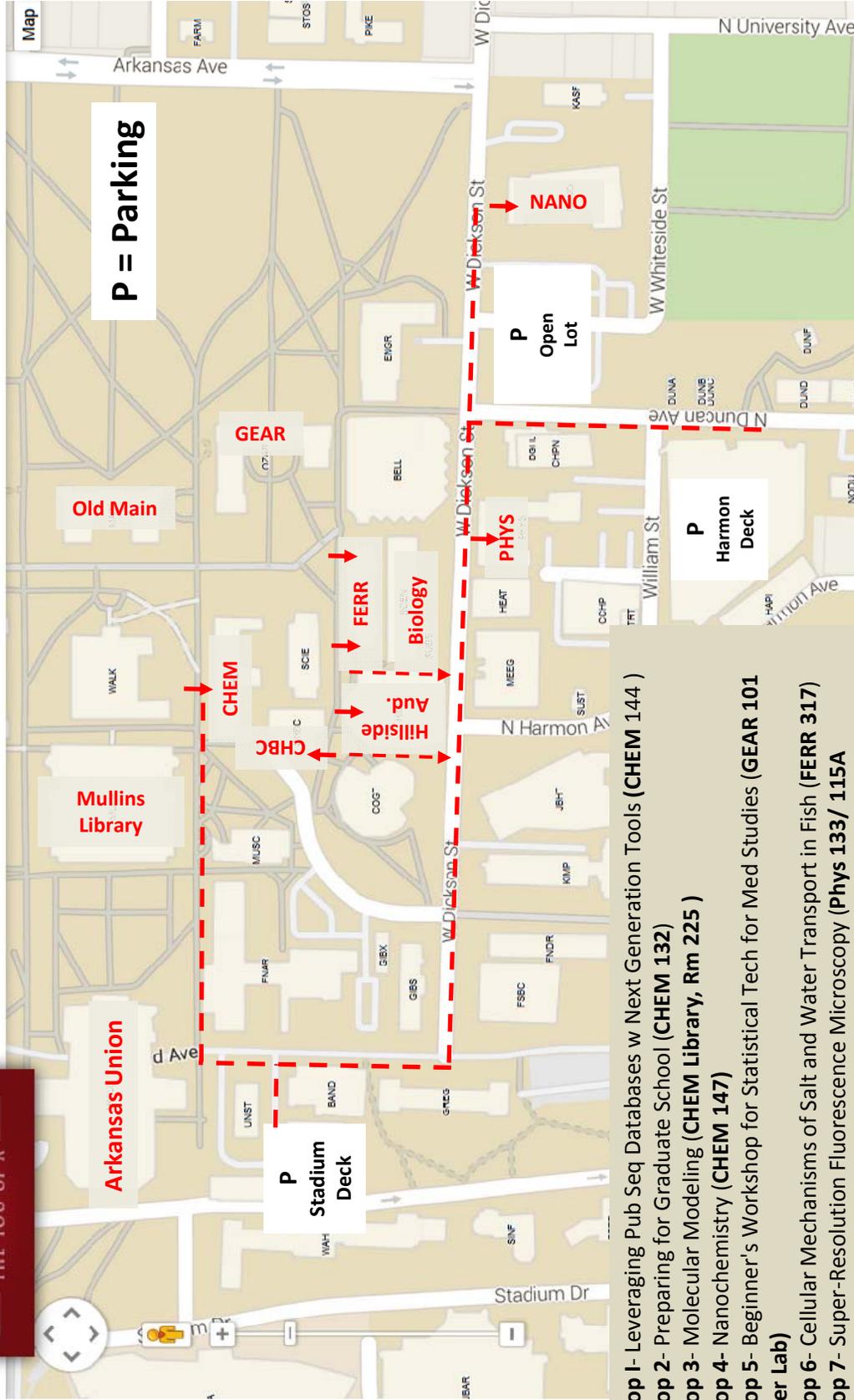
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