

IDeA Network of Biomedical Research Excellence

Arkansas INBRE Research Conference

2021

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October 29-30

Arkansas INBRE Research Conference Arkansas IDeA Network of Biomedical Research Excellence

Schedule of Events

Mask Mandate: Both the city of Fayetteville, and the University of Arkansas Campus is currently under a mask Mandate. Wearing of masks at all times when in door is required.

Location: The Graduate Hotel and University of Arkansas Campus

Friday, October 29, 2021

Graduate Hotel

12:00 p.m.– 1:30 p.m.	Registration – Graduate Hotel Atrium, Second Floor Information Tables		
1:30 p.m. – 2:30 p.m.	. Keynote Speaker – Graduate Hotel		
	Telling your story: Communicating and Advocating for Science in Challenging Times		
	Dr. Jessica N. Snowden, University of Arkansas for Medical Sciences		
3:00 p.m. – 4:30 p.m.	Invited Student Platform Sessions – physics, chemistry, biology		
6:00 p.m. – 7:00 p.m.	Boxed dinner – Graduate Hotel, Second Floor		

Saturday, October 30, 2021

University of Arkansas Campus

7:45 a.m.	Breakfast – Hillside Auditorium and Physics Building, until 9:30
8:00 a.m.	Poster session A (posters come down at 9:00 a.m.) - Hillside Auditorium (Biology), Verizon
	Ballroom* (Chemistry) and Physics Building (Physics)
9:15 a.m.	Poster session B (posters come down at 10:15 a.m.) - Hillside Auditorium (Biology), Verizon
	Ballroom (Chemistry) and physics building (Physics)
10:30 a.m.	Workshops – assigned locations

There will be no award ceremony this year.

^{*} Chemistry participant breakfast is at Hillside Auditorium

Registration Information

The INBRE registration desk will be open:

- Friday 12:00 p.m. to 5:00 p.m., Graduate Hotel Atrium (2nd floor)
- Saturday 7:30 to 10:00 a.m., Hillside Auditorium, Upper Lobby

Lodging will be at the Graduate Hotel,

70 N. East Avenue, Fayetteville, AR 72701 and at the Holiday Inn Express, 1251 N. Shiloh Drive, Fayetteville, AR 72704. The list of schools staying off-site will be rotated each year.

Parking: Friday parking is complimentary in the Municipal Parking Garage, third level only (first level card access for registered guests of the Graduate Hotel).

Saturday parking is free on the UA campus in designated yellow sign lots and parking decks.

Arkansas INBRE

https://inbre.uams.edu/

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.

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

Ines Pinto and Christian Tipsmark; biological sciences Jingyi Chen, Heather Jorgensen, Feng Wang, and Ying Yuan; chemistry and biochemistry

Reeta Vyas; physics

INBRE Steering Committee

Lawrence Cornett, Ph.D., UAMS, PI & Chair Jerry Ware, Ph.D., UAMS, PC & DRP Program Director Alan Tackett, Ph.D., UAMS, Biotechnology Core Director Feng Wang, Ph.D., UAF, Outreach Core Director Galina Glazko, Ph.D., UAMS, Bioinformatics Co-Director Liz Pierce, Ph.D., UALR, Bioinformatics Co-Director Nathan Reyna, Ph.D., Ouachita Baptist University Ann Wright, Ph.D., Hendrix College Thomas Risch, Ph.D., Arkansas State University Stephen Addison, Ph.D., University of Central Arkansas Joel Funk, Ph.D., John Brown University Mansour Mortazavi, Ph.D., UAPB Nancy Rusch, Ph.D., UAMS, Executive Associate Dean for Research Jeff Shaver, Ph.D., UAFS Richard Schoephoerster, Ph.D., Arkansas Tech University Frank Knight, Ph.D., University of the Ozarks Jeffery Massey, Ph.D., Harding University Caroline Miller Robinson, UAMS Diane McKinstry, UAMS

Staff

Diane McKinstry, UAMS, Program Coordinator Caroline Miller Robinson, UAMS, Business Manager Heather Jorgensen, UAF, Outreach Coordinator

Participating Institutions

Arkansas Tech University, Russellville Emory University, Atlanta Harding University, Searcy Henderson State University, Arkadelphia Hendrix College, Conway Louisiana Tech University, Ruston Lyon College, Batesville Missouri Southern State University, Joplin Missouri State University, Springfield Northeastern State University, Tahlequah NWACC, Bentonville Oklahoma Baptist University, Shawnee Ouachita Baptist University, Arkadelphia Rhodes College, Memphis University of the Ozarks, Clarksville University of Arkansas, Fayetteville University of Arkansas, Fort Smith University of Arkansas, Little Rock University of Arkansas, Monticello UA Medical Sciences, Little Rock University of Arkansas, Pine Bluff University of Central Arkansas, Conway

Featured Speaker

Friday, 1:30 p.m., Graduate Hotel, Presiding: Christian Tipsmark

Telling your story: Communicating and Advocating for Science in Challenging Times

Dr. Jessica N. Snowden, MD. MS. MHPTT.



Associate Professor Professor of Pediatrics, University of Arkansas for Medical Sciences, Little Rock, AR

Division Chief, Pediatric Infectious Disease, University of Arkansas for Medical Sciences co-Director, Translations Research Institute, University of Arkansas for Medical Sciences Vice-chair for Research, Department of Pediatrics, University of Arkansas for Medical Sciences Associate Director for Clinical and Translational Research, Arkansas Children's Research Institute Principal Investigator, Data Coordinating & Operations Center, ECHO IDeA States Pediatric Clinical Trial Network

Awards

Awards: Prizes will be awarded to the top oral and poster presentations by undergraduate students in each discipline. There will be no award ceremony this year.

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.

Student Oral Presentations

Friday, 3:00 p.m. to 4:30 p.m. Graduate Hotel No registration required

Biology Oral Presentations

Brodie Payne Ballroom C-D - Cindy Cisar, Chair

03:00 PM. Grace E. Tidwell

Ouachita Baptist University

Bird diversity and abundance in relation to habitat complexity at jack mountain wildlife management area

03:15 PM. Regan Massey

University of Arkansas

Elevated levels of external cysteine inhibit nitrogen fixation by the methanogenic archaeon Methanosarcina acetivorans

03:30 PM. Nhi Le

Missouri State University

An investigation of the intracellular trafficking of cadmium selenide zinc sulfide quantum dots in yeast cells

03:45 PM. Lydia Ostmo

Northeastern State University - Broken Arrow DNA polymerase epsilon mutants exhibit delayed recovery after DNA damage

04:00 PM. Jade Dorman

Ouachita Baptist University Lung Carcinoma Exosomes Modify Tumor Microenvironment

04:15 PM. Claire Burton

Harding University

Exposure to iron and copper in Caenorhabditis elegans mutants produces elevated levels of reactive oxygen species

Chemistry Oral Presentations

Trammel Room - Martin Edwards, Chair

03:00 PM. Joshua Thammathong

University of Arkansas - Fort Smith Molecular modeling based screening to identify potential small molecule therapeutics for treatment of resistant bacterial infections.

03:15 PM. William Strickland

University of Arkansas - Fayetteville Spike protein structural dynamics of SARS coronaviruses studied using molecular dynamics

03:30 PM. Joshua Spiva

Ouachita Baptist University Incorporating a bioengineered protein and a collagen analog into modern wound dressings

03:45 PM. Abbey Bryan

Harding University Lead detection using Raman scattering

04:00 PM. Gisela Xhafkollari

Rhodes College

Using UV-vis spectroscopy to determine the pKa values of catechols

04:15 PM. Johanna Lasiter

University of Central Arkansas

An inexpensive and efficient approach to cure Chagas Disease

Physics Oral Presentations

Brodie Payne Ballroom A - Hugh Churchill, Chair

03:00 PM. Hypatia Meraviglia

University of Central Arkansas Effects of microgravity and radiation on rat bone strength and composition

03:15 PM. Zach Kauffman

Missouri State University What is friction at the atomic level? Adhesion and shear force

03:30 PM. Apoorva Bisht

University of Arkansas - Fayetteville Field programmable gate array for correlation measurements and data acquisition system

03:45 PM. Seth Williams

Arkansas Tech University Motility dynamics of E. coli in dense environments using differential dynamic microscopy

Poster Sessions

Poster set-up begins at 7:45 a.m. on Saturday Hillside Auditorium - Biology Verizon Ballroom- Chemistry Physics Building – Physics

> Session A – 8:00 to 9:00 a.m. Session B – 9:15 to 10:15 a.m.

Presenters are expected to be present during the scheduled time. Business or business casual dress is encouraged.

Workshops

Saturday, 10:30-11:45 a.m. Various locations on the U of A campus Registration for Workshops will be at Conference Registration Table

Workshop 1 – Enabling the Teaching of Bioinformatics Core Competencies in the Classroom

Location: Hillside 202 Elizabeth Pierce, PhD, Dept. of Information Science, UALR

In this mini-workshop, Dr. Liz Pierce (UALR) will be sharing the results of a recent survey of bioinformatics education among the 4 year schools in Arkansas followed by a Q&A session to gather information from faculty and students as to what kinds of support (training, lab modules, computing/software platform, wetlab resources) would best help schools to incorporate bioinformatics skills into the curriculum of life science majors.

Workshop 2 – The NIH R15 and SuRE R16 Mechanisms

Location: Hillside 206 Jerry Ware, PhD, Professor of Physiology & Biophysics, UAMS

The NIH Academic Research Enhancement Award (AREA) program supports faculty research at campuses that have not received significant NIH funding in the past. This workshop highlights unique factors that distinguish the R15 mechanism

from other RPG mechanisms, such as the RO1, where scientific merit and the investigators are major score driving criteria. New funding opportunities, the Support for Research Excellence (SuRE) Program and SuRE-First Program (R16s) have been released with the first-ever submission deadline of September 2021. Comparing the 2 FOAs and appropriateness for PUI faculty to apply for either will be discussed. Both the R15 and R16 have three main goals, 1) to support meritorious science 2) to strengthen the institution's research environment, and 3) to expose students to research. Thus, special consideration for how/where to incorporate all three goals into the application will be discussed. The presenter has been part of recent NIH R15 Special Emphasis Panels and will share experiences with a goal of benefitting interested faculty and providing a perspective on how to write a competitive AREA application. Discussions will include what reviewers are "coached" to look for during peer review and some of the most common mistakes that can temper reviewer enthusiasm.

Workshop 3 – Preparing for Graduate School Location: CHEM 132 Colin Heyes, PhD, Dept. of Chemistry & Biochemistry, UAF

This workshop is targeted towards under-graduate 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:

Prof. Mahmoud Moradi, department of Chemistry and Biochemistry, UAF

Prof. Michelle Evans-White, department of Biological Sciences, UAF

Prof. Adnan Alrubaye, Cell and Molecular Biology Graduate Program, UAF Prof. David Ussery, Department of Biomedical Informatics, UAMS

Mamello Mohale, Graduate Student, department of Chemistry and Biochemistry, UAF

Patience Okoto, Graduate Student, Cell and Molecular Biology, UAF

Allie Litmer, Graduate student, department of Biological Sciences, UAF

Aaron Kemp, Graduate student, Neurocognitive Dynamics Lab, University of Arkansas for Medical Sciences (UAMS)

Workshop 4 – Molecular Modeling

Limited to 8 active participants (more people can listen but there are no computer seats for them) Location: GEAR 101 *Peter Pulay, PhD, Dept. of Chemistry & Biochemistry, UAF*

This workshop will demonstrate the use of small or personal computers to model molecules, calculate their geometry, infrared and Raman spectra, relative stability, NMR chemical shifts and other properties.

The software has two components:

(1) A Graphical User Interface allows the construction of molecules and, after the calculation, show the results, and display of molecular orbitals and electron density.

(2) A Quantum Mechanical program allows the determination of molecular geometries and other properties.

Several such programs are available but most have a fairly steep price. We will use the Parallel Quantum Solutions software developed in Dr. Pulay's group because a free version is available. Calculations will run on a cloud server at the workshop but the same programs can be installed free on Windows, Mac and Linux PCs from Dr. Feng Wang's Web site.

Several examples have been prepared for the workshop but we will probably able to finish only one. The following projects are available: Singlet and triplet states of methylene, CH2 A strange molecule: SF4 The thermal ring opening of cyclobutene Geometry and NMR chemical shifts of cyclohexene

Workshop 5 – XRD new capability for art restoration, pharmaceutical development, and structure determination of pharmaceutical targets both small and large.

Limited to 20 participants Location: CHEM 144 also on zoom (Meeting ID: 865 7532 2038 Passcode: XRD@Uark21) participant limit does not apply to online participants.

Josh Sakon, PhD, Dept. of Chemistry & Biochemistry, UAF/ Eric Reinheimer, PhD, Rigaku Co.

The X-ray diffraction system, in the X-ray Core laboratory has played a role in the statewide research efforts in the structure determination of biomolecules. His involvement in the Arkansas INBRE began in 2001 when the Arkansas BRIN was first funded through a grant from the National Center for Research Resources. XRD replacement funded in 2021 by NIH will increase the functionality and usability of the system. The new generation of X-ray detector will produce higher quality data than what can be done with the existing X-ray detector and the software that now comes with the detector/goniometer. The replacement leverages advanced new algorithms developed in the recent decade and will enable the extraction of more accurate information with better confidence even with the same signal to noise ratio. The instrument will extend the capacity of the instrument from being a system dedicated to protein crystallography to one that is capable of also generating high-quality small molecule results, which will help the core facility to stay at the cutting edge of biomedical research, as well as provide needed service to additional research labs in the state.

The fundamental theory for XRD and small molecule structure determination will be discussed by Eric Reinheimer of Rigaku. Joshua Sakon (Director of X-ray Core Facility) will discuss macromolecule structure determination application. Rigaku's near noiseless solid-state detector will enable the extraction of weak with better confidence from smaller samples than the systems currently used at Smithsonian and Getty Museums. The instrument will gain ability to identify pigments from paintings or fresco particles.

Workshop 6 – Use of fluorescence microcopy in quantitative Biology

Limit to 10 participants Location: PHYS 228 & PHYS Lab 126 *Pradeep Kumar, PhD, Dept. of Physics, UAF*

The workshop will provide hands-on experience on working with yeast and bacterial cells under a microscope. First, we will provide a brief introduction of the fluorescence microscopy and its usage in Biology. Participants will then have the opportunity to participate in demo laboratory projects such as –visualizing DNA inside yeast and bacteria, quantifying dead and alive cells, and playing with glowing bacteria

Workshop 7 – Playing with lasers

Limit to 15 participants Location: PHYS 132 & Phys Lab 123 *Hiro Nakamura, PhD, Department of Physics, UAF*

The workshop will provide hands-on experiences on lasers. We first provide a brief introduction on the type of lasers we use in the lab, and some optical effects such as diffraction. Then participants will move to a physics lab and join a few short demo projects: 1) drilling a hole in a paper or card (feel free to bring one); 2) make a rainbow using grating; 3) attempt to "see" ultrafast laser pulses.

Workshop 8 – Nanotechnology and Public Health

Limit to 25 participants Location: PHYS 133 *Yong Wang, PhD, Dept. of Physics., UAF*

This workshop will first introduce and explain what nanotechnology and public health are, followed by how they overlap and impact each other. Participants will identify how nanotechnology can influence public health, learn about epidemiological investigations, and applications of engineered nanomaterials for vaccine developments. In addition, the workshop will discuss how training in both fields can prepare students for a wide range of career options – in academia, nonprofit organizations, and industry.

Workshop 9 – Physics "Graduate Application" Location: PHYS 134 Reeta Vyas, PhD, Dept. of Physics, UAF

In this workshop 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 10 – CRISPR-Cas9-mediated targeted mutagenesis

Limit to 5 participants Location: FERR 214, 323 and SCEN 122 *Nagayasu Nakanishi, Ph.D., Dept of Biological Sciences, UAF*

CRISPR-Cas9 is a powerful genome editing tool whose applications are rapidly expanding across diverse fields from biomedicine to evolutionary biology. In this workshop, participants will learn how the CRISPR-Cas9 genome editing technology is used to investigate gene function in sea anemones. The hands-on session will involve microinjection of guide RNAs and Cas9 protein into zygotes of sea anemones to generate knockout mutations at a targeted locus.

Facility Tours

Saturday, 10:30-11:45 a.m. Hillside Auditorium, Top level Entrance *Registration for Tours will be at Conference Registration Table*

Facility Tour 1 | Arkansas High Performance Computing Center

Raymond Weldon. – Department of Chemistry and Biochemistry, University of Arkansas and Pawel D. Wolinski, Ph. D., AHPCC, University of Arkansas

Oral Abstracts Biology

03:00 PM. Bird diversity and abundance in relation to habitat complexity at jack mountain wildlife management area

<u>Grace E. Tidwell</u>, Kelsey M. Bester, and Christin L. Pruett, Biology, Ouachita Baptist University

Since 1973, North America has lost 2.9 billion birds due to habitat loss and fragmentation (Rosenberg et al. 2019). To assess the effects of habitat complexity on bird diversity, 88 locations were

Facility Tour 2 | Department of Chemistry and Biochemistry

Julie Stenken Ph. D. – Department of Chemistry and Biochemistry, University of Arkansas

surveyed at Jack Mountain Wildlife Management Area (WMA) using ten-minute point counts. All birds seen and heard at each point were documented and habitat complexity was assessed by examining the percentage of ground cover, shrub layer, midstory tree layer, and canopy layer at each point. A habitat complexity index was generated from these plant surveys. Previous research at Jack Mountain has shown that habitats dominated by pine trees had the highest bird species diversity and abundance. Habitat complexity has been associated with an increase in bird species diversity (Sam K. et al 2019) and thus, we hypothesized that pine habitats would have greater habitat complexity and that

habitat complexity would be positively correlated with bird diversity and abundance. Statistical tests were performed in R to assess these hypotheses. In comparisons between species diversity (r=0.116; P=0.28) or abundance (r=0.115; P=0.28) with habitat complexity index no significant correlation was observed. We then compared each of the four aspects of the habitat complexity with species diversity and abundance and found a significant negative correlation between species diversity (r=-0.383, P<0.001) and abundance (r=-0.372, P <0.001) versus canopy coverage. Also, significant positive correlations were found between species diversity (r=0.378, P<0.001) and species abundance (r=0.405, P<0.001) versus ground cover (Figure 6) and species abundance was also positively correlated with amount of shrub cover (r=-0.097, P=0.366). Each point location was also assigned to a habitat class based on the percentage of pine and deciduous tree cover. As found in previous summers by students at OBU, a comparison among habitat classes and species diversity showed higher numbers of species in pine habitats (F=3.755, P=0.0274) however, the habitat complexity index did not differ among habitat classes (F=2.05, P=0.135). To further evaluate, the drivers of larger numbers of birds in pine habitats, aspects of the habitat index were then compared to habitat classes. We found smaller amounts of canopy coverage (F=0.4538, P=0.0134) and larger amounts of ground cover (F=4.538; P=0.0134) and shrub cover (F=6.879, P=0.0017) in pine habitats than in deciduous or mixed habitats. These findings suggest that there are more bird species and individuals among pine habitats at Jack Mountain because of less canopy coverage. A reduction in canopy coverage in pine habitats could lead to an increase in ground and shrub coverage, which are both correlated with an increase in the diversity and abundance of birds. In conclusion, we reject our initial hypothesis about bird diversity and pine habitats being associated with increasing habitat complexity. Our findings suggest that the population dynamics of birds at Jack Mountain are associated with a diverse set of habitat variables that cannot be simplified into a single habitat complexity index.

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03:15 PM. Elevated levels of external cysteine inhibit nitrogen fixation by the methanogenic archaeon Methanosarcina acetivorans

<u>Regan Massey</u>, Ahmed E. Dhamad, Melissa Chanderban, Faith H. Lessner, and Daniel J. Lessner, Biological Sciences, University of Arkansas

Methanogens are nitrogen fixing and methane producing archaea that play a key role in the cycling of carbon and nitrogen on earth. Methanogens are the only archaea that contain nitrogenase, the enzyme required for the reduction of dinitrogen (N2) to ammonia (NH3) by the following reaction: $N2 + 16ATP + 8e^{-} + 8H^{+} \rightarrow 2NH_{3} + H_{2} + 16ADP +$ 16Pi. Due to the high demand for ATP, nitrogenase is only used to fix N₂ when no other nitrogen source is available. The overall goal of this study was to determine the effect of amino acids as nitrogen and sulfur sources on nitrogenase usage in the model methanogen Methanosarcina acetivorans. Strain DJL74 was used to test the ability of M. acetivorans to use amino acids as a nitrogen source, since it is a knockdown strain that was created using the CRISPRi-dCas9 system, where dCas9 blocks transcription of the nitrogenase genes preventing N2 fixation. Of the amino acids tested, only glutamine that contains a second amino group could be used as a nitrogen source and support growth similar to the control ammonium (NH4⁺). Interestingly, under prolonged incubation without a usable fixed nitrogen source strain DJL74 was able to overcome dCas9-dependent repression of nitrogenase and began to fix N₂, as revealed by immunoblots specific to the catalytic subunit of nitrogenase. However, cultures that were given the sulfurcontaining amino acid cysteine never overcame dCas9 repression and failed to produce nitrogenase. Cysteine can be used as a sulfur source but not as a nitrogen source by M. acetivorans. Cysteine is typically provided at 3 mM when given as a sulfur source, but in the nitrogen source study it was given at 10 mM. To test whether the inhibitory effect of cysteine is concentration dependent, growth studies were performed with strain DJL74 provided 0-10 mM cysteine and either NH_4^+ or N_2 as the nitrogen source. Cysteine concentrations of 0 and 3 mM did

not inhibit growth with NH4+ and the strain was able to eventually overcome dCas9 repression and fix N₂. Cysteine at 10 mM inhibited growth with both NH₄⁺ and N₂, indicating cysteine at this concentration overall inhibits growth of M. acetivorans. However, cysteine at 5 mM did not inhibit growth with NH4+ but inhibited the ability of strain DJL74 to overcome dCas9 repression of nitrogenase and grow by fixing N2. Thus, elevated external cysteine levels specifically inhibit nitrogenase usage by M. acetivorans, revealing for the first time a connection between sulfur source and N₂ fixation in any N₂-fixing prokaryote.

03:30 PM. An investigation of the intracellular trafficking of cadmium selenide zinc sulfide quantum dots in yeast cells

<u>Nhi Le</u>, Cameron Kirk, and Kim Kyoungtae, Biology, Missouri State University

Quantum dots (QDs) are semiconductor nanoparticles capable of emitting strong and stable light of various colors. For this reason, quantum dots have been utilized in many research and medical applications. Recently, some studies have suggested the toxicity of quantum dots on cells, but the exact mechanism is unknown. The primary focus of our project was to investigate the traffic route of Cadmium Selenide Zinc Sulfide quantum dots (CdSe/ZnS QDs) in Saccharomyces Cerevisiae yeast cells. We hypothesized that QDs are internalized into yeast cells by receptor-mediated endocytosis pathway and then transported to various locations of yeast cells. In an attempt to determine the trafficking route of QDs in yeast cell, we treated budding yeast expressing: Plasma membrane reference marker GFP-2PH; receptor-mediated early endocytosis reference marker ABP1-GFP; trans-Golgi network/ late Golgi reference marker FAPPI-GFP; and late endosome reference marker Vps10-GFP, with red CdSe/ZnS QDs over a period of 24 hours. In treatment of low concentration of red CdSe/ZnS QDs (4µg/mL), we found that QDs associated with the outer layer of yeast cell immediately after treatment. However, ODs did not co-localize with the plasma membrane reference marker GFP-2PH at this time, suggesting that QDs

may only associate with the cell wall of yeast cell in the early hours. At about three hours after treatment, a minimal amount of QDs co-localized with the plasma membrane, indicating that at least three hours is needed for QDs to start internalizing into veast cells. After six hours of treatment, a large amount of QDs was found at the plasma membrane of the yeast cell, a decent amount of QDs colocalized at the early endocytosis vesicle, and a low amount of QDs showed co-localization with the late Golgi. From eight hours to twenty-four hours after treatment, the amount of QDs in yeast cell decreased drastically, likely due to the aggregation of QDs in culture media, as a large number of aggregated clusters of QDs were observed in the media in later time point. ODs did not co-localize with the late endosome reference marker Vps10-GFP at any time point, suggesting that late endosome is not a destination for QDs trafficking route. We concluded that QDs associated with the outer layer of yeast cell immediately after treatment, took around three hours to get to the plasma membrane, arrived at the early endocytosis vesicle then traveled to the late Golgi at around six hours. As of now, the rest of the trafficking route of QDs in budding yeast cells remained unknown and needs further investigation.

03:45 PM. DNA polymerase epsilon mutants exhibit delayed recovery after DNA damage

<u>Lydia Ostmo</u>, Michael Smith, Sarah Woller, Dr. Subhas Das, and Dr. Sapna Das-Bradoo, Natural Sciences, Northeastern State University - Broken Arrow

DNA replication requires many proteins to interact together to keep copies of our DNA intact and free of errors. Recent work in our lab with budding yeast has shown that Mcm10 plays an integral role in DNA polymerase epsilon (Polɛ) functionality. Polɛ contains three structural subunits and one essential catalytic subunit known as POLE1 in mammals and Pol2 in budding yeast. The N-terminal half of Pol2 contains functionally characterized DNA polymerase and exonuclease domains but the Cterminal half contains no experimentally characterized domains aside from two putative Zn-

finger modules that are conserved from yeast to humans. Previously, we have shown that the Cterminus of Pol2 interacts with Mcm10 in budding veast. Expanding on this research, we constructed mutation in yeast Pol2 that interrupted interaction with Mcm10. The current project studied cell cycle progression in the yeast POL2 mutants after exposure to DNA damage. Our results suggest that the specific mutants of Pol2 take longer to complete chromosome replication when treated with hydroxyurea. Our second project investigated the interaction of MCM10 and POLE1 in human cells. Co-immunoprecipitation experiments confirmed the interaction in HEK293T cells. Future experiments are needed to shed light on the function of this interaction in the maintenance of genome stability.

04:00 PM. Lung carcinoma exosomes modify tumor microenvironment

<u>Jade Dorman</u>, Gracen Hambrick, Lauren McCann, and Dr. Nathan Reyna, Department of Biology, Ouachita Baptist University

Cancer uses intercellular communication to induce tumor growth and metastasis. Fibroblasts can become specifically transformed and associated with cancer to aid in the process. Extracellular vesicles, specifically exosomes, contain proteins, RNA, and DNA that are taken up by local cells to affect cellular behavior. Exosomes were isolated from lung carcinoma using total exosome isolation reagent and quantified. These exosomes were used to treat lung fibroblasts and enrich lung carcinoma cells, and the effects of exosomes on cancerous properties, cell viability and cell migration, were studied. An increase of cell viability was found with exosome treatment for both cell lines while migration only increased for enriched lung carcinoma cells. Additionally, mass spectrometrybased proteomics of exosomes isolated from hepatocellular carcinoma was analyzed. Through a survey of differentially expressed proteins between high and low grade hepatocellular carcinomas against normal liver cells, several pathways of interest were identified. Some common motifs in underexpressed genes were the regulations of cell signaling, cell metabolism, and cell death.

04:15 PM. Exposure to iron and copper in Caenorhabditis elegans mutants produces elevated levels of reactive oxygen species

<u>Claire Burton</u> and Dr. David Donley, Department of Biology, Harding University

The production of, and detoxification of reactive oxygen species (ROS) are important cellular pathways that regulate metabolism and other functions. The buildup of ROS in cells--termed oxidative stress--results in damage to macromolecules that can alter cellular function. Oxidative stress contributes to aging and neurodegenerative diseases like Alzheimer's Disease (AD). Buildup of the amyloid-beta peptide $(A\beta)$ is associated with AD progression, increased ROS, and buildup of metals. The goal of this study was to use Caenorhabditis elegans as a model to determine if $A\beta$ altered the sensitivity to redox active metals including copper and iron. To accomplish this, ROS levels were measured in three C. elegans strains with and without exposure to metals in a factorial design. The transgenic smg-1 mutant produces the human A β in C. elegans; the smg-1/rol-6 strain was used as a control for the smg-1 strain because it has low transgene expression, modeling A β production in a healthy, non-AD brain. Mutant strains were compared to the wild type (N2) strain of C. elegans. The levels of ROS were measured using 2',7'-dichlorofluorescin diacetate (DCFDA). Each mutant strain was incubated in CuSO₄, FeSO₄, or phosphate buffered saline (PBS), after which ROS were quantified using DCFDA fluorescence. Both mutant strains were more sensitive to oxidative stress than the N2 strain (main effect p<0.001). Furthermore, ROS production was significantly higher in the smg-1 strain with high A β production compared to the other two strains in pairwise comparisons (interaction p=0.0135; p<0.05 vs. smg-1/rol-6; p<0.01 vs. N2). These results demonstrate that $A\beta$ production in C. elegans increases the sensitivity to redox active metals and are consistent with a model where ROS production in AD results from altered cellular sensitivity to ROS-generating compounds. More work is needed to fully elucidate

mechanism(s) for these effects and determine point(s) of intervention.

Oral Abstracts Chemistry

03:00 PM. Molecular modeling based screening to identify potential small molecule therapeutics for treatment of resistant bacterial infections.

<u>Joshua Thammathong</u>, Harmeet Cohan, Kairy Galvez, Souvik Banerjee, and Sayo O. Fakayode, Chemistry, University of Arkansas - Fort Smith

Novel antibacterial scaffolds have been in high demand for the treatment of infections caused by antibiotic-resistant bacteria. The ESKAPE panel of bacteria, which includes Enterococcus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acetinobacter baumanii, Pseudomonas aeruginosa, and Enterobacteriaceae species, is responsible for the majority of antibiotic-resistant bacterial infections. A pharmacophore and molecular modeling-based virtual screening against penicillin binding protein 2x co-crystal structure (PBP 2X) from Streptococcus pneumoniae (PDB: 2ZC3) showed that a group of small molecules from the MolPort library may have antiviral activity. QSAR analysis was performed on the 20 most promising hits from molecular docking demonstrating ability to predict binding energy with impressive high accuracy. Top 5 docking hits were subject to ADMET screening to identify top three potential small molecule therapeutics with drug-like properties. Further research is needed to biologically evaluate top two hits.

03:15 PM. Spike protein structural dynamics of SARS coronaviruses studied using molecular dynamics

<u>William Strickland</u>, Mahmoud Moradi, and Mortaza Derakhshani Molayousefi, Biology, University of Arkansas - Fayetteville

Coronavirus disease 2019 (COVID-19), caused by severe acute respiratory syndrome coronavirus 2

(SARS-CoV-2), has overwhelmingly impacted the global population, accounting for millions of infections and deaths over the last year and a half. The virus's rapid influence on the health and safety of individuals, the economy, and daily life has been disruptive and devastating. Understanding the differential behavior of the present SARS-CoV-2 variants, and specifically, the spike proteins that play a crucial role in receptor recognition, could expedite the process of developing vaccines and antivirals that identify the sites as potential drug targets. In this study, we aim to investigate the activation process of the spike protein and the conformational changes that must occur for the receptor-binding motif (RBM) to be made available for binding to the human receptor (ACE2). Using all-atom molecular dynamics simulations, we will be able to visualize a detailed account of spike protein activations and compare one variant to another and see if any similarities arise. The differential behaviors that are analyzed will aid in determining the dynamical changes of the spike proteins in the activation process and not just their inactive and active states.

03:30 PM. Incorporating a Bioengineered Protein and a Collagen Analog into Modern Wound Dressings

Joshua Spiva, and Dr. Sharon Hamilton, Chemistry and Physics, Ouachita Baptist University

Collagen is a vital part of wound healing and has been incorporated into a variety of modern wound dressings including electrospun fiber mats. The limitations of human collagen include high costs and limited availability. Chitosan, another biopolymer used in wound healing, possesses antimicrobial properties, and offers protection against biofilms which hinder healing of the wound bed. Previously, our lab has electrospun chitosan and PVA (poly(vinyl alcohol)) with collagen to produce fiber mats that have shown promise as modern wound dressings. Additionally, the Hamilton lab has developed a cost-effective collagen analog that has been incorporated into nanofiber scaffolds. The resulting nanofiber mats have been designed to mimic the morphology of the

extracellular matrix in the body for use in biomedical applications including wound healing. These biomimetic electrospun scaffolds show promise for releasing molecules into the wound bed including proteins and other large molecules. Our lab has incorporated s-HFGF1 (super-human fibroblast growth factor), a bioengineered protein based on HFGF1, into nanofiber mats. Studies have shown that the direct application of s-HFGF1 to cells results in increased proliferation in vitro. The protein paired with the biomimetic and antimicrobial properties of the novel nanofiber scaffolds should result in a faster regrowth of the wound bed as well as preventing bacterial infection. The protein release capabilities of our nanofiber mats in physiological conditions have been assessed. In the future, protein release studies will be performed in vitro and analyzed using cell migration assays. It is anticipated that these experiments will verify the release of biomolecules from novel nanofiber scaffolds and a synergistic healing effect will be observed.

03:45 PM. Lead Detection Using Raman Scattering

<u>Abbey Bryan</u>, Dr. Maggie He, adn Babitha Machireddy, Engineering and Physics, Harding University

Lead has adverse effects on all age ranges by causing health problems in a child's growth and various diseases in adults. The widespread lead (Pb2+ ion) contamination in drinking water and its severe health consequences to the people in Flint, Michigan has received immense attention and health awareness. Realizing the deleterious effects of lead on human health, we sought to develop a lead sensor using graphene enhanced Raman scattering. Our sensor consists of an appropriate probe molecule that reacts and responds to the presence of lead ion in solution. Reaction with lead causes the spirocyclic structure of the probe molecule to undergo spiro ring-opening to form a π conjugated molecule, which we expect will interact strongly with a graphene surface. Graphene is used as a substrate for the enhancement of Raman scattering from the probe molecule. The goal is that

the change in molecular structure is reported through Raman spectroscopy. This lead sensor is synthesized from the starting materials, Rhodamine B and Ethylenediamine. Through a 6-step synthesis, the desired probe was successfully synthesized and characterized through nuclear magnetic resonance (NMR). Preliminary Raman measurements were carried out on 1 μ M of the probe in acetonitrile in the presence of various concentrations of Pb2+ ranging from micromolar to nanomolar. The Raman spectra observed in these measurements were rather small. Most likely due to unsuccessful adsorption of probe molecule on the surface of graphene. Future work will focus on attaching the probe molecule on the surface of graphene covalently.

04:00 PM. Using UV-vis spectroscopy to determine the pKa values of catechols

<u>Gisela Xhafkollari</u>, Larryn W. Peterson, Alexa Alana, and Keri L. Colabroy, Biochemistry and Molecular Biology, Rhodes College

There are a number of important catechols, including dopamine, catecholic nitriles, 3,4dihydroxyhydrocinnamic acid (DHHCA), and L-3,4-dihydroxyphenylalanine (L-DOPA) that serve as substrates for enzymes, including catechol-Omethyltransferase (COMT), L-DOPA dioxygenase, and cytosolic sulfotransferases (SULTs). We have synthesized a number of novel derivatives of these catechols with a range of substituents on the aromatic ring to investigate the mechanism and substrate selectivity of the enzymes. As the abstraction of the proton is a key step in many of the enzymatic reactions, determining the pKa values of these compounds is an important step in understanding their reactivity and identity. Experimental determination using UV-vis spectroscopy of the pKa values of these catechols allows for insight as to how they behave and interact in the active site. The pKa values of the analogues correlate well with the electron donating/withdrawing ability of the substituent.

04:15 PM. An inexpensive and efficient approach to cure chagas disease

<u>M. Johanna Lasiter</u>, and Gregory R. Naumiec, University of Central Arkansas, University of Central Arkansas

Neglected Tropical Diseases (NTDs) pose an enormous threat to those in poverty-stricken regions of the world such as Central and South America. NTDs have affected the lives of nearly 2 billion people worldwide. With limited funds and resources, research on NTDs is lacking. Chagas disease, one such NTD, is a parasitic infection that is now becoming increasingly common throughout the southwest United States. Chagas disease is caused by the parasite Trypanosoma cruzi, carried by an insect known as the "kissing bug". Once infected, the insect passes parasites through their feces and can eventually cause "Chagas heart disease," resulting in death. There are currently two drugs in the market for treating Chagas, benznidazole and nifurtimox. Benznidazole is the only drug of the two that is FDA-approved (only in children), and both drugs have severe side effects along with alarming reports of treatment failures due to drug resistance in T. cruzi. We aim to make a new class of anti-Chagastic compounds using disquaramide structural motifs. Disquaramides have shown to have anti-parasitic activity and are facile and cost-efficient to synthesize. Our research has incorporated the use of diamines in order to make cyclic disquaramides. To date, we have successfully synthesized three of these compounds with moderate to high yield (21-96%). The main focus of this research is to create inexpensive drugs to aid in the fight against Chagas disease.

Oral Abstracts Physics

03:00 PM. Effects of microgravity and radiation on rat bone strength and composition

<u>Hypatia Meraviglia</u>, Rahul Mehta, and Brent Hill, Department of Physics and Astronomy, University of Central Arkansas

The effect of prolonged exposure to microgravity and cosmic radiation on bone strength has long been

of critical pertinence to human spaceflight. Previous studies have shown that these deep space conditions reduce bone strength and elasticity and increase levels of calcium and phosphorus. We investigate these effects in male Sprague-Dawley rats, divided into four groups: a control group, a group exposed to cumulative 2.4 Gy radiation, a group suspended with hind legs up to simulate low-gravity conditions, and a group subjected to both 2.4 Gy radiation and simulated low gravity. The strength and chemical composition of right-side tibias and femurs of sacrificed rats were tested through threepoint bending and a scanning electron microscope (SEM). We applied force to the center of each of the four anatomical sides of each bone with a force transducer. We measured the cortical area of slices from the center of each bone and the relative percentages of carbon, oxygen, phosphorus, and calcium under a scanning electron microscope (SEM). Hind-leg suspension reduced bone strength statistically significantly, while radiation had no significant impact in either test (three-point bending and spectroscopy via SEM). We present additional findings, discuss implications for bone health in deep space conditions, and propose future research. Acknowledgement: This work is supported by the Arkansas Space Grant Consortium (ASGC). The authors also acknowledge the assistance of Manling Cheng, Natalie King, and Parimal Chowdhury (University of Arkansas for Medical Sciences).

03:15 PM. What is friction at the atomic level? Adhesion and shear force

<u>Zach Kauffman</u> Dr. Greg Salamo Mohammad Zamani Alavijeh, Physics, Missouri State University

Atomic force microscopy (AFM) is a hallmark of scanning probe technology; it uses nanoscale contact to map the surface's morphology, but the mechanism can also be used to investigate the friction qualities of the material. This series of experimentation focused on analyzing three facets of atomic-scale friction: First, this study analyzed the relationship between tip surface area and adhesion force. Second, this study produced a relationship between tip surface area and overall lateral friction. Lastly, this study analyzed the wear process on AFM tips as a function of normal forces are applied over time on different surfaces. Investigating each of these aspects of friction will improve our understanding of surface-to-surface interactions absent confounding variables such as interlocking asperities or surface roughness. It was found through these results that surface area and elasticity had notable implications for friction measurements which deviates from traditional understandings of friction.

03:30 PM. Field programmable gate array for correlation measurements and data acquisition system

<u>Apoorva Bisht</u>, and Hiro Nakamura, Physics, University of Arkansas - Fayetteville

A photon correlation measurement system has been developed using field programmable gate array (FPGA). This has been tested for classical light sources like coherent and bunched light. These were generated via unmodulated and modulated laser respectively. We will further use FPGA for advanced photon manipulations such as temporal multiplexing of single photons. FPGA specifically will be used for implementing the routing logic for the single photons to generate a regular sequence of single photons.

03:45 PM. Motility dynamics of E. coli in dense environments using Differential Dynamic Microscopy

<u>Seth Williams</u>, Pradeep Kumar, Department of Physics, Arkansas Tech University

Motility of bacteria has traditionally been studied by having a sparse population of bacteria moving in a quasi-2D environment whereas positions of cells can be tracked in real time under a microscope. Such methods fail to work for a dense population of bacteria where tracking single cells become difficult, and in some cases impossible. Dynamics of dense bacterial environments can be studied by using a method coined Differential Dynamic Microscopy (DDM). In this talk, I will describe the method and its implementation with bright field microscopy using colloidal beads as an example. Furthermore, I will discuss the dynamics of Escherichia coli cells at various concentrations of magnesium sulfate.

Poster Abstracts Biology

1A. ML-1 Thyroid Cancer Cells are more resistant to platinum-based chemotherapeutic agents over HeLa Cervical Cancer Cells

<u>Daniel Kim</u>, Min Zhang, Nhi Le, Kyoungtae Kim, Biology, Emory University

Recent literature demonstrates that platinum-based chemotherapeutic drugs in physiological solvents display higher efficacy in destabilizing cancer cells. As human cells come in over 200 different varieties, it would be beneficial to test the efficacy of these drugs using a wider spectrum of cancer cells. Utilizing the well-tested HeLa Cervical cancer cells as a control for the effects of these drugs, we assessed the impact of the platinum-based cisplatin, carboplatin, and oxaliplatin on ML-1 Thyroid cancer cells. Through the XTT Viability assay, we found that ML-1 cells are more resistant to cisplatin and oxaliplatin with an IC50 value two times higher than for the same drugs in HeLa cells. It has been consistently shown that the oxidative stress caused by these chemicals were more pronounced in HeLa cells than in ML-1 cells, but the only measurable results were found 24 hours after treatment. We also show that a high percentage of HeLa cells displayed apoptosis with even 20µM of these chemicals, which is directly comparable in effect to the 100µM of chemicals in ML-1 cells. Upon comparing the expression levels of caspase-3 in HeLa and ML-1 cells, we observed that when treated with 40µM of cisplatin, the levels of caspase-3 were statistically higher for HeLa cells than for ML-1 cells. We propose that ML-1 cells are more resistant to these platinum-based chemotherapeutic agents by adopting higher levels of multi-drug resistant (MDR) properties. We are currently testing the expression levels of MDR-1 in both cell strains. This will provide new insight into the different capacities of each cell line in regard to MDR

mechanisms and the treatment regimen for cancer patients in the future.

1B. Expression and function of a putative barrier claudin in opercular epithelia and gill of fundulus heteroclitius, a euryhaline teleost fish

<u>Olivia G. Parker</u>, Allison C McFarland, Julie A. Staling, Christian K. Tipsmark, Biological Sciences, University of Arkansas - Fayetteville

Atlantic killifish (Fundulus heteroclitius) are euryhaline fish that can live in both fresh water and seawater and there have to limit passive ion fluxes across their surface epithelia, gill and skin, to safeguard ion homeostasis. Claudin tight junction proteins largely determine epithelial permeability and transcriptomic studies in killifish suggests that the putative barrier forming claudin-30c is the most abundant paralog expressed in the gill. We studied claudin-30c and select other paralogs (10c, 10d, 10e, 10f, 32a) testing 3 hypotheses: i) these claudin paralogs are most highly expressed in gill and skin; ii) expression in opercular skin is similar to gill; iii) claudin-30c in killifish provides protection from detrimental passive salt fluxes and are up-regulated or down-regulated based on environmental salinity. Organ distribution experiments confirmed that claudin-30c (and 10c, 10d, 10e, 10f, 32a) have higher expression in the opercular skin and gill than in the other examined organs (kidney, anterior intestine, posterior intestine, skeletal muscle, brain, liver). The similar expression in this simpler twodimensional opercular skin as in the complex tridimensional gill structure independent of salinity helps validate the use of the former organ as a gill model in Ussing type electro-physiological set-up. We also compared claudin mRNA expression in gill and opercular skin from fish acclimated long-term to dilute (freshwater), physiological (brackish water) and concentrated (seawater) environments. There was no effect of salinity on claudin-30c transcript levels and studies at the protein levels are underway and will be presented.

2A. Microglia polarize in response to transactive response DNA-binding protein-43 (TDP-43)

and display partial recovery after removal of the stimulus

<u>Alicen Wilcox</u>, and David Donley, Department of Biology, Harding University

The proper response to protein signals is necessary for a healthy central nervous system (CNS), and protein dysregulation is a feature of neurodegenerative diseases. Transactive response DNA-binding protein-43 (TDP-43) is an intranuclear protein, but mislocalization is associated with amyotrophic lateral sclerosis (ALS). TDP-43 is released into the extracellular space where it is sensed by microglia, the CNS-resident immune cells. Our data and the literature suggest that microglia respond to TDP-43 dysregulation by increasing CNS inflammation. The goal of this study was to determine the impact of TDP-43 on microglial function and the extent to which microglia recovery. To study the inflammatory response, microglia were stimulated with TDP-43 in a 2x2 factorial design with other inflammatory stimuli. Using iNOS and arginase colorimetric assays, we found that TDP-43 caused microglia to lose the ability to appropriately respond to inflammation. To study recovery, cultured microglia were stimulated with TDP-43 or a vehicle; then the media was changed to remove the stimuli and allow a recovery period. Markers of activation were measured using flow cytometry and metabolic assays. After recovery, microglia had a slight decrease in phagocytic capability as compared to TDP-43 stimulation without recovery. Microglia also demonstrated a metabolic shift toward glycolysis, consistent with a proinflammatory phenotype but returned to baseline levels of metabolic activity after recovery. These data demonstrate that dysregulated TDP-43 shifts the balance of signaling pathways toward an inflammatory phenotype, but microglia begin to recover after removal of the inflammatory stimuli.

2B. Exposure to reactive oxidative species in Caenorhabditis elegans promotes phosphorylation in epidermal growth factor receptors

<u>Eliana John</u>, Dr. David Donley, Biology, Harding University

Regulation of cellular processes is important for proper functioning. One of the ways regulation is maintained is through the growth cycle. If this is disturbed, there is a higher risk for disease, or cancer if proliferation is not properly regulated. Environmental factors, including stress, can interfere with cellular regulation. Cellular stress can come in several different forms: chemicals, ultraviolet light, as well as heat. When regulation is disrupted via certain chemicals, cell interactions can be inhibited or increased. Either of these can negatively impact the cell. One of the diseases caused by cellular regulation disturbance is cancer. Epidermal Growth Factor (EGF) is a protein that is involved in the regulation of cell growth and differentiation. This protein binds to a receptor known as Epidermal Growth Factor Receptor (EGFR). At the EGFR level, activation can be detected by measuring protein phosphorylation levels. The goal of this study was to use the hermaphroditic nematode model, Caenorhabditis elegans, to understand the impact of cellular stress on EGFR signaling. The let-23 gene in C. elegans is a homologue to the human EGFR. Using the let-23 knockout strain of C. elegans, phosphorylation levels are measured with a phosphorylation assay after exposure to Reactive Oxidative Species (ROS)-inducing compounds. These data will help elucidate the impact of ROS and other cellular stressors on EGFR signaling and potential ways to target cell regulation in disease states.

3A. Rev1-Mediated replication of Gquadruplexes

<u>Bethany Paxton</u>, Dr. Robert Eoff, Dr. Leena Maddukuri, Biology, Henderson State University

DNA replication is an important cellular process that generally requires a high degree of accuracy and efficiency to maintain cellular homeostasis. Replication can be especially challenging in some regions of the genome, particularly in motifs that have the capacity to adopt non-canonical structures. One such non-canonical structure is the four-

stranded G-quadruplex (G4) formed in some guanine-rich regions of the genome. Failed G4 bypass leads to the formation of single-stranded DNA (ssDNA), which can further collapse into strand breaks, causing chromosomal fragmentation and genomic instability. Furthermore, efficient bypass of G4 motifs ensures that regulatory histone post-translational modifications are maintained in the wake of the replisome; if histone recycling is hindered, overall chromatin structure can be disrupted, resulting in genetic and epigenetic instability. The translesion synthesis polymerase Rev1 has been implicated in G4 maintenance, but mechanistic details related to fork dynamics are incomplete, especially for human Rev1. Understanding the role of Rev1 in G4 replication will provide new insight into replication mechanisms that promote bypass of endogenous barriers to fork progression. In this study, CRISPR-Cas9 gene editing was used to generate a HEK 293 Flp-InTM T-RExTM (FT) Rev1 knockout (REV1KO) cell line. We then performed a clonogenic survival assay to measure EC50 values for WT and REV1KO cells treated with pyridostatin (PDS), a G4 stabilizer. REV1KO cells were almost three times more sensitive to PDS than WT cells. These results are supportive of the idea that Rev1 is a critical barrier to the anti-proliferative effects of PDS. To test the impact of Rev1 loss on ssDNA gap formation, we performed non-denaturing immunofluorescence with CldU incorporation. REV1KO cells showed higher levels of CldU incorporation compared to controls. Addition of menadione, an oxidative stressor, and PDS caused a further increase in CldU signal in REV1KO cells compared to WT. These results suggest that the formation of global ssDNA gaps is elevated in REV1KO cells experiencing G4-induced stress. indicative of the importance of Rev1 in resolving G4 structures during replication.

3B. Analysis of a Unique Tennessee Cave System: A Potentially Sulfur Speleogenic, Chemolithoautotrophic Cave Supporting Multiple Trophic Levels

<u>Lauren Camp</u>, Kaylie Wheeless, Aspen Huseman, Maya Robles, James Engman, Michael Ray Taylo, Biology, Henderson State University

While most biological communities require energy from sunlight and photosynthesis, a few powered solely by chemical energy have been discovered, primarily in deep sea hydrothermal vents and a few unique cave systems around the world. Secret Squirrel Cave in Central Tennessee is a presumptive chemolithoautotrophic cave. Deep in the cave is an area called the Petroleum Passage because of its pervasive petroleum smell. Within the passage lies a perched pool. Its sandy bottom contains crude oilreleasing "mini vents," surrounded by colored bands of sediment. Initial metagenomic analysis of nine selected samples identified 593 different bacteria and Archaea, indicating diverse microbial communities in the bands. These included thermophiles/hyperthermophiles, and taxa that oxidize sulfur, methane, ammonia, and hydrocarbons, similar to those found in previously described chemoautotrophic systems. Gas chromatography mass spectrometry (GC/MS) analysis of oil from the pool reveals degraded hydrocarbon chains, five to ten carbons long, compared to "typical" crude oil composed of chains of fourteen to sixteen carbons. Recent observations found unusually high densities of salamanders and millipedes in the passage of interest, further supporting the hypothesis that chemolithoautotrophy in and below the pool is the basis for a system with multiple trophic levels. The presence of large gypsum formations led to the hypothesis of potential sulfur speleogenesis within Secret Squirrel. Future study will involve targeted genetic sampling in the pool, a photo documentation system to record temporal variation in the pond system and animal populations, more thorough water chemistry analysis, scanning electron microscopy (SEM), and stable isotope analysis to determine potential flow of energy through trophic levels. This survey and future studies could provide insight to the cave's possible speleogenic origin, microbial species in extreme environments on Earth, and offer an example of a system previously suggested as a potential model for life in subsurface environments on Mars.

4A. Determining the ability of type I IFNs to promote IL-10 production directly or indirectly by CD4+ T cells.

<u>Sarah Vue</u>, Jason Stumhofer, Ph.D., Kara O'Neal, Andrea Harris, Chemistry, Henderson State University

Interleukin-10 (IL-10) has a prominent immunoregulative role in protecting against inflammation, particularly in the context of Plasmodium Falciparum infection in mice and humans. Although much is known about the role of IL-10 in reducing inflammation during this infection, the factors and signaling pathways that induce IL-10 expression are still poorly understood. Here we report that interferon- β (IFN- β) and IL-27 individually induce the production of IL-10 by CD4+ T cells in vitro. However, when combined, they have a synergistic effect on the production of IL-10. Furthermore, the ability of IFN- β to induce T cell production of IL-10 was dependent on the presence of the transcription factor interferon regulatory factor-1 (IRF-1). Also, our initial data indicate that IFN- β can induce T cell production of IL-10 directly but not indirectly in vitro. Together our in vitro data confirm that type I IFNs are a potent inducer of IL-10 production by CD4+ T cells, and these cytokines can act directly on T cells to promote an immunoregulatory phenotype.

4B. Docking low-energy ligand conformations to human μ -opioid receptor complex model to verify the model's reliability

<u>Alaina Ivers</u>, Dr. Caitlin E. Scott, Department of Biology, Hendrix College

Monish Shukla, Lauren Jones, Brenna Outten, Dr. George C. Shields Lauren, Brenna, and Dr. Shields, Furman University

Opioids are commonly used medications that manage chronic pain, which affects approximately 50 million individuals in the U.S. Opioids are agonists that activate the μ -opioid receptor, a type of G-protein coupled receptor (GPCR). When the μ opioid receptor is bound to the Gi protein, analgesia occurs without tolerance and addiction, but when opioids bind to β -arrestin, tolerance, addiction, and respiratory dysfunction occur. Our goal is to design an agonist that activates the μ -opioid receptor when it is bound to the Gi protein. Previously, we used computational techniques to construct a model of the human µ-opioid receptor bound to the Gi protein based on the mouse μ -opioid receptor in complex with the human Gi protein (PDB ID: 6DDE). However, the mouse μ -opioid receptor has been crystallized in the activated state in the presence of the agonist BU72, but the conformation of the bound BU72 is in the high-energy state. Here, we show that: 1) the low-energy ligand conformations can bind to the μ -opioid receptor, and 2) our human u-opioid receptor model is reliable. First, we used the Induced Fit and Glide Docking programs to dock poses that are similar to the crystal structures to the crystallized receptors to show that the docking program is reliable. Then, we docked lowenergy conformations of BU72 and β -FNA (modified to naltrexone) to the active and inactive crystal structures (PDB ID: 5C1M and PDB ID: 4DKL) and to the human μ -opioid receptor model. The results demonstrated that our human µ-opioid receptor model is reliable. We then used LigPrep and Jaguar software to prepare the conformations and charges of 36 ligands that have been experimentally shown to bind strongly to the µopioid receptor. The next step will be to dock the compounds to the human μ -opioid receptor model. With opioids currently being the only effective chronic pain medication, the significance of this research is to eventually develop opioids that are safer and non-addictive. In knowing how these ligands bind, we can design more agonists that make the Gi protein-coupled µ-opioid receptor more favorable for pain relief, and they can be further developed into pain medication.

5A. Investigating the role of DNA Ligase K during DNA repair in bdelloid rotifers

<u>Halie J. Booth</u>, and Andrew M. Schurko, Biology and Health Sciences, Hendrix College

Bdelloid rotifers are an all-female lineage of microscopic invertebrates found in aquatic habitats.

These animals are unique because they possess an extraordinary DNA repair system for recovery from DNA damage encountered during desiccation. While this is an important survival strategy for bdelloids, the mechanism for DNA repair is not understood. Previous work determined that the gene encoding DNA ligase K (LIGK) is upregulated during recovery from DNA damage in the bdelloid Adineta vaga. The objective of this project was to investigate the role of LIGK during DNA repair by using (i) RNA interference (RNAi) to silence LIGK, and (ii) CRISPR/Cas9 genome editing to inactivate LIGK. For RNAi, an E. coli feeder strain that expresses a double stranded RNA (dsRNA) copy of LIGK was fed to rotifers at various concentrations and for different lengths of time. However, realtime PCR failed to show strong evidence for a gene knockdown. We also used CRISPR/Cas9 genome editing to inactivate LIGK. A single guide RNA (sgRNA) was used to cut LIGK with in vitro assays. We designed a template for homology-directed repair that would introduce stop codons in LIGK resulting in a truncated protein. Rotifers were then electroporated with sgRNA/Cas9 complexes and the template. PCR with mutation-specific primers showed evidence of genome editing and introduction of the desired mutation in the genome. PCR and DNA sequencing of LIGK from individual CRISPR-treated rotifers will be done next to identify mutants. Future work will explore the effects of desiccation recovery on RNAi-treated rotifers and LIGK mutants derived from CRISPR treatment to investigate the role of this protein in DNA repair.

5B. LADCAP: Launchable Automated Device for Collecting Airborne Particles

<u>Olivia G. Echols</u>, Marleigh Dodson, Briar Miller, and David J. Thomas, Ph.D, Science Division, Lyon College

Our lab studies extreme environments as analogs for potential habitats elsewhere in the solar system. Currently, our research focus is on atmospheric microbes. Microorganisms at high altitudes survive in low temperatures and pressure, desiccation, and high UV flux. Thus, the atmosphere is an "extreme

environment." Previous research has shown that microbes can be carried around the globe by prevailing winds. Not only do these microbes survive the trip, some are metabolically active while airborne. In order to sample atmospheric microbes, we are developing a small, cost-effective collection apparatus that can be flown on balloons, rockets, and/or drones. LADCAP (Launchable Automated Device for Collecting Airborne Particles) was built to collect microbes and/or other atmospheric particulates. The present version of LADCAP has a mass of approximately 120 grams and fits within a diameter of four centimeters. For atmospheric testing, it is flown on a custom mid-power rocket dubbed "G-Lifter Mark-2," which can attain a maximum altitude of 1200 meters and flight time of 230 seconds with a G-class motor. Using standard 25 mm diameter, 0.45 µm membrane filters, the LADCAP's vacuum pump can intake >2.5 L/min using a lithium-ion, nine-volt battery. Further, our lab is modifying high-power rockets including LOC Precision Hi-Tech, Madcow Mini-DX3, and Wombat high-power rocket kits for higher and longer flights that will be able to contain LACAPs. These kits are commercially available with extensive flight records, and their payload bays allow for multiple LADCAPs to be flown at once. For example, the Hi Tech/LADCAP combination can reach 2800 m altitude with 430 s flight duration and can collect up to eight samples. During flight, LADCAP passes air (and microbes) through the filter at a predetermined time or altitude. Anything larger than the filter's pore size gets trapped on its surface. After retrieval, the filter can be placed directly onto culture media for growth or examined under a microscope. Extensive ground-testing was required to calibrate airflow, determine optimal sampling duration, and ensure the device was functional. During ground tests, the device was activated for 30-120 seconds, and filtered microbes were on general-purpose media (nutrient agar, tryptic soy agar, R2A agar, etc.). To date, we have launched LADCAP three times, but with only one successful collection of microbes. During summer 2021, students learned how to assemble commercial rocket kits, design custom rockets, and determine stability. By the end of the summer session, students built the high-power, fiberglass rocket, Wombat,

which has the potential to lift multiple LADCAPs to over four kilometers altitude. Flight and ground tests continue. This work was supported by a grant from the Arkansas Space Grant Consortium.

6A. An investigation of the intracellular trafficking of cadmium selenide zinc sulfide quantum dots in yeast cells

<u>Nhi Le</u>, Cameron Kirk, Kim Kyoungtae, Biology, Missouri State University

Quantum dots (QDs) are semiconductor nanoparticles capable of emitting strong and stable light of various colors. For this reason, quantum dots have been utilized in many research and medical applications. Recently, some studies have suggested the toxicity of quantum dots on cells, but the exact mechanism is unknown. The primary focus of our project was to investigate the traffic route of Cadmium Selenide Zinc Sulfide quantum dots (CdSe/ZnS QDs) in Saccharomyces Cerevisiae yeast cells. We hypothesized that QDs are internalized into yeast cells by receptor-mediated endocytosis pathway and then transported to various locations of yeast cells. In an attempt to determine the trafficking route of QDs in yeast cell, we treated budding yeast expressing: Plasma membrane reference marker GFP-2PH; receptor-mediated early endocytosis reference marker ABP1-GFP; trans-Golgi network/ late Golgi reference marker FAPPI-GFP; and late endosome reference marker Vps10-GFP, with red CdSe/ZnS QDs over a period of 24 hours. In treatment of low concentration of red CdSe/ZnS QDs (4µg/mL), we found that QDs associated with the outer layer of yeast cell immediately after treatment. However, QDs did not co-localize with the plasma membrane reference marker GFP-2PH at this time, suggesting that QDs may only associate with the cell wall of yeast cell in the early hours. At about three hours after treatment, a minimal amount of QDs co-localized with the plasma membrane, indicating that at least three hours is needed for QDs to start internalizing into yeast cells. After six hours of treatment, a large amount of QDs was found at the plasma membrane of the yeast cell, a decent amount of ODs colocalized at the early endocytosis vesicle, and a low

amount of ODs showed co-localization with the late Golgi. From eight hours to twenty-four hours after treatment, the amount of QDs in yeast cell decreased drastically, likely due to the aggregation of QDs in culture media, as a large number of aggregated clusters of ODs were observed in the media in later time point. QDs did not co-localize with the late endosome reference marker Vps10-GFP at any time point, suggesting that late endosome is not a destination for QDs trafficking route. We concluded that QDs associated with the outer layer of yeast cell immediately after treatment, took around three hours to get to the plasma membrane, arrived at the early endocytosis vesicle then traveled to the late Golgi at around six hours. As of now, the rest of the trafficking route of ODs in budding yeast cells remained unknown and needs further investigation.

6B. Comparing the loading of DNA polymerase epsilon on origins in wild type and mutant yeast

<u>Carlos Cuza,</u> Sapna Das Bradoo, Natural Sciences, Northeastern State University

DNA Polymerase Epsilon (Polɛ) and Minichromosome maintenance protein 10 (Mcm10) are essential proteins for cell cycle progression. DNA Pole is the polymerase responsible for leading strand synthesis during DNA replication, while Mcm10 is a multifunctional protein that participates in replication initiation, replication progression and DNA damage response. Studies from our group have shown that Pole and Mcm10 interact during DNA replication. To gain insight into the nature of Pole-Mcm10 interactions, we planned to investigate the presence of both proteins on early and late firing origins during DNA replication. To test for the presence of Pole and Mcm10 at sites of origin, we performed Chromatin Immunoprecipitation (ChIP) to pull down our proteins of interest in yeast cells synchronized in the early S phase. DNA in the ChIP samples was purified and tested for enrichment of early and late origins by Polymerase Chain Reaction (PCR). Immunoblotting verified the presence of Pole and Mcm10 proteins in yeast lysate after crosslinking with formaldehyde. Furthermore, Mcm10 successfully coimmunoprecipitated with Pole in S phase cells. Importantly, we observed Pole associated with early origin sequences in S phase synchronized cells. The data suggest that Pole and Mcm10 are present at early origins during the S phase and may coordinate the early DNA replication process. Further experiments with mutant yeast suggest that Pole mutants that have reduced interaction with Mcm10 display reduced affinity for early origin activation. To further elucidate the nature of this interaction,we plan to repeat these experiments with additional time points in G phase, as well with the addition of real time PCR.

7A. Fluorescent UPEC: A tool to study UTI pathogenesis

<u>Alissa D. Eberhard,</u> Janaki K. Iyer, Gregg Wadley College of Science and Health Professions, Northeastern State University

Urinary tract infections (UTIs) caused by uropathogenic E. coli (UPEC) are the most common type of bacterial infections seen in women. UPEC express many virulence factors including adhesins and fimbriae that aid the bacteria adherence to the bladder epithelium and in some cases even invade into tissues. The pathogenic mechanisms employed by UPEC that promote adhesion and invasion are not fully explored. We propose to study the mechanisms of adherence and invasion of UPEC to bladder cells by producing UPEC expressing the green fluorescent protein (GFP). We hypothesize that the GFP-expressing UPEC will have similar properties to the non-fluorescent UPEC and thereby assist in studying host-pathogen interactions. To test this hypothesis, we transformed UPEC with a GFP encoding plasmid and generated fluorescent UPEC. These fluorescent UPEC were utilized to infect human bladder epithelial cells (5637) at increasing multiplicities of infection (MOI) to study adherence and invasion. We successfully detected and quantified adherence and invasion of the fluorescent UPEC by fluorescent microscopy, flow cytometry, and gentamicin-based invasion assays. Thus, the GFP-expressing UPEC will enable us to identify host proteins that mediate adherence and invasion of UPEC. These findings will provide more insight

on the mechanisms of pathogenesis employed by UPEC, which will aid in the design of more effective therapies for the prevention and treatment of UTIs.

7B. Visualization of the conserved MCM10:POLE interaction in human embryonic kidney cells by confocal microscopy

<u>Sarah Woller</u>, Lydia Ostmo, Michael Smith, Shwetanshu Das, Subhas Das, and Sapna Das-Bradoo, Natural Science, Northeastern State University

DNA replication includes spectacular interactions among replication proteins stimulated in the S phase of the cell cycle. Polymerase epsilon (POLE) is required for leading strand replication and activation of the DNA damage response pathway. Mutations in Polymerase epsilon are linked to cancerous predispositions. Our laboratory has shown that MCM10 plays an integral role in the functionality of POLE in budding yeast. Our project's goal is to investigate if the roles of MCM10 and POLE are conserved in human cells. To achieve this goal, we cloned MCM10 and POLE into GFP and RFP vectors, respectively. DNA sequencing confirmed the insertion of the genes into the respective vectors. The vectors were transfected into HEK293 cells and expression of the tagged proteins were visualized by fluorescence microscopy. Importantly, we observed interaction between MCM10 and POLE in human cells. This was achieved using co-localization fluorescence studies. We utilized Click EDU technology to study the dynamics of the MCM10:POLE interaction during the cell cycle. By Incorporation of the thymidine analog EDU (5-ethynyl-2'-deoxyuridine) into DNA during active DNA synthesis we were able to identify localization patterns of MCM10 and POLE in the nucleus during the S phase. Interestingly, MCM10 and POLE interaction is only seen in mid to late S phase even though they are both present throughout the S phase. Our data suggests that both proteins interact to carry out specific function/s during DNA replication

8A. An in-vitro model to study the effects of progesterone on cystitis caused by UPEC

<u>Mackenzie Bonnewitz</u>, Abigail McNabb, Alexandra Head, and Janaki K. Iyer, Gregg Wadley College of Science and Health Professions, Northeastern State University

Urinary tract infections (UTIs) are increasingly becoming more difficult to treat, as many uropathogens that cause UTIs acquire mechanisms that allow them to evade antibiotic treatment. UTIs and recurrent UTIs are frequently seen in women with fluctuating hormones – as characterized during menses, menopause, and post-menopause. Such changes in steroid sex hormone levels negatively affects the tissues of the reproductive and lower urinary tract, creating a window of opportunity for infection by uropathogens, including Escherichia coli (E. coli). There is evidence that estrogen offers protection against UTIs but it unclear if progesterone, another major steroid hormone, mediates protection against UTIs. In the current study, we utilized the human bladder cancer cell line 5637 as a model of the urinary tract, and E. coli strain CI5 as our uropathogen. Our findings show that 5637 cells express the progesterone receptor and that treatment with different concentrations of progesterone does not detrimentally affect cell viability. We also provide evidence of E. coli CI5's ability to infect and invade bladder cells via gentamicin protection assays. These results provide a basis for future experiments with progesterone to determine its ability as a potential therapeutic in treating UTIs caused by E. coli.

8B. Comparisons of corbicula mimicry pollination methods in Brassica rapa

<u>Will Dockery</u>, and Gary Bates, Biology, NorthWest Arkansas Community College

A substantial portion of agricultural crops are pollinated by insects. Many of these pollinator insects have, in recent years, had a serious drop off in population numbers. The perceived threats that have caused these precipitous declines are myriad but include a host of human-made problems; global climate change, pollution, fragmentation of habitat, increased parasite load, and industrial farming techniques. The decline of natural pollinator animals and changing agricultural methods – like an increase in controlled environment agriculture may necessitate the near future need for mass artificial pollination. Brassica rapa were used to compare pollination methods using corbicula mimicry, which is the primary way Hymenoptera species (such as honeybees (Apis spp.) and bumble bees (Bombus spp.)) transport and spread pollen. Both quality and number of seed produced were compared based on the artificial pollination methods.

9A. Bioinformatic analysis of genes CUL3, KEAP1 and NFE2L2 within specific cancer types

<u>Kaili Ralston</u>, and LaShall Bates, Biology, NorthWest Arkansas Community College

Mutations in the oxidative stress pathway KEAP1-NFE2L2 has been associated with resistance to treatments and rapid progression of specific cancers. The KEAP1-NFE2L2 pathway regulates redox and metabolic homeostasis on an intracellular level. KEAP1, an adaptor protein, recruits CUL3, a E3 ubiquitin ligase complex important for protein degradation, and continuously targets transcription factor NFE2L2. After oxidative and toxic stress, NFE2L2 is released from KEAP1 allowing transcription of its target genes. A study was conducted comparing gene mutations for this pathway and associated data between different cancer data sets in cBioportal to determine significance and associations.

9B. Analyzing viral and host gene expression in Gammaherpesviruses

<u>Rylie Davis,</u> Craig Forrest, Shana Owens, Biology, Ouachita Baptist University

Gammaherpesviruses (GHVS) are defined by their capacity to establish life-long latency in their hosts. Most humans are chronically infected with at least one GHV, either Epstein-Barr virus or Kaposi sarcoma-associated herpesvirus (KSHV). These viruses undergo lytic infection, in which the virus

produces new virions to infect neighboring cells, and latency, in which the virus lies dormant awaiting lytic reactivation1. The Forrest lab studies the mechanisms by which gammaherpesviruses infect their hosts and lead to cancers such as Burkitt lymphoma and Kaposi sarcoma in humans. The lab uses murine gammaherpesvirus 68 (MHV68) as a small animal model of gammaherpesvirus infection. Gammaherpesviruses have mechanisms by which they regulate both viral and host gene expression. It is through these mechanisms that they establish latency, drive lytic infection, and eventually cause cancer. The MHV68 protein MTA, or the mRNA transcript accumulator, was found to differentially regulate the expression of two other immediate early genes, the latency- associated nuclear antigen (LANA) and the replication and transcription activator (RTA). This project focuses on determining whether kMTA also differentially regulates kLANA and kRTA. After preparing DNA samples of each of these genes, a transfection and Western blot will be performed to assess protein production. In a second portion of this project, the oncogenic properties of KSHV were investigated using endogenous fluorescent tagging by CRISPR/Cas9. P53 and p21, cell cycle control/tumor suppressor proteins were fluorescently-tagged within the cell to visualize protein localization in virally infected cells. In a control HEK 293T cell line, cells successfully took up the red fluorescent protein insert as shown by the production of proteins p21 that displayed red fluorescence. After optimizing this procedure with a blue fluorescent protein insert and p53 guide, the 293 cells will be transfected with KSHV bacterial artificial chromosome DNA, and the production and localization of tumor suppressor proteins will be compared to that of the control cell line.

10A. Crosstalk between vitamin D receptor signaling and glucocorticoids in musculoskeletal induced atrophy

<u>Seth Curl</u>, Dr. Teresita Bellido, Dr. Amy Sato, Biomedical Sciences, Ouachita Baptist University

Accumulation of glucocorticoids occurs through exposure to chemotherapy drug cocktails,

immunosuppressants, stress, and aging, and leads to a loss of bone and muscle mass. Excess of glucocorticoids induces musculoskeletal atrophy and is now the third leading cause of osteoporosis. The goal of this project is to investigate whether increased vitamin D receptor (VDR) signaling interferes with glucocorticoid induced atrophy in bone and skeletal muscle, and to investigate the role of VDR signaling in skeletal muscle within this frame. Four-month-old mice that either expressed VDR in their skeletal muscles or had expression of VDR suppressed through genetic excision with cre recombinase enzyme activity were used in this project. The mice were treated with either a placebo or glucocorticoids, and then the same mice were either dosed with the active metabolite vitamin D (1,25-dihydroxyvitamin D3) or a vehicle control. After 4 weeks of treatment, the lean body mass, gastrocnemius muscle weight, and bone mineral density of each mouse was collected. The lean body mass of the mice was decreased by glucocorticoids, and vitamin D intervention protected from this loss. The gastrocnemius muscle weight was decreased by glucocorticoids, and vitamin D prevented this loss only in mice that have skeletal muscle VDR expression, but not in mice that lack this expression. Glucocorticoids decreased bone mineral density, but vitamin D provided a partial protection from this loss. These findings indicate that vitamin D intervention might simultaneously protect against glucocorticoid induced musculoskeletal atrophy in immunosuppressant patients.

10B. Bird diversity and abundance in relation to habitat complexity at Jack Mountain Wildlife Management Area

<u>Grace E. Tidwell</u>, Kelsey M. Bester, and Christin L. Pruett Ph.D, Biology, Ouachita Baptist University

Since 1973, North America has lost 2.9 billion birds due to habitat loss and fragmentation (Rosenberg et al. 2019). To assess the effects of habitat complexity on bird diversity, 88 locations were surveyed at Jack Mountain Wildlife Management Area (WMA) using ten-minute point counts. All birds seen and heard at each point were documented and habitat complexity was assessed by examining

the percentage of ground cover, shrub layer, midstory tree layer, and canopy layer at each point. A habitat complexity index was generated from these plant surveys. Previous research at Jack Mountain has shown that habitats dominated by pine trees had the highest bird species diversity and abundance. Habitat complexity has been associated with an increase in bird species diversity (Sam K. et al 2019) and thus, we hypothesized that pine habitats would have greater habitat complexity and that habitat complexity would be positively correlated with bird diversity and abundance. Statistical tests were performed in R to assess these hypotheses. In comparisons between species diversity (r=0.116; P=0.28) or abundance (r=0.115; P=0.28) with habitat complexity index no significant correlation was observed. We then compared each of the four aspects of the habitat complexity with species diversity and abundance and found a significant negative correlation between species diversity (r=-0.383, P<0.001) and abundance (r=-0.372, P<0.001) versus canopy coverage. Also, significant positive correlations were found between species diversity (r=0.378, P<0.001) and species abundance (r=0.405, P<0.001) versus ground cover (Figure 6) and species abundance was also positively correlated with amount of shrub cover (r=-0.097, P=0.366). Each point location was also assigned to a habitat class based on the percentage of pine and deciduous tree cover. As found in previous summers by students at OBU, a comparison among habitat classes and species diversity showed higher numbers of species in pine habitats (F=3.755, P=0.0274) however, the habitat complexity index did not differ among habitat classes (F=2.05, P=0.135). To further evaluate, the drivers of larger numbers of birds in pine habitats, aspects of the habitat index were then compared to habitat classes. We found smaller amounts of canopy coverage (F=0.4538, P=0.0134) and larger amounts of ground cover (F=4.538; P=0.0134) and shrub cover (F=6.879, P=0.0017) in pine habitats than in deciduous or mixed habitats. These findings suggest that there are more bird species and individuals among pine habitats at Jack Mountain because of less canopy coverage. A reduction in canopy coverage in pine habitats could lead to an increase in ground and shrub coverage, which are both

correlated with an increase in the diversity and abundance of birds. In conclusion, we reject our initial hypothesis about bird diversity and pine habitats being associated with increasing habitat complexity. Our findings suggest that the population dynamics of birds at Jack Mountain are associated with a diverse set of habitat variables that cannot be simplified into a single habitat complexity index.

11A. Identification of miRNA targets as lung cancer therapeutics

<u>Lauren McCann</u>, Dr. Robert Griffin, Azemat Jamshidi-Parsian, and Dr. Nathan Reyna, Biology, Ouachita Baptist University

The environment of tumors is hypoxic and becomes even more so after exposure to radiation therapy. Activation of the HIF1 gene enhances the ability of the cancer cells to survive this treatment, and the knockout (KO) of this gene has been shown to decrease cancer cells' resistance to radiation therapy (See "HIF1 and Resistance to Radiation"). By targeting HIF1-dependent genes in the HIF1 signaling pathway, cell viability can be reduced after radiation exposure, therefore increasing patient recovery and survival. The available drugs and treatments for HIF1 knockout have been found to be toxic and using miRNA as treatment could avoid this toxicity. After identifying target genes, miRNAs were found that could be mimicked or inhibited in order to produce the desired gene expression. Future analysis should be done to investigate the effect of these miRNAs on genes other than the found target genes so that unwanted side effects can be avoided. Experiments should be done to show the effect of the miRNA mimics and inhibitors in hypoxic and normoxic conditions.

11B. The effects of light wavelength and gravity on physarum polycephalum growth

<u>Reese Chesshir</u>, Dr. Jim Taylor, Thomas Harrington, and Taylor Barnhart, Biology, Ouachita Baptist University

Physarum is a slime mold in the genus of mycetozoan and the family of Physaraceae. It is a single cellular, multinuclear organism that is not classified as an animal, plant, or fungi. The purpose of this experiment is to study the effect of different light wavelengths and the influence of gravity on Physarum growth patterns. The Physarum is grown in a bacteriological agar with distributed oats as its food base. Red, green, blue, red and blue, and no light was studied and expansion was documented. The possible effects of gravity conditions were introduced by a clinostat. The experiments showed that different light and gravity environments had no effect on the expansion and growth of the Physarum in these conditions. The experimental results were analyzed using a single factor ANOVA test, concluding, all p-values showed statistical indifference between each condition. Therefore, the search for a food source has more influence on Physarum growth than different wavelengths of light and clinostat conditions.

12A. Lung carcinoma exosomes modify tumor microenvironment

<u>Jade Dorman</u>, Gracen Hambrick, Lauren McCann, Dr. Nathan Reyna, Department of Biology, Ouachita Baptist University

Cancer uses intercellular communication to induce tumor growth and metastasis. Fibroblasts can become specifically transformed and associated with cancer to aid in the process. Extracellular vesicles, specifically exosomes, contain proteins, RNA, and DNA that are taken up by local cells to affect cellular behavior. Exosomes were isolated from lung carcinoma using total exosome isolation reagent and quantified. These exosomes were used to treat lung fibroblasts and enrich lung carcinoma cells, and the effects of exosomes on cancerous properties, cell viability and cell migration, were studied. An increase of cell viability was found with exosome treatment for both cell lines while migration only increased for enriched lung carcinoma cells. Additionally, mass spectrometrybased proteomics of exosomes isolated from hepatocellular carcinoma was analyzed. Through a survey of differentially expressed proteins between

high and low grade hepatocellular carcinomas against normal liver cells, several pathways of interest were identified. Some common motifs in underexpressed genes were the regulations of cell signaling, cell metabolism, and cell death.

12B. Extracellular vesicles and their interactions between cell lines

<u>Gracen Hambrick</u>, Dr. Nathan Reyna, Biology, Ouachita Baptist University

Extracellular vesicles play a major role in cell signaling and the deliverance of supplementary materials. Understanding cell signaling has an important role in finding treatments for cancer. The main signaling molecules that are studied are exosomes, however, they may not be the only form of communication utilized by the cell. Using the idea of extracellular vesicles and their role in cancer cell signaling, the extracellular vesicles from A549 Lung Carcinoma cells were extracted by collecting the media nourishing the cells. This media was then applied to HFL1 Lung Fibroblast as well as the A549 cells to identify the changes that these vesicles may produce. Through a range of experiments, they each showed that the extracellular vesicles tended to change the behavior of the A549 and HFL1 cells after treatment, including increased and decreased migration, as well as decreased cell viability.

13A. Establishing a zebrafish colony: considerations for animal husbandry, regulatory guidance, and undergraduate research and coursework

<u>Rebecca Holiman</u>, and Dr. Joshua Kwekel, Biology, Ouachita Baptist University

Zebrafish (Danio Rerio) are a tropical fish that serve as a key comparative model for human health and disease. The anatomical and genetic similarities shared by humans and zebrafish make establishing a fish colony advantageous for undergraduate research and coursework. Laboratory setup took into consideration current best practices, regulatory guidelines, and the evaluation of costs for and

potential obstacles to effective aquaculture. Establishing protocols for the use and care of fish include all aspects of zebrafish lifestyle such as: feeding, breeding, nursery management, water quality, and health monitoring. Operational considerations include number and size of tanks, racks, water filtration systems, cleaning protocols, laboratory layout, records and documentation, and emergency planning. The brine shrimp hatching trials were conducted to optimize efficiency for future feeding protocols. The 24-hour incubation time resulted in a substantially higher observable survivability and displayed a heavier weight of hatched brine shrimp. Possible future research may include investigations of sex-differences in susceptibility to disease and adverse drug effects.

13B. A systematic review on malnutrition assessments and interventions for elderly persons

<u>Cannon Fisher</u>, Jorie Beaumont, and Dr. Detri Brech., Nutrition and Dietetics, Ouachita Baptist University

Background Elderly persons are at significant risk of becoming malnourished. Specific assessment tools that take into account the common difficulties and challenges associated with aging are needed. Nutritional interventions that are successful in treating elderly malnutrition need to be employed in the right circumstances to slow down the increasing rate of malnutrition in the United States (U.S). Objective To systematically review the evidence from intervention and nonintervention studies on current practices for screening for malnutrition and interventions that are applied as well as the outcomes of the malnourished older persons. Methods Four electronic databases were searched (ProQuest, EBSCOhost, PubMed, and JSTOR) for intervention and nonintervention studies published until July 1, 2020. Studies focused on elderly persons with information on screening tools or intervention strategies for malnutrition. Results The literature search resulted in a successful 24 articles that included the research criteria. Of the 24 articles, 16 included interventions, while eight included malnutrition screening geared towards the older

population. The Mini-Nutritional Assessment shortform was identified as a successful screening when implemented with anthropometric measures or lab tests. Interventions that included dietary supplementation for an extended period of time were successful in improving the subjects' health. Conclusions The systematic review resulted in a plethora of data on the malnourished elderly population in the U.S. Many interventions were identified to improve the targeted population's nutritional status. Articles found that pertained to diagnosing malnutrition often used several approaches to diagnosing, including anthropometric measures, interviewing, and lab testing. However, the review includes diagnoses that include only one type of assessment.

14A. Genetic diversity and population structure of Rock Sandpipers (Calidris ptilocnemis) with a focus on a population of conservation concern

<u>Hyland Alfonso</u>, and Christin L. Pruett, Biology, Ouachita Baptist University

Rock Sandpipers (Calidris ptilocnemis) are a species of shorebird only found in the Bering Sea region whose subspecies, C.p. ptilocnemis, is categorized as high conservation status due to small population size and isolation. Rock Sandpipers could lose over half of their habitat in the next decade due to maritime pollution, invasive mammal species, and rising sea levels associated with climate change. The aim of this study is to determine the genetic diversity of two island populations of C. p. ptilocnemis and compare these populations with each other and with Rock Sandpipers found in other locations. This study has implications for conservation since other Bering Sea bird species that breed on islands often have lower genetic diversity than mainland populations and thus less adaptive ability in the face of climate change and habitat loss.

14B. The Study of gasdermin D mutation in cancer research

<u>Gabrielle Roberts,</u> Dr. Yang, and Dr. Wang, Biology, University of Arkansas - Little Rock Gasdermin D (GSDMD) is a protein located on chromosome 8 within humans, and it is an essential protein in the process of pyroptosis, a type of lytic cell death. During pyroptosis, GSDMD is cleaved into two fragments, the N and C fragments, which results in the N fragments coalescing to form a pore in the cellular wall, effectively lysing the cell and releasing its contents. This process means that GSDMD has a plethora of potential uses, such as acting as a plausible cancer treatment, due to its tumor-suppressing nature. Through computational analysis, we have been able to note trends in certain cancers in relation to GSDMD. Therefore, we have worked in the wet lab to start the process of purifying proteins for future study.

15A. Melanoma, Metabolism, and Immunotherapy

<u>Bria Hampton,</u> Analiz Rodriguez, and Megan Reed, Biology, University of Arkansas - Little Rock

Melanoma is a type of skin cancer that emerges when a person's melanocytes have undergone oncogenic mutations. This disease proliferates steadily and has the potential to become life threatening without proper detection and treatment. Currently, the most common forms of treatment include surgical resection, chemotherapy, and ionizing radiation. While research and clinical trials have shown that these therapies can be effective. they are also known for their potential harmful side effects towards the patient. As a result, immunotherapy research in relation to cancer treatment has surged in the last decade. Despite the medicinal breakthroughs that have been achieved when using the immune system to fight cancer, there is still a significant number of patients that do not respond to immunotherapy. Prior research has indicated that a cancer cell's viability is highly dependent on its availability to glucose, as a result of the cell wanting to complete anaerobic glycolysis for proliferation. Additionally, researchers found that the tumor microenvironment is important because without lymphocytes recognizing the cancer cells as 'foreign', the body does not attack. Therefore, we hypothesized that manipulating the tumor microenvironment via glucose availability

and upregulating the major histocompatibility complex (MHC) class I, could lead to an increase in cancer cell detection and killing. The results from multiple assays confirmed our hypothesis that altering nutrient availability alongside overexpression of MHC, allows for an increase in cancer killing.

15B. Investigating the transcriptomic responses in rice roots during interactions with plant growth-promoting bacteria, Burkholderia unamae

John Cook, Qinqing Yang, <u>John Pope</u>, Yasir Rahmatallah, Devyn Ruiz, Jayden Carter, Galina Glazko, and Arijit Mukherjee, Biology, UCA

Major crops such as rice and maize can benefit from associations with different plant growth-promoting bacteria (PGPB). Studies have shown that these PGPB (e.g., Azospirillum, Herbaspirillum, Burkholderia) promote plant growth primarily via nitrogen fixation and phytohormone secretion. However, our current understanding of the underlying molecular mechanisms involved in these associations is limited. For instance, very little is known about the associations between plants and the symbiotic Burkholderia species, B. unamae, at a molecular level. Earlier, we set up an experimental system where PGPB such as Azospirillum brasilense could colonize rice roots and promote plant growth. In this study, we used the same experimental system and showed that B. unamae could promote growth and colonize the roots of rice plants. Next, using RNA sequencing, we identified the transcriptomic responses in rice roots, one day post-inoculation. We identified 1128 differentially expressed genes (DEGs) in rice roots and validated the expression pattern of few genes via RT-PCR. We identified genes involved in the flavonoid biosynthesis pathway, defense, hormone signaling, and photosynthesis to be differentially expressed. We also identified several genes encoding for transcription factors, protein kinases, and transporters in our dataset. Comparison of our dataset to existing RNA-seq datasets in rice roots during interactions with other plant-beneficial Burkholderia species (Burkholderia vietnamiensis,

Paraburkholderia kururiensis, Paraburkholderia phytofirmans) indicated downregulation of defense genes during these interactions. We also identified 398 differentially expressed genes in rice roots during interactions with B. unamae and A. brasilense. Some of these genes are likely to play important roles during these interactions. Overall, our study has identified several promising targets for future genetic studies.

16A. Microstate analysis in parkinson's patients experiencing freezing of gait

<u>Joshua Adams</u>, Dr. Linda Larson-Prior, and Mr. Aaron Kemp, Biomedical Engineering, University of Arkansas

Parkinson's disease (PD) is a progressive nervous system disorder that primarily affects movement, characterized by the presence of bradykinesia in addition to muscular rigidity, postural stability, or tremors at rest. Currently knowledge regarding quantifiable determinates of PD severity is incomplete. Electroencephalogram (EEG) and Behavioral data were collected during a set of behavioral and cognitive task to assess differentiation of individuals displaying different levels of cognitive and motor function. EEG data was quantified, and microstate analysis was performed. Microstates, quasi-stable instances of specific dynamic configurations of the brain, were obtained in an effort to distinguish set differences between patients experiencing PD symptoms with healthy controls. Statistical assessment revealed there to be implications of microstate analysis potential to assess PD presence and condition.

16B. Anti-glioblastoma activity of monensin and its analogues in 3-dimensional cancer model

<u>John Gaydos</u>, Alicja Urbaniaka, Billie Heflin, Megan R. Reed, Adam Huczyński, Analiz Rodriguez, Timothy C. Chambers, Robert L. Eoff, and Angus M. MacNicol, Department of Biochemistry, University of Arkansas

Characterized by extensive vascularization with poor prognosis, glioblastoma multiforme (GBM) is

the most aggressive form of brain tumor in adults. With limited treatment options ranging from surgery, chemotherapy, and radiotherapy, GBM's survival rate is remarkably poor with only 2% of patients living three years or longer post diagnosis. One of the main problems contributing to limited effective treatment options and poor overall survival is the lack of the models of the disease which could reliably recapitulate tumor heterogeneity. Organoids, are 3D, self-organized structures which mimic the endogenous tumor architecture, microenvironment, and cellular interactions, which makes them an improved model for anti-cancer drug discovery. Monensin (MON) is a polyether ionophore antibiotic with antiparasitic, antibacterial, antifungal, antiviral, and anticancer properties. It has been approved by FDA for the use in veterinary medicine as an anti- parasitic agent, but despite its promising activity it has not yet been approved as a therapy for humans. In this work, we investigated the effect of MON and its analogues on GBM organoids. We identified seven analogues characterized by lower IC50 values towards those organoids than parent molecule. All of those compounds induced significant DNA fragmentation after 72 h of treatment. Further studies revealed that MON and its most potent analogue NS-001 induced PARP cleavage and its degradation, increased the expression of the autophagy marker LC3II, and increased the expression of yH2AX, a marker of DNA damage. Additional studies are warranted in order to investigate therapeutic potential of those promising molecules as anti-GBM agents.

17A. Identifying intercalated motifs and targeting MYD88 and associated oncogenic pathways

<u>Mark Alexander Ball,</u> Susie Brown, and Dr. Samantha Kendrick, Biology, University of Arkansas - Little Rock

Diffuse large B-cell lymphoma (DLBCL) is the most common form of Non-Hodgkin's Lymphoma with discouraging disease-free survival rates and an intense treatment program. Overexpression of myeloid differentiation factor 88 (MYD88) is related to harsher prognostic factors like tumor

recurrence and low recovery rates. The MYD88 gene is responsible for triggering the NF- κ B signaling pathway which reduces cell death in lymphoid malignancies and enables proliferation of cancerous cells. DNA secondary structures like the intercalated motif (i-motif) and the guanine-rich (G4)-Quadruplex are associated with gene expression and are studied in conjunction with lymphoma in an effort to target oncogenic pathways and provide therapeutic treatment to patients diagnosed with DLBCL. The overall objective of this project is to investigate the relationship between gene expression of MYD88 and i-motif stability. To achieve this end, a viral model was employed to characterize the environmental and genetic conditions in which a stable i-motif forms. Various experimental techniques like circular dichroism and quantitative polymerase chain reaction (qPCR) were employed to study the relationship of i-motif viability and oncogenic expression.

17B. Population dynamics of hard ticks in Southeastern Arkansas 2020-2021

<u>Ty Say</u>, Taylor Ludwig, Mark Hairston, and Keith Blount, Biology, University of Arkansas -Monticello

Tick populations have increased, and their geographic range is expanding in the United States. At the start of this study in 2020, no other studies that met the definition of active surveillance had been completed in Arkansas for nine years. The lone star tick, Amblyomma americanum, was the most abundant species collected with a total of 1796 ticks collected. Additional species observed were A. maculatum (67 ticks), Dermacentor variabilis (127 ticks), and Ixodes scapularis (188 ticks). In this study, we examined the prevalence of tick populations in southeast Arkansas over a period of 14 months. More research is needed to assess the populations in southeast Arkansas and well as surrounding areas

18A. Energy content of seeds of Palmer's pigweed (Amaranthus palmeri) in the diet of

scaled quail (Callipepla squamata) in Southeastern New Mexico

<u>Faith Johnson</u>, John L. Hunt, Matthew E. Grilliot, Troy L. Best, Isaac C. Castillo, Paige E. Eddington, Faith A. Johnson, Tyneshia L. Kilgore, and Jacob H. Courson, Mathematics and Natural Sciences, University of Arkansas - Monticello

Palmer's pigweed (Amaranthus palmeri) is a common grassland plant that occurs across much of North America. It is often considered a weed but is an important source of food for many game birds. We analyzed the energy content of seeds of Palmer's pigweed obtained from the crops of scaled quail (Callipepla squamata) collected from plainsmesa sand-scrub habitat in Eddy and Lea counties, New Mexico. Seeds were dried for 48 hours at 60 degrees Celsius to remove moisture and then analyzed for gross caloric value (i.e., energy content) in an oxygen bomb calorimeter. energy content of seeds of Palmer's pigweed from New Mexico averaged 16.6 J/kg (4.0 kcal/g), and was among the lowest values obtained when compared to those of many seeds previously reported from the diet of scaled quail and other granivorous birds.

18B. Role of differentially expressed genes involved in suppression of tumorigenesis by CREB3L1 in breast cancer.

<u>Syan Tyler</u>, Heaven Mister, Biology, University of Arkansas - Pine Bluff

Role of differentially expressed genes involved in suppression of tumorigenesis by CREB3L1 in breast cancer. Syan Tyler and Heaven Mister Department of Biology, University of Arkansas at Pine Bluff Abstract Breast cancer is the most frequently diagnosed cancer in women globally. Although metastatic breast cancer accounts for a small percentage of initial diagnosis, the overall survival rate of these patients is low. CREB3L1 (cyclic AMP [cAMP]-responsive element-binding protein 3-like protein 1), a member of the unfolded protein response (UPR) plays an important role in breast cancer development and metastasis. CREB3L1 acts as a suppressor of metastasis by

regulating expression of genes involved in cell growth, angiogenesis, and migration in breast cancer. The elucidation of the role of differentially expressed genes and major pathways involved in the CREB3L1 related suppression of metastatic breast cancer is of much importance. Differential gene expression (DEG) analysis was performed on a CREB3L1 associated gene expression dataset using statistical software R. Gene Ontology enrichment analysis and pathway analysis were performed to identify pathways in which the DEGs were significantly enriched. Finally, gene modules were explored for their biological significance. The role of the significantly differentially expressed genes in major pathways identified will facilitate understanding of molecular mechanisms and to conduct functional studies.

19A. Dictyostelium discoideum as a host microbe model for screening quinazolinonebased drugs for anti-virulence properties

<u>Danielle Randolph</u>, Sandhya Baviskar, Sayo Fakayode, Souvik Banerjee, Jeff Shaver, Roger Lightner, Zane Neal, Josh T, Harmeet Chohan, Kairy Galvez, Chemistry, University of Arkansas -Fort Smith

Antibiotic resistance is one of the biggest threats to our health as it reduces our ability to treat infectious diseases. Many of the available antibiotics are ineffective because they target few bacterial processes such as protein synthesis and cell membrane functions. Thus, there is a need for searching anti-virulence drugs that do not kill the host and bacterial pathogen, but disrupt the production of virulence factors that damage the host. Recently, Dictyostelium has been used as a biomedical model for studying the targets and mechanisms of action of known and novel drugs. Dictyostelium is a bactivorous, soil-dwelling amoeba, and its growth and development is affected by pathogenic microorganisms. The Dictyostelium host-microbe model system is suitable for preliminary screening of anti-virulence agents because it is simple, reproducible, robust, and easy to manipulate compared to many non-mammalian and mammalian models. To characterize the effects

of Quinazolinone-based drugs, we will use cell proliferation and starvation induced-assays and to evaluate the anti-virulence properties, Dictyostelium developmental virulence and antivirulence assays will be used. The results of this study can be further validated in mammalian models.

19B. Testing of quinazolinone-based drug candidates as treatments for antibiotic resistant bacterial infections

<u>Kairy Galvez</u>, Sandhya Baviskar, Roger Lightner, Jeff Shaver, Biology, University of Arkansas - Fort Smith

Quinazolinone-based scaffolds have been studied as potential treatments of resistant bacteria. Most antibiotic resistant bacterial infections are attributed to ESKAPE bacteria, including Enterococcus faecium, Staphylococcus aureus, Klebsiella pneumoniae, Acetinobacter baumanii, Pseudomonas aeruginosa, and Enterobacteriaceae species. The goal is to design, synthesize and evaluate the efficacy of 2,3-disubstitued-quinazolinone (DSQZNE) based drugs targeting pathogenic bacteria with Dictyostelium discoideum, a grounddwelling amoeba that feeds on bacteria, used as a model eukaryotic host. To determine the antibacterial properties of each drug candidate, we utilize traditional disk diffusion assay and minimum inhibitory concentration (MIC) determination tests. The lowest concentration of the drug candidate that inhibits the growth of the bacterium is the MIC. Test results are utilized to determine which drug candidates exhibit antimicrobial properties against safe standard (Staphylococcus epidermidis, Escherichia coli, and Pseudomonas aeruginosa) and pathogenic bacteria (Methicillin-resistant S. aureus (MRSA) and P. aeruginosa). Promising antimicrobial drug candidates are advanced to pathogen-Dictyostelium system testing.

20A. Investigate the molecular mechanisms by which plant growth-promoting bacteria, Azospirillum brasilense, mediate salt stress tolerance in rice.

Zachariah Degon, John Pope, John Cook, and Arijit Mukherjee, Biology, University of Central Arkansas

Abiotic factors (e.g., salt stress, heat and drought stress, nutrient deficiency) are major concerns for crop productivity. For instance, most food crops, such as rice and maize, display severe yield losses (50-80%) under moderate to extreme salinity. Problems associated with soil salinity are anticipated to worsen because of adverse climatic conditions. For improving crop performance under saline conditions, it is necessary to implement sustainable agricultural strategies. One option is to take advantage of beneficial plant-microbe associations. Plants can form associations with different beneficial microbes including, arbuscular mycorrhiza, rhizobia bacteria, plant growthpromoting bacteria (PGPB). Several studies have suggested that PGPB improve plant growth via multiple mechanisms, including biological nitrogen fixation, hormone synthesis, protection against biotic and abiotic stresses, etc. Azospirillum brasilense is one of the most studied PGPB to mitigate salinity stress in different crops such as maize and wheat. However, not much is known about the molecular mechanisms by which A. brasilense mitigates salt stress. Recently, we optimized an experimental system where rice growth was improved in A. brasilense-inoculated plants compared to the uninoculated plants when these were grown under high salt concentration (200 mM NaCl). Using plate count assays, we determined that colonization of rice roots by A. brasilense under high salt concentration was not affected at this time point (7 days post-inoculation). Currently, we are investigating the expression pattern of a few salt-sensitive reporter genes in rice plants inoculated with or without A. brasilense and grown under high salt concentration. In the future, we will perform an RNA-seq experiment to identify the transcriptomic responses in rice plants during A. brasilense-mediated salt stress tolerance. Overall, the results from this project will provide important insights into salt stress mitigation in rice by A. brasilense.

20B. Microbiome analysis of cactophilic drosophila arizonae

<u>Thomas B. Crook</u> and Tamara S. Haselkorn, Department of Biology, University of Central Arkansas

The microbiome, or the total sum of microorganisms residing within a host, drastically increases the metabolic capabilities of organisms by contributing to the total amount of expressed genes. Furthermore, this complex symbiotic relationship affects much more than metabolic pathways, and manipulations of the gut microbiome of mice have been shown to affect development, immune functions, nutrition processes, and the organism's susceptibility to disease. A better understanding of these interactions between microbiomes and their host is crucial in treating many diseases like diabetes and autoimmune disorder brought on by unfavorable diets and excessive use of antibiotics interacting with the microbiome. Drosophilids, or common fruit flies, have quickly become one of the most popular model organisms in the studies examining the relationship between microbiomes and their host because of their wide range of ecological niches and their relatively simple and short life cycles. For example, the life cycles of cactophilic species of Drosophila depend entirely on different species of cactus for shelter and the nutrition, although these cactus rots do also contain toxins. While many organisms could have great difficulties digesting the toxins produced by cactus plants, it is suspected the microbiome of these hosts enables the Drosophilids to exploit the cactus as their primary food source. Through the combination of DNA extractions using the DNeasy Blood and Tissue kit and next-generation sequencing, we extract and sequence the microbiomes of five different Drosophila species. The microbiome composition will be identified using bioinformatics and the giime2 pipeline, quantifying and identifying species through a reference database. If our hypothesis is supported, the microbiomes of cactophilic Drosophilids will be primarily comprised of bacterial species different from other non-cactophilic Drosophlid species, suggesting that the microbiome plays a role in enabling them to digest the cactus' toxic tissues.

21A. Evidence of coevolution in the phylogenies of chlamydiae bacteria and social amoebae

<u>Hailee Gerner</u>, Terry Uhm, Mackenzie Hoogshagen, James DuBose, and Tamara S. Haselkorn, Department of Biology, University of Central Arkansas

Symbiosis is a range of interactions between two organisms that can span from pathogenic to mutualistic depending on many factors including the length of time of the interaction and the environment. Amoebae are good organisms to use when researching bacterial symbiosis because they consume bacteria through phagocytosis and add pressure for the bacteria to evolve to avoid digestion. Certain bacteria in the phylum Chlamydiae have been found to be symbionts in D. discoideum and other species of amoebae. While Chlamydiae bacteria are mostly considered pathogens, the role of Chlamydiae in amoebae is currently unknown, and mutualistic interactions have been observed in some species. Recently Chlamydiae bacteria have been found to be highly prevalent in natural populations of D. discoideum and other species of social amoeba. The D. discoideum Chlamydiae endosymbionts are novel bacterial lineages and they do not seem to have any fitness costs when measured in the lab. Preliminary DNA sequencing has shown several different Chlamydiae lineages infect different species of social amoeba. I hypothesize that if Chlamydiae bacteria have a mutualistic relationship with social amoebae then there will be evidence of coevolution in the phylogenies of the Chlamydiae bacteria and the social amoeba. We are in the process of sequencing full length 16rRNA genes for the Chlamydiae bacteria from six different social amoeba species to reconstruct a robust phylogeny and look for evidence of coevolution that might suggest a mutualistic relationship.

21B. The hidden diversity of social amoebae in Arkansas

<u>Kira Gibbs</u>, and Tamara S. Haselkorn, Department of Biology, University of Central Arkansas

Terrestrial, soil dwelling protozoans, particularly amoebae, play a key role in primary production and contribute to decomposition, mineralization, and have a significant role in nutrient cycling transferring nutrients to higher order consumers in the soil food web; this is an important link connecting subterranean ecological components to those above ground. While some amoebae have been observed and studied in laboratory conditions, soil amoebae are still largely understudied, particularly in their natural habitat. The soil microbiome is one of the most diverse ecosystems with a broad and variable array of soil microorganisms; and the full extent of amoebae diversity is currently unknown. It is estimated that 70% on species are missed due to under-sampling. Sampling microbial eukaryotes is challenging given their microscopic nature and inability of many to be cultured in the lab. Furthermore, only a small proportion of microbes can be seen at any point in time due to optimal conditions varying throughout a year that impact activity. We are using newly developed molecular methods to PCR amplify social amoeba DNA directly from soil samples. Thus far we have sampled 10 sites in Woolly Hollow State Park and have completed DNA extractions. We have also PCR amplified and cloned the social amoebae 18S rRNA genes, identifying amoeba species using NCBI Blast. We are currently comparing these molecular identification methods to traditional morphological methods and assessing how amoeba diversity varies by season and microhabitat. This study will shed light on the variability of this important group of soil-dwelling microorganisms and the ecological factors that affect them.

22A. Prevalence of burkholderia and chlamydiae bacterial symbionts in natural populations of social amoeba

<u>Bailey Skinner</u>, Jordan Bowen, Phong Nguyen, Britteny Berumen, Erin Golden, and Tamara S. Haselkorn, Department of Biology, University of Central Arkansas

As single-celled eukaryotes that feed on bacteria in nature, amoebae are thought be evolutionary

training grounds for bacteria to develop an intracellular lifestyle. If bacteria can evolve to evade the phagocytic digestion of amoebae, then they can potentially survive in other hosts, evading digestion of the macrophage cells of the immune system and becoming important pathogenic or mutualistic symbionts. Thus, it is important to identify the bacterial symbionts of natural populations of amoebae. Social amoebae are particularly useful for this endeavor, as they go through a social lifecycle. This consists of thousands of single cells aggregating together to ultimately form a fruiting body consisting of a stalk with a ball of spores on top. This fruiting body can easily be screened for bacterial symbionts. To do this we collected soil samples from 18 locations throughout Arkansas and neighboring states. Samples were plated and fruiting bodies of 10 different amoebae species were collected for DNA extraction, PCR, and sequencing. Amoeba-specific primers were used to confirm amoeba species identity. Burkholderia and Chlamydiae specific primers were used to identify the presence of particular bacterial genera that have previously been found in other amoeba species. These PCR products were sequenced for additional identification of bacterial species. Preliminary data shows an infection rate of over 75% throughout all locations that were screened for Burkholderia and Chlamydiae. Both Burkholderia and Chlamydiae were found to infect multiple species of social amoebae. In these other species we have found the farming symbiont B. agricolaris, as well as other Burkholderia species: B. phenazium, B. arboris, and B. caledonica. We also found 27 different Chlamydiae haplotypes. The widespread prevalence of Burkholderia and Chlamydiae suggests that these bacteria play an important role in the ecology of many social amoebae. Further research into this topic can reveal how these symbionts are able to effectively form this relationship and what the effects are of these other symbiont species are on their amoeba hosts.

22B. The Effects of Time of Year and Microhabitat on the Prevalence of Bacterial Symbionts in Social Amoebas

<u>Alexis Villalobos</u>, Kira Gibbs, and Tamara S. Haselkorn, Department of Biology, University of Central Arkansas

The social amoeba Dictyostelium discoideum is a common model organism to use for a variety of reasons including studying eukaryotic host cell interactions with bacteria. The D. discoideum social amoeba is unique in that it has a unicellular and multicellular stage. When bacterial food becomes scarce in the amoeba's environment, the amoebas congregate together to form a slug that allows migration to the surface of the soil, where it forms a fruiting body. Not all bacteria are digested, though, and D. discoideum is known for forming mutualistic relationships with bacteria in the genus Paraburkholderia, which allows for the amoebas to farm. The farming ability allows for D. discoideum to incorporate edible bacteria into their fruiting bodies, which the spores carry to new sites. In addition to Paraburkholderia, bacteria in the phylum Chlamydiae have also been found in D. discoideum and other social amoeba species, although the function of these bacteria is currently unknown. For my research I am measuring the effects of time of year and microhabitats on the prevalence of bacterial symbionts within populations of different species of amoebas. The goal is to understand what drives the distribution of Paraburkholderia and Chlamydiae symbionts in natural populations of social amoeba species. We are sampling three different microhabitats at different times of year and plating the soil samples to allow for amoeba fruiting body formation. We then have been extracting the DNA from the fruiting bodies and are using PCR with bacteria-specific primers to screen for our symbionts and determine prevalence. Our null hypothesis is that the prevalence of the bacterial symbionts will be consistent across different times of year and microhabitats. Deviations from this may suggest circumstances in which the symbionts are beneficial or detrimental. If prevalence varies significantly from the time of year the samples are collected, this could indicate that the relationship between the bacterial symbiont and amoeba is temperature dependent and can alter which symbionts we see in different amoeba populations. Varying prevalence in different amoeba species

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may suggest host-specific benefits to those hosts with high symbiont prevalence.

23A. H2AX in the DNA damage response

<u>Ganell Jones</u>, Jessica Kelliher, and Justin Leung, Department of Biology, University of Central Arkansas

Double strand breaks (DSBs) caused by ionizing radiation can result in chromosomal translocations, loss of genomic information, and tumorigenesis. DNA damage repair (DDR) pathways such as homologous recombination (HR) and nonhomologous end-joining (NHEJ) function to repair DSBs. The phosphorylation of Serine 139 on H2AX, a histone variant of H2A, signals the initiation of the NHEJ pathway. Conservation along the c-terminal of H2AX throughout evolution suggests that other amino acids along the c-terminal may also be significant. This report investigates the contribution of c-terminal amino acids to the recruitment of DDR-associated protein 53BP1.

23B. Slower eye movements to incongruent targets may underlie the size congruity effect in digit perception.

<u>Nickolas Paternoster</u>, Emily Andrews, Julia Williams, Taylor Dague, Amrita Puri, and Ken Sobel, Computer Science, University of Central Arkansas

The size congruity effect occurs in tasks in which digits are either congruent or incongruent regarding numerical size (a semantic feature) and physical size (a perceptual feature). For example, participants are slower to identify a physically large target digit as numerically small (incongruent; e.g., a physically large "2") compared to when it is physically small (congruent), and vice versa. Although this phenomenon is well established, the stage of processing at which the conflict between semantic and perceptual information occurs is still unclear. Participants searched for either a numerically large or small digit (regardless of physical size) and reported its location within an array of digits (left or right). Participants' eye

movements were recorded to gain insight into their attentional shifts. We hypothesized that if the interaction between semantic and perceptual information occurs at an early stage, the time until the first fixation (TFF) on incongruent targets may be longer than for congruent targets, as participants may experience interference immediately upon viewing the display, prior to attending to the target. Alternatively, if the two types of information interact only later, at a decision stage, we predict similar TFF across conditions, but longer total duration and/or number of fixations on incongruent targets. We found that TFF was significantly longer for incongruent targets, suggesting early interaction. Furthermore, these differences between the TFF for incongruent compared to congruent targets were positively correlated with differences in the time to respond between conditions. To test whether participants' attention was captured by distractors in the incongruent condition, we next examined eye movements to distractors. However, TFF on distractors was also longer for incongruent compared to congruent trials, suggesting otherwise. Instead, the number and duration of fixations to distractors, which were also longer for incongruent trials, may account for the delay in TFF to targets.

2<u>4</u>A. Using liquid chromatography mass spectrometry for metabolic profiling and analysis of lung cancer tumor cells.

<u>Amy Tran</u>, Gunnar Boysen, and Azemat Jamshidi-Parsian, Biology, University of Central Arkansas

Glutamine is the most abundant amino acid in the body and facilitates as an energy source for cells, tissues, and organs. In previous studies, lung tumors have shown to consume excessive amounts of glutamine, to make, and excrete glutathione. Glutathione is an important antioxidant that increases the cellular defense, making lung cancer cells more resistant to radiation and chemotherapy. With a glutamine inhibitor called CB839, the production of glutathione has shown to decrease in tumor cell lines, in tumor tissues, and in clinical tumor specimen studies. The relative viability and ability to form colonies can be measured using established CCK8 and clonogenic assays. To determine tumor specificity of CB839, the effects in LLC cells (mice lung tumor cells) are compared to the effects in NRK cells (normal epithelial rat kidney cells). In addition, to elucidate the molecular mechanism of CB838-induced cytotoxicity, we apply LC/MS/MS to monitor potential metabolic reprogramming. The data suggest dose dependency due to cytotoxicity by CB839 in LLC cells, but not in NRK cells. Metabolomics shows major CB839 induced changes in the relative culture media concentrations of several metabolites, including most of the amino acids, in LLC cells but not in NRK cells. The metabolic alterations suggest reduced consumption of glutamine and other amino acids due to inhibition of glutaminase by CB839.

Poster Abstracts Chemistry

101A. Optimization of Single-pot, Solid-phase Sample-preparation (SP3) for use in the National Resource for Quantitative Proteomics

<u>Audrey Lawrence</u>, Humphrey Wanjala, Rick Edmondson, and Dennis Province, Chemistry, Harding University

Proteomics is a field that studies the abundance and types of proteins. In the realm of the National Resource for Quantitative Proteomics, these cells often come from clinical trials and must be lysed, usually with deter-gents, to extract the proteins before they can be analyzed. Single-pot, solid-phase sample-preparation (SP3) is a lysate digestion method developed to remove detergents from protein samples while breaking samples into peptides for proteomic analysis via LC-MS. Detergents used for cell lysis clog columns and limit the speed and efficacy of the mass spectrometer. The SP3 method uses magnetic beads with a carboxylate coat-ing that binds to the proteins in a sample, allowing for effective detergent removal. This method also works at low protein concentrations and with shorter digestion and incubation times, allowing for higher sample throughput. The goal is to get the same level of depth with small amounts/time in the LC-MS and a broad-ened research scope through a larger possible number of samples. By modifying digestive enzyme amounts and digestive conditions, the protocol was successfully optimized down to $10 \ \mu g$ of protein with a three-hour digestion time, with future work focusing on the automation of the process.

101B. Determination of ascorbic acid produced in Martian regolith

<u>Darby Mohon</u>, and Rebekah Rampey, Department of Chemistry and Biochemistry, Harding University

The National Aeronautics and Space Administration plans to go to Mars in the 2030s. To have sustained life on another planet, nutritional supplements that can be produced in plants grown in Martian regolith must be found. Initial research indicated that the Oxalis genus of plants have been reported to have high concentrations of Vitamins C and E. However, Thymus vulgaris (thyme) prevailed as a safer alternative for ascorbic acid. Deep space voyages to Mars will require a two year commitment from astronauts to travel, work and return back to earth. Medicinally-important plants like thyme might be the key to sustaining humans both physically and emotionally during this time as they provide both nutrients and greenery. While confirming the quantity of vitamins in this plant group via the polymolybdate and Folin phenol reagent methods, these data showed the effectiveness of growth in Martian regolith when compared to traditional Earth soils. Thyme was determined to be viable in Martian regolith. Ascorbic acid standards were established in these methods. Estimated daily requirements of Vitamin C (Ascorbic Acid) are 1000 mg, according to the American Drug Association. This means that these plants could potentially provide the daily vitamin content that astronauts on Mars need for their diet.

102A. Computational drug design to target the cannabinoid type 2 receptor to develop safe and effective pain medication

<u>Theresa Thomas</u>, and Caitlin Scott, Chemistry, Hendrix College The cannabinoid system, a biological network involved in regulating physiological and cognitive processes, consists of the Cannabinoid Type 1 Receptor (CB1) located in the central nervous system and the Cannabinoid Type 2 Receptor (CB2) located within the immune system. Activation of both these receptors mediates pain, however, CB1 is associated with physiological side effects, like addiction from opioids. The CB2 receptor plays a vital role in the regulation of immune responses, inflammation, pain, and other metabolic processes, and agonist targeting this receptor have been proposed as treatments for these conditions, however, there are currently no drugs on the market that targets the CB2 receptor. This research aims to develop a drug that relieves pain without the adverse side effects of opioids, more specifically, a drug that selectively targets the CB2 receptor. This research was conducted computationally through Schrodinger to stabilize the CB2 ligands. We first used LigPrep to prepare the crystallized structure of the ligand to edit for further simulations. To calculate the partial charges using quantum mechanics of each ligand, we performed Jaguar and then Superimposition to compare the crystal structure and experimental structure of each ligand. Finally, to obtain an empirical score that approximates the ligand binding free energy, we used GlideScore to dock the ligands into the CB2 receptor. My simulations indicate that the Ki values and binding scores from docking and the experimental ligands correlated with the crystallized structures. These findings indicate further development in a more selective drug design, bring new hope for the therapeutic potential of CB2 and a greater understanding of the endocannabinoid system.

102B. Elucidation of the regiochemistry of daphnegiratriprenylone A by quantum chemical calculations

<u>Lara Kockaya</u>, Pankaj Pandey, Lingzhi Li, Mark T. Hamann, and Robert J. Doerksen, Chemistry and Biochemistry, Henderson State University

Natural products have been used for medicinal purposes for centuries, and newly isolated

compounds open up the possibility of alternative treatment methods for medical issues. Here, we report our findings on the correct regioisomer of Daphnegiratriprenvlone A, a triprenvlated flavonoid isolated from Daphne giraldii Nitsche, a promising new drug for treating cancers caused by mutations occurring in fibroblast growth factor receptor 1 (FGFR1). Mutations affecting FGFR1 give rise to several types of human cancers, such as lung, breast, prostate, ovarian, and liver cancer. To confirm the structural assignment of Daphnegiratriprenylone A, four possible regioisomers were subjected to thorough conformational searches, and further geometry optimizations were performed utilizing DFT calculations. Theoretical isotropic shielding tensors (NMR chemical shifts) were obtained using the PW1PW91/6-311+G(d,p) method in DMSO. Finally, we compared the calculated NMR shifts to the experimental NMR shifts of Daphnegiratriprenylone A using DP4+ probability analysis and other statistical parameters. We found that the 2',5'-diprenyl-B-ring regioisomer (Daphnegiratriprenylone A) was closest to the experimental data with 100% DP4+ probability (considering both 1H and 13C shifts). These results demonstrate the utility of applying the DP4+ method for assigning the correct regioisomer of natural products.

103A. Using computational methods to calculate the stability of the CB1 receptor's structure to design a positive allosteric modulator

<u>Emma Chavez</u>, Dr. Caitlin Scott, and Erin R. Borst, Biochemistry, Hendrix College

The cannabinoid CB1 receptor, a target for drug design, is activated when it binds to an endocannabinoid, leading to down-field signaling which causes physiological responses such as pain relief. CBD oil and medical marijuana are currently used to treat pain but cause undesirable psychoactive affects. Positive allosteric modulators modify the duration and location of the agonist's effect within the body by binding to a distinct site than the agonist does, which make PAMs attractive to drug design. There is no FDA-approved drug that

yet target the CB1 receptor. The goal of this research is to use molecular dynamics and computational chemistry to monitor the CB1 receptor's structure. When we obtain a stable structure of the CB1 receptor, we will design a CB1-targeted PAM that does not cause adverse side effects. To calculate the CB1 receptor's stability and structure we performed 100ns molecular dynamic simulations using AMBER software of the CB1 receptor bound to agonist AM841 in a physiological environment. CHARMM-GUI, a web-based server, was used to generate the physiological environment consisting of POPC lipids, TIP3P water molecules, 0.15 M NaCl and protonated residues. Our simulations indicate a stable structure of the activated CB1 receptor that we will use to dock known compounds using Phase and Glide software. We performed principal component analysis, PCA, to compare the experimental structures of the Cannabinoid Receptor 1 and Cannabinoid Receptor 2. We hypothesize that principal component 3 will distinguish when the protein is activated and can bind to the Gi protein. With a stable confirmation of the CB1 receptor, we can continue to research and design a PAM that is based on the activated confirmation of our protein. Positive allosteric modulators enhance the effect resulting from the biding of the orthosteric ligand. Design of a positive allosteric ligand that binds to the CB1 receptor can lead to the physiological response of pain relief without adverse side effects.

103B. Virtual ligand screening and docking to identify possible antagonists to be used as antidepressants that target the kappa opioid receptor

<u>Emily Pickering</u>, Graham T Anderson, and Dr. Caitlin Scott., Biochemistry and Molecular Biology, Hendrix College

G-protein coupled receptors (GPCRs) are a family of membrane proteins activated by various stimuli that are targeted by a large number of drugs currently on the market. The kappa opioid receptor is a type of GPCR that when activated by an agonist can lead to depression. Current antidepressants have numerous flaws such as varying effects among users, long incubation periods, and unpredictable side-effects. Research suggests that the binding of an antagonist to the receptor stabilizes its inactive structure causing antidepressant-like effects. The goal of this project is to design a drug antagonist that strongly binds to the kappa opioid receptor which can be developed into an antidepressant. Previous work was done using Schrodinger software Protein Prep Wizard and 100 ns molecular dynamics with Desmond software to create a stable model of the kappa opioid receptor bound to the antagonist JDTic. Using the computer software Glide, we docked 15 antagonists to the model that were prepared using LigPrep to generate minimized 3D structures of the ligands and Jaguar to determine the Mulliken charges of the ligands. Docking ligands structurally similar to the crystal ligand JDTic validated our model of the kappa opioid receptor and indicated that ligands in the binding site interact with the residue D138. Ligands docked that differed from JDTic also interacted with D138; so, drugs designed to strongly bind to the kappa opioid receptor should also bind to D138. Glide's energy score predicted ligand conformations that had the best agreement with the crystallized JDTic conformation in the binding site. We found a positive correlation between experimentally determined binding affinity and the computational docking score. Using the best docked poses of each of the 15 ligands, we created pharmacophores with Phase software and ran pharmacophore-based ligand screening. We also ran structure-based ligand screening using the webserver MTIOpenSource. With these two screening methods, we were able to find two possible drug candidates that were not originally designed to interact with the kappa opioid receptor and have never been tested on the kappa opioid receptor. Docking these ligands to our model of the kappa opioid receptor resulted in favorable docking scores. Thus, we have made progress in the creation of an antidepressant that interacts with the kappa opioid receptor, a protein different from what current medicines on the market target.

104A. S100A1 protein and its interaction with antagonist drugs

<u>Megan Pelley</u>, and Caitlin Scott, Chemistry, Hendrix College

S100A1 is a protein that undergoes a large conformational change when it binds to calcium, which allows S100A1 to interact with many targets such as neurotransmitters, cytoskeletal and filament-associated proteins, transcription factors and their regulators, enzymes, and other calciumactivated proteins. S100A1 modulates muscle contraction and relaxation, which is important for cardiac function. The goal of this research is to understand how the S100A1 protein interacts with the antagonist-drugs olopatadine, cromolyn, pentamidine, amlexanox, fluphenazine, and propranolol because studies have shown that a decrease in the S100A1 protein in the heart contributes to beneficial effects of cardiac function. These drugs are specifically chosen for this project, because they block the activation of the S100A1 protein. We want to visualize the binding site of these antagonists with S100A1, because that will provide insight into the design of therapeutics to prevent certain heart diseases. First, to verify that the experimental NMR structures are stable conformations, we performed 100 ns molecular dynamics on the solvated and neutralized inactive and activated S100A1 proteins (PDB ID: 2L0P and PDB ID: 2LP3, respectively) using AMBER software. We then docked the known drugs to our structures using Glide software. From previous biochemical experiments concerning the S100A1 protein and the ryanodine receptor, we can confer that my compounds, specifically cromolyn and pentamidine, bind to the same site as the ryanodine receptor. Therefore, these drugs would inhibit the physiological responses of the activation of the S100A1 protein. In the future, we will develop a pharmacophore that will enable the discovery of compounds and will be possible candidates for further development into medication. These therapeutics will be beneficial in treating a multitude of different diseases, such as diabetes mellitus, heart failure, and several types of cancer.

104B. Building a flexible electrochemical microscope

<u>Nicholas Jones</u>, Dr. Martin Edwards, College of Engineering and Science, Louisiana Tech University

Building a Flexible Electrochemical Microscope Nicholas Jones 1.2 and Martin Edwards 1 1. Department of Chemistry and Biochemistry, University of Arkansas, Fayetteville, AR 2. College of Engineering and Science, Louisiana Tech University, Ruston, LA Electrochemical measurements quantify how materials exchange electrons and ions. This information is important to understanding the functioning of materials that make up batteries, fuel cells, electrochemical sensors, electrodes for electrochemical synthesis, etc. and for understanding electrochemical processes, such as corrosion. Electrode surfaces are never uniform. Nanoscale features, such as materials defects, nanoparticles, inclusions, and grain boundaries contribute to the electrochemical behavior of an electrode. Conventional electrochemical measurements electrically characterize entire electrodes, which are typically mm to cm in size. In these macro-electrochemical measurements, the current is the sum response of the entire surface, obscuring local variability. By measuring on the nanoscale, we can evaluate how different surface structures, influence electrochemical properties. To perform such measurements, we built an electrochemical microscope. Our electrochemical microscope uses pipettes with tips that have a diameter of ~100 nm to measure electrochemical behavior with nanoscale resolution. These pipettes contain an electrode that is immersed in an electrolyte which forms a meniscus at the tip of the pipette. When this meniscus is touched to the surface of the sample, it completes a circuit and measurements are made only in the area where the meniscus contacts the surface, a region which is about the size of the pipette tip. The microscope was designed to be modular, which allows components to be easily modified or replaced to allow for the usage of probes and pipettes and thus a large range of measurements with a single instrument. The flexibility of the microscope makes it suitable for measuring a large variety of samples in reduced the time. We developed a parts list based on

specifications and designed custom parts to integrate the different components into a modular and flexible microscope with nanoscale resolution. We shared our electrochemical microscope as open source to encourage adoption of nanoscale electrochemical analysis using flexible and modular base. This microscope assists in minimizing time to setup, costs, and learning of a new instrument, which removes significant barriers in the study of nanoscale electrochemical properties. Understanding the electrochemical performance at the nanoscale could ultimately lead to the designing of better electrochemical materials (e.g., for batteries, fuel cells).

105A. Simple Click Chemistry on Complex Rifamycin Core Leads to Novel Antimicrobials

Jake Smith, Dailyn Crain, Hattie Milligan, Daniel Armstrong, Marissa Fullerton, Amanda Dragan, Daniel E. Voth, and Irosha N. Nawarathne, Chemistry Department, Lyon College

Simple Click Chemistry on Complex Rifamycin Core Leads to Novel Antimicrobials Jake Smith1, Dailyn Crain1, Hattie Milligan1, Daniel Armstrong1, Marissa Fullerton2, Amanda Dragan2, Daniel E. Voth2, Irosha N. Nawarathne1 1Division of Mathematics and Sciences, Lyon College, Batesville, AR, United States. 3Department of Microbiology & Immunology, University of Arkansas for Medical Sciences, Little Rock, AR, United States. In 1999, the World Health Organization estimated that one-third of the world's population had latent tuberculosis (TB) infection. Recently, this has been updated to one-fourth of the world. The worrisome connection between COVID-19 and latent TB is that contraction of coronavirus by someone with latent TB could activate the Mycobacterium tuberculosis (MTB), the opportunistic pathogen (bacterium) causing TB, making the individual severely ill or potentially dead and also a transmitter of both diseases to others. Consequently, coronavirus indirectly helps in spreading TB faster while also continuing to slow global progress against TB due to health disruptions. While an estimated 60 million lives were saved through TB diagnosis and treatment

between 2000 and 2019, the multidrug-resistant TB (MDR-TB) is increasingly becoming a public health threat in the midst of the pandemic. Rifamycins, particularly rifampicin, are a mainstay of TB treatment since 1960's; they bind to the β subunit of MTB RNA polymerase (RNAP) and block RNA synthesis. Also, they become futile in TB therapy when MTB RNAP mutations disrupt various key interactions between the drug and the target. By taking advantage of the 'enabling reaction' of the rifamycin core and coupling it with simple click chemistry, we have exploited the broadly-used and thoroughly-studied rifamycin scaffold to target MDR-TB and potentially treat other notorious bacterial infections. Our work highlights the first report of the synthesis, isolation-purification, and biological significance of rifamycin derivatives with azido, alkyne, and triazole functionalities, the innovative products of coupling between complex rifamycin chemistry and simple click chemistry. This project was supported by the Arkansas INBRE program, with a grant from the National Institute of General Medical Sciences, (NIGMS), P20 GM103429 from the National Institutes of Health.

105B. Optimization & synthesis propargylic ethers for use in the synthesis of metabotropic glutamate receptor antagonists

<u>Asa Borup</u>, Dr. James Donelson, and Dr. Lynell Gilbert-Saunders, Chemistry, Missouri Southern State University

Recent studies have found elevated concentrations of glutamate, an excitatory neurotransmitter, in the blood and certain regions of the brain of those affected with autism spectrum disorders (ASD). It is theorized that hyper-glutamate concentrations in specific regions of the brain could potentially contribute to some ASD. Therefore, inhibition of the glutamate receptor is a potential mechanism for treating ASD, though there are currently no glutamate receptor antagonists approved for the treatment of ASD. A series of potential allosteric antagonists of the metabotropic glutamate receptor 5 (mGluR5) has been designed. The synthesis of these inhibitors involve the [3+2] cycloaddition of a aryl-substituted benzyl azides and aryl-substituted propargylic ethers. 4-bromophenol was used as the preliminary substrate for the synthesis of the first propargylic ether. Using a microwave reactor, a variety of reaction conditions were attempted in order to optimize the synthesis. Reaction progress was monitored using gas chromatography. Using a solution of tert-butoxide in tert-butanol led to complete reaction of the starting reactants and produced 1-bromo-4-(prop-2-yn-1-yloxy)benzene. Using these optimized conditions, the synthesis of a small library of substituted aryl propargyl ethers is reported.

106A. Microwave-assisted synthesis of 4aryloxymethyl-1-arylmethyltriazoles as potential glutamate receptor antagonists

<u>Mary Schad</u>, and Dr. James Donelson, Chemistry, Missouri Southern State University

It is well known that glutamate is the major excitatory neurotransmitter in the brain and plays a vital role in basic functioning. Elevated glutamate levels have been observed in individuals with autism spectrum disorders (ASD) and these elevated levels are theorized to be one of the etiologies for ASD. With this in mind, interest has fallen on targeting the metabotropic glutamate receptor 5 (mGluR5) for treatment of ASD, as evidence suggests glutamate transmission dysfunction at this receptor in ASD. Using Dipraglurant, a known mGluR5 allosteric antagonist as a model, a series of 4-aryloxymethyl-1-arylmethyltriazoles were designed and targeted for synthesis. The final triazoles are synthesized using a [3+2] cycloaddition between various benzyl-substituted azides and aryl-substituted propargylic ethers. The benzyl-substituted azides were synthesized from the corresponding benzyl bromide and sodium azide. The aryl propargylic ethers were synthesized via a SN2 from the corresponding phenol and propargyl bromide under microwave conditions. Coupling of the azides and alkynes proceeded using CuSO4 as a catalyst under microwave conditions. Using this 3step combinatorial sequence, a small library of 4aryloxymethyl-1-arylmethyltriazoles is reported.

106B. Synthesis of biomimetic polymers towards modern wound healing materials

<u>Reagan Neal</u>, and Sharon Hamilton, Chemistry, Ouachita Baptist University

One area of the medical field that has potential to make great strides is the area of wound dressings. Conventional wound dressings do not promote cell growth and if not treated with care can cause more injuries when taken off improperly. Modern wound dressings should promote tissue growth and model the extra cellular matrix. Collagen is needed because it influences tissue growth and the restoration of the epithelium. However, Collagen is expensive and is not easily acquired. Our bPAA synthetic collagen mimic has similar properties to human collagen because of the amino acid mimics functional groups that we have added on are like those found on normal collagen. The collagen mimic can be spun with PVA and Chitosan which help with electrospinning capability and antimicrobial properties which are important in the wound healing process. Electrospinning also helps model the extra cellular matrix by spinning the fibers in a random fashion rather than having a pattern or order like traditional wound dressings. Collagen not only has properties that promote tissue growth, but also helps control bacterial growth. Chitosan is useful in wound healing because of its antibacterial properties. Although Chitosan and Collagen have great properties for wound healing, they can be difficult to electrospin. Therefore, in most cases they are spun with a co-polymer such as poly(vinyl alcohol) to help stabilize charges. With the intention of making a cost affective synthetic collagen, functional groups were added to poly(acrylic acid) was modified via amide coupling that closely resemble the amino acids found in Collagen.

107A. Alternative to modern wound dressings: developing a biodegradable collagen analog

<u>Andrew Tarlton</u>, and Dr. Sharon Hamilton, Chemistry, Ouachita Baptist University

Recent studies in modern wound dressings have focused on producing materials that promote wound healing by mimicking biofunctions in the wound healing process. Breakthroughs in this field have been achieved by electrospinning nanofibers from collagen to best mimic the morphology and components of the extracellular matrix. However, these dressings are expensive, not always degradable, and do not always contain antibacterial properties. Polycaprolactone (PCL) is a biodegradable polyester that could be used with chitosan, an antibacterial biomacromolecule, to develop electrospun nanofibers that can be incorporated into wound dressings. The ideal wound dressing would be a hemostatic material that is biodegradable, inexpensive, inherently antibacterial, and promotes rapid wound healing. Therefore, the overall goal of this project is to develop a material that incorporates these properties and can be electrospun into a nanofiber scaffold. Towards this effort, this project has focused on the synthesis of a novel biomimetic polycaprolactone (bPCL) prepared by modifying PCL via amide coupling reactions to attach molecules that mimic the amino acids naturally occurring in collagen. It is anticipated that these moieties will promote healing and hemostatic properties essential for wound dressings. Thus far, electrospinning protocols for PCL/chitosan fiber mats have been established through electrospinning trials and it is anticipated that these protocols can be applied to bPCL/chitosan solutions to prepare degradable, biomimetic, antibacterial nanofiber scaffolds. These novel mats will be analyzed via degradation and in vitro assays. It is expected that these studies will help assess the utility of these mats in biomedical applications.

107B. The development of a new water-soluble zinc porphyrin ZnTPP-3AP, and its potential as photodynamic therapy agent

<u>Emma Rouse</u>, and Dr. Joseph E. Bradshaw, Biology, Ouachita Baptist University

A promising new treatment method for cancer and other medical disorders known as photodynamic therapy (PDT) is being developed. PDT uses the radiant energy of light and a photosensitive agent for treatment. In this research a novel water-soluble zinc(II) porphyrin was developed as a potential PDT agent. When the porphyrin is activated by light, singlet oxygen is generated which affects the surrounding cells. The goal of this research was to synthesize and characterize a new water-soluble zinc(II) porphyrin incorporating the amine, 3amino-1-propanol, to be used as a possible PDT agent. The novel porphyrin, ZnTPP-3AP, was purified using column chromatography, and characterized using IR, UV-vis, and NMR spectroscopies. The purity of the desired compound was determined using HPLC. Additionally, an MTT assay utilizing A549 lung cancer cells was completed to evaluate the cytotoxicity of the ZnTPP-3AP in both light and dark conditions. Preliminary results of the exposure of ZnTPP-3AP to light have indicated that ZnTPP-3AP has promise as a potential PDT agent.

108A. The potential advancement of photodynamic therapy using a novel watersoluble zinc porphyrin, ZnTPP-5AP

<u>Sidney Pigott</u>, Joesph Bradshaw, Emma Rouse, and Marly Welborn, Biology, Ouachita Baptist University

Photodynamic therapy (PDT) is a type of cancer treatment that uses light and a photosensitizing agent to kill malignant cells. This research focused on synthesizing and analyzing a new water-soluble zinc(II) porphyrin compound as the photosensitive agent. The specific porphyrin compound ZnTPP-5AP was synthesized by the addition of 5-amino-1pentanol to the porphyrin, ZnTPPC. The new product was purified by column chromatography through Sephadex G-50 and LH-20 columns to ensure the purity of the product before characterization. The identification of ZnTPP-5AP was verified by infrared spectroscopy (IR), nuclear magnetic resonance spectroscopy (NMR), and ultraviolet-visible spectroscopy (UV-vis). Purity of the new material was determined by high performance liquid chromatography (HPLC). Finally, the utility of the ZnTPP-5AP as a photosensitizing agent was determined by

examining the cytotoxicity of ZnTPP-5AP by MTT assay on the A549 lung cancer cell line, in the presence and absence of white light.

108B. Effects of shipment temperature and duration on the release of bisphenol-A from infant toothbrushes

<u>Emma Bynum</u>, and Sara E Hubbard, Biology, Ouachita Baptist University

Effects of Shipment Temperature and Duration on the Release of Bisphenol-A from Infant Toothbrushes Emma Bynum and Sara E. Hubbard, Ph.D. Bisphenol-A (BPA) is a structural component in many plastic products, which acts as an endocrine-disruptor mimicking estrogen. This hormonal disruption has been linked to obesity, reproductive issues, cardiovascular problems, and the neurodevelopment disorders. Infants are at the highest risk of BPA exposure compared to any other stage of life. Because an infant's endocrine system is developing, exposure to an endocrine-disruptor, such as BPA, can be especially harmful. While the FDA monitors products like baby bottles, canned goods, and plastic containers for BPA, infant oral hygiene products are not closely monitored. Bisphenol-A fluoresces at an excitation wavelength of 278 nm and an emission wavelength of 304 nm. Previous research in our lab used fluorescence spectroscopy to test several brands of infant toothbrushes and found that many contain and leach BPA into their surroundings. Further research on the effects of temperature of the oral cavity and the pH of the saliva on the release of BPA from toothbrush samples showed an increased amount of BPA leaching from the toothbrushes when tested at the average body temperature, 37°C. For this project, toothbrushes were tested by storing them at higher temperatures, 50oC and higher, prior to testing for longer amounts of time to resemble that of shipment in semi-trucks. Large shipments spend an average of 3-7 days in semi-truck containers and the shipment temperature on average reach 50C. Toothbrushes were then placed in 1:1 methanol/water for several hours, aliquots were removed over time, and the amount of BPA leaching from the samples were monitored using an

FS5 Spectrofluorometer from Edinburgh Instruments.

109A. BPA presence in daily use panty liners and its ability to disrupt normal reproductive functioning

<u>Keren Fernandez</u> and Dr. Sara Hubbard, Biology, Ouachita Baptist University

BPA presence in daily use panty liners and its ability to disrupt normal reproductive functioning. Keren Fernandez and Sara E. Hubbard, Ph.D. Bisphenol-A is an industrial chemical that is widely utilized in products such as resins, plastic bottles, and thermal receipt paper. A study was recently performed at NYU Medical School, testing several different feminine hygiene products including panty liners, tampons, pads, feminine washes and deodorants. One of the results of this study showed that BPA is found in feminine products, and that panty liners contained the highest amount of BPA. This is concerning because BPA exposure in women can lead to the dysfunction of the endocrine and reproductive systems, especially during reproductive and post-menopausal ages. Panty liners come in direct contact with sensitive skin for an extended time, and panty liners are used daily for many women. Furthermore, the vaginal absorption rate is significantly higher than that of any other dermis of the skin. This research project sought to monitor the leaching of BPA from panty liners at hourly intervals from 0-4 hours. For each sample, the top layer of three panty liner samples were placed into a 1:1 solution of methanol/water, aliquots were removed over time, and fluorescence intensity data were obtained using the FS-5 spectrofluorometer from Edinburgh Instruments. Each sample was prepared in quadruplicate by submerging the top surface of 3 panty liners into 100 ml of M/W. The top surface of the panty liners was selected because it comes in direct contact with the vulva. Due to the complex matrix of the panty liner materials, this research was conducted using the standard addition method, where a known volume of the analyte was placed in a flask with varying volumes of a BPA stock solution.

109B. Using UV-vis spectroscopy to determine the pKa values of catechols

<u>Gisela Xhafkollari</u>, Larryn W. Peterson, Alexa Alana, and Keri L. Colabroy, Biochemistry and Molecular Biology, Rhodes College

There are a number of important catechols, including dopamine, catecholic nitriles, 3.4dihydroxyhydrocinnamic acid (DHHCA), and L-3.4-dihydroxyphenylalanine (L-DOPA) that serve as substrates for enzymes, including catechol-Omethyltransferase (COMT), L-DOPA dioxygenase, and cytosolic sulfotransferases (SULTs). We have synthesized a number of novel derivatives of these catechols with a range of substituents on the aromatic ring to investigate the mechanism and substrate selectivity of the enzymes. As the abstraction of the proton is a key step in many of the enzymatic reactions, determining the pKa values of these compounds is an important step in understanding their reactivity and identity. Experimental determination using UV-vis spectroscopy of the pKa values of these catechols allows for insight as to how they behave and interact in the active site. The pKa values of the analogues correlate well with the electron donating/withdrawing ability of the substituent.

110A. Computational design and synthesis of potential inhibitors of LpxC enzymatic activity

<u>Gabriella A. Krisanic</u>, Jacob D. Greenberg, Emma J. Chow, Eleanor A. Fontana, Campbell A. Brown, and Larryn W. Peterson, Chemistry, Rhodes College

Computational Design and Synthesis of Potential Inhibitors of LpxC Enzymatic Activity Gabriella A. Krisanic, Jacob D. Greenberg, Emma J. Chow, Eleanor A. Fontana, Campbell A. Brown, Larryn W. Peterson Department of Chemistry, Rhodes College, 2000 N. Parkway, Memphis, TN 38112 Abstract: As strains of multidrug resistant (MDR) Gram-negative bacteria continue to emerge, development of novel treatments for bacterial infections remains critical. The enzyme LpxC exists as an attractive target in inhibitor development due to its role in the first committed biosynthetic step in production of Lipid A, a main component of lipopolysaccharide, which is responsible for limited permeability of the cell membrane. Several analogues have been designed to bind within the three specific targets of the LpxC active site: a zinc ion, a polar region, and a hydrophobic pocket. Specifically, potential inhibitors with a more polar side chain as well as a hydrophobic tail have been investigated in silico using UCSF Chimera. The compounds were also docked using AutoDock Vina to determine a docking score and key interactions within the LpxC active site. Differences in strength of interaction and binding between the various analogues and the LpxC active site was elucidated. Progress toward the synthesis of the most promising compounds will be discussed.

110B. Synthesis of 6-substituted L-DOPA Analogues

<u>Kudzai L. Nyamkondiwa</u>, Trevor Squires, Erykah Starr, Rishabh Mazumder, Keri L. Colabroy, and Larryn W. Peterson, Chemistry, Rhodes College

L-3,4-Dihydroxyphenylalanine (L-DOPA) dioxygenase is implicated in several metabolic pathways. The enzyme is a member of the vicinal oxygen chelate (VOC) superfamily, which can cleave aromatic rings in catechols using metal chelation. Currently, L-DOPA dioxygenase's mechanism is not fully characterized, especially due to the lack of diverse substrates. This work focuses on the synthesis of 6-substituted L-DOPA analogues to expand the library of L-DOPA dioxygenase substrates, particularly those with electron-withdrawing nitro, cyano, and bromo substituents. Once the chemistry of breaking open a catecholic aromatic ring is well established, chemists may be able to utilize this enzyme in bioremediation or the synthesis of novel antibiotics.

111A. Design and synthesis of novel antibacterial compounds to combat gram-negative bacterial resistance and infections <u>Emma Chow</u>, Dr. Larryn Peterson, Gabriella Krisanic, Ellie Fontana, Campbell Brown, and Jacob Greenberg, Chemistry Department, Rhodes College

Design and Synthesis of Novel Anti-Bacterial Compounds to Combat Gram-negative Bacterial Resistance and Infections Emma J. Chow, Gabriella A. Krisanic, Jacob D. Greenberg, Eleanor A. Fontana, Campbell A. Brown, Larryn W. Peterson Department of Chemistry, Rhodes College, 2000 N. Parkway, Memphis, TN 38112 Abstract: The development of chemical compounds with broadspectrum activity against Gram-negative bacteria, which cause life-threatening illnesses, is imperative to source our limited stores of antibiotics and to combat the growing resistance of bacteria to antibiotics. These novel compounds, which include a hydrophobic moiety amide coupled to a propargylglycine-based hydroxamic acid, will provide additional options for the treatment of Gram-negative bacterial infections. Gram-negative bacteria with the TolC-mediated efflux pump have effectively removed propargylglycine-based antibacterial compounds with a biphenyl tail, resulting in limited activity of these compounds. However, the design of novel compounds that avoid the efflux pump with better overall antibacterial activity have been investigated. The pathways to successful synthesis of these novel compounds will be presented.

111B. Synthesis of 3, 4-dihydroxyhydrocinnamic acid derivatives with electron withdrawing substituents and the effect on pKa and oxidation potential

<u>Jessica L. Steiner</u>, Ryan N. Marasco, Mark Betonio, Keri L. Colabroy, Larryn W. Peterson, Chemistry, Rhodes College

L-DOPA dioxygenase is an enzyme that uses metal chelation to catalyze the cleavage and catholic rings. A thorough understanding of the mechanism and substrate space of L-DOPA dioxygenase is limited by the focus of current research on type V topology, while this enzyme has type IV topology, and further by a lack of substrates available for study. In order to more fully understand the mechanism of L-DOPA dioxygenase, we wanted to expand the available substrates. Although our work began with a series of 6-substituted dopamine derivatives, it is now focused on 6-substituted 3, 4dihydroxyhydrocinnamic acid analogues, specifically with bromo, nitro, and cyano substituents. The synthesis of these derivatives and their potential as substrates of L-DOPA dioxygenase, based on pKa and oxidation potential, will be discussed.

112A. Extraction and analysis of medicinal biomolecules in witch hazel

<u>Alaina Glover</u>, Alaina, Taylor, Lauren, Van Dee, Lauren, and Williams, Andrew, Math and Sciences, University of Arkansas - Monticello

Dating back millennia, plants have been used for their medicinal properties. Witch hazel (Hamamelis virginiana) is commonly known to calm skin irritants and commercially used in dermatological topical agents. As a native to plant it is readily available, and due to its biological activity, it presents itself as an interesting study. For this reason, we have begun to extract and analyze the active compounds found in witch hazel, and determine the quantities of each. Once this data has been analyzed, more studies will be done on the medicinal functions they have and the practicality of using them. These biologically active molecules can be extracted in aqueous solution, so we have a green method to extract these molecules. The compounds found in witch hazel will possibly be a safe and green way to improve health.

112B. Determination of fatty acid concentrations in algae

<u>Lauren Taylor</u>, Alaina Glover, Payton Ashcraft, Blake Martinez, Jason Rodriguez, Randa Jacks, and Andrew Williams, Math and Sciences, University of Arkansas - Monticello

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: lypholization, 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.

113A. Installing a carboxyl group onto the covalent organic framework backbone for dye adsorption/removal

<u>Davis Lee</u>, and Suraj Gupta, Department of Biological Sciences, University of Arkansas

Covalent organic frameworks (COFs) are an emerging class of crystalline porous materials which are synthesized by the combination of appropriate monomer organic molecules into extended structures. Undoubtedly, adsorption technologies have played a vital role in the removal of toxic organic pollutants including dyes from waste-water. For this, ultraviolet-visible spectroscopy has proved to be a simple yet efficient way of measuring adsorption. Due to the porous structure and flexibility to tune the pore size, COFs have proven to be promising candidates for adsorption and removal of dyes from waste-water. Besides, modifications onto the functional groups of COF architectures would influence the selectivity towards target compounds. For example, carboxylfunctionalized COFs provide enhanced adsorption through electrostatic interactions and $\pi - \pi$

interaction with the benzene rings and ionic quaternary amines of triphenylmethane dyes. With this background, we are expecting to observe increased adsorption and removal of dyes when installing a carboxyl group onto the backbone of the COF. Two COFs, (COF)-0-COOH and (COF)-1-COOH, were synthesized using the building blocks: tetrakis(4-aminophenyl)ethylene (tetraamine), 1,1':4',1"-terphenyl-4,4"-dicarbaldehyde (DiAld-0-COOH), and 4,4"-diformyl-[1,1':4',1"-terphenyl]-2'-carboyxlic acid (DiAld-1-COOH). The monomers were characterized through proton nuclear magnetic resonance (1HNMR) and matched with reported 1HNMR spectra reported in literature. Further, the COFs were characterized through infrared (IR) spectroscopy, powder X-ray diffraction (PXRD), and matched with similar patterns reported in literature. Finally, the absorbance of two dyes, Brilliant Green (BG) and Crystal Violet (CV), were measured using ultraviolet-visible spectroscopy (UV-Vis). (COF)-0-COOH removed 14% of CV and 24% of BG while (COF)-1-COOH removed 46% of CV and 75% of BG, suggesting that the installation of a carboxyl group onto the COF does increase dye adsorption.

113B. Characterization of interaction between microtubules and ruthenium-based compounds using fluorescence spectroscopy

<u>Chloe Hutchison</u>, Dr. Paul Adams, and Dr. Djamali Muhoza. This research has been supported by an Honors College Research Grant, Biology, University of Arkansas

Cancer is a disease at the cellular level that is caused by uncontrolled cell proliferation. Small molecules can bind proteins that promote cell growth and proliferation to disrupt their natural physiological roles and thus interfere with mitosis progression. Microtubule (MT) dynamic instability plays an essential role in the separation of chromosomes during cell division. Taxol, a current chemotherapeutic agent, binds MT's and stabilizes their polymerized state, stalling cell cycle progression and leading to apoptosis. Research has identified novel Ruthenium Polypyridyl Complexes (RPCs) that also act as Microtubule Stabilizing

Agents (MSAs). The focus of this research is to characterize the binding interactions of other RPC small molecules and polymerized Tubulin through the use of fluorescence spectroscopy. DB ([Ru(dip)2bpy]Cl2) and DP ([Ru(dip)2phen]Cl2) are RPC small molecules that are water soluble and are the interest of this work. Fluorescence titrations have been completed to study the intrinsic fluorescent signals from tryptophan, an amino acid, in the MT to characterize this binding interaction. Titrations were performed with increasing concentration of the RPC to calculate its dissociation constant to the MT by fitting the emission spectra at 330nm to a Hill Plot. The Kd for the DP small molecule was calculated to be 15.61x10⁻⁶ M. The Kd for the DB small molecule was calculated to be 19.1×10^{-6} M. The hyperbolic curve of the fluorescence plot and Kd in the micromolar range show that these molecules are binding to the MTs and binding in ranges similar to other RPCs. Current and future work to further characterize the binding interactions will be Differential Scanning Calorimetry (DSC) to identify the effects of small molecule binding on polymerized Tubulin stability by assessing the melting temperature (Tm) of the protein and the protein and small molecule. Additionally, studies will be performed at an increasing temperature and specific concentration of the RPC, to indirectly measure the thermodynamics of the binding interaction by creating an Arrhenius plot. Expected results should aid in the characterization of this small molecule interaction with the MT and subsequently translated to a description of how the RPC influences important properties of MTs.

114A. Structure based design and synthesis of substituted heterocyclic pyrimidine based colchicine binding site inhibitors

<u>Bobbi Evans</u>, Joshua Thammathong, Neal Zane, and Souvik Banerjee, Physical Sciences, University of Arkansas - Fort Smith

Abstract The disruption of microtubule assembly by colchicine binding site inhibitors (CBSIs) is a wellestablished therapeutic approach in cancer chemotherapy. Treatment with CBSIs, on the other

hand, might cause serious problems including multi-drug resistance and toxicity in otherwise healthy cells. As a result, demand for potent CBSIs with wider therapeutic utilities is strong. Azixa was first developed for the treatment of glioblastoma, however it was never approved for use due to the compound's cardiovascular toxicity. The drugs of the Azixa class have exceptionally high potency, which is accompanied by significant toxicity, resulting in a limited therapeutic index. CBSIs from the Azixa family have recently been reported by our group to suppress tumor development in the A375 melanoma xenograft model. Furthermore, in a paclitaxel-resistant prostate cancer xenograft model, these CBSIs effectively overcame multi-drug resistance. We continue to develop new Azixa derivatives with enhanced therapeutic utilities for future in vivo experiments.

114B. Analysis of collagenase G and model protein (hen egg white lysozyme) by dynamic light scattering and X-ray crystallography respectively

<u>Harmeet Kaur Chohan</u>, and Josh Sakon, Department of Physical Sciences, University of Arkansas – Fort Smith

Bacterial collagenases can efficiently degrade extracellular matrices of animal cells, due to their ability to digest native collagen. The bacterial collagenases are used to remove fibrosis in Dupuytren's contracture, Peyronie's disease and cellulite. The enzyme firstly unbundles fibril, then unwinds triple-helical collagen to expose peptide bonds for hydrolysis. Presumably, the enzyme uses various segment to carry out the complex task. Biophysical analyses identified the purity and ideal solution for isolated and purified natural collagenase G from Hathewaya histolytica (Clostridium histolyticum). The size distribution profile of natural collagenase G from in different calcium environments (pCa = -log[Ca2+]) by dynamic light scattering (DLS) was used to assess the stability of the enzyme in solution. The information will be useful in future works investigating structural changes of the enzyme at the different pCa environments using small angle

X-ray scattering technique (SAXS). To learn various biochemical techniques, protein used for analyses were initially hen egg white lysozyme. Lysozyme was crystallized, and X-ray crystallography was performed on the tetragonalshaped crystal. It had a size of 400x300nm and symmetry of primitive cubic unit cell. Sodium Dodecyl Sulfate-Polyacrylamide Gel Electrophoresis (SDS PAGE) was performed on both lysozyme and collagenase G, and the molecular weights were estimated to be 14 and 120kDa respectively, as expected. The latter was also used to estimate protein purity using the Image J software, and the value was 98.6%. DLS on 1 mg/ml of lysozyme showed aggregation and relatively low kcps (kilo counts per second) values until the concentration was ramped up to 8 mg/ml. However, the hydrodynamic diameter was inconsistent with literature. A second model protein, bovine serum albumin (BSA) was used to obtain better results concerning kcps values, stability, and measured hydrodynamic diameter in consistence with literature. DLS was performed on various distilled water sources to be used for pCa buffer preparations. Distilled water from the lab in the Nanoscale Material Science and Engineering Building exhibited little particulate matter. After buffer preparation and buffer exchange with natural collagenase G, DLS was performed on the samples in pCa 3 and pCa 6. The hydrodynamic diameter was approximately 12 d.nm but varied slightly depending on the pCa buffer. This study showed that different concentrations of calcium ions may affect particle size and overall structure of natural collagenase G.

115A. Site-directed mutagenesis to alter autolysin protein binding affinity

<u>Ibraheem Abbood</u>, Blake Katz, Rahul Yadav, Joanna X. Xu, Radha P. Somarathne, Nicholas C. Fitzkee, and Nawab Ali, Department of Chemistry and Biology, University of Arkansas - Little Rock

Bacterial biofilms can form on many different types of surfaces and are a leading cause of hospitalrelated infection. The bacteria in biofilms typically resist antibiotic treatments and are therefore a

serious global health concern. Bacterial biofilms are dependent on extracellular polymeric substances (EPS) surrounding and protecting the cells, and these substances interact with surfaces during the early stages of biofilm formation. R2ab is a domain of the autolysin protein from Staphylococcus epidermidis, and it has a high affinity to polystyrene surfaces. R2ab is implicated in biofilm formation, and removal of this domain significantly reduces biofilms in S.epidermidis. However, the molecular mechanism of how R2ab interacts with polystyrene is not well understood. Based on prior research on isolated amino acids, we hypothesize that aromatic residues in R2ab drive the binding to polystyrene. In this study, we use site-directed mutagenesis to identify important amino acid residues in R2ab as it binds to polystyrene surfaces and polystyrene nanoparticles We have designed mutagenesis primers and used the polymerase chain reaction (PCR) to generate two variants so far, Y722A and Y844A. Fluorescence-monitored protein denaturation experiments reveal a preliminary unfolding stability of $\Delta G = 3.5 \pm 0.3$ kcal mol-1 for Y722A. These variants were grown in 15N media for characterization by NMR spectroscopy Based on two-dimensional HSQC spectra, both proteins are folded and appear to adopt similar structures to the wild-type (WT) R2ab domain. The Y722A and Y844A amino acid substitutions, therefore, do not appear to affect R2ab itself, making these variants suitable for surface binding studies. Work is ongoing to characterize polystyrene binding as well as to assess whether these variants are effective at interfering with S. epidermidis biofilm growth. Our long-term goal is to identify key surface binding residues as a means of developing new treatments for preventing biofilm growth such as photothermal therapy.

115B. Refolding of S. aureus MTA nucleosidase to analyze biological activities

<u>Tripti Shukla</u>, Lauv Patel, and Dr. Shanzhi Wang, Department of Chemistry, University of Arkansas -Little Rock

Staphylococcus aureus (S. aureus) is a grampositive bacteria that is purple-stained in a gram test, cocci-shaped, and usually arranged in chunks. This bacteria is capable of growing aerobically or anaerobically. Bacterial enzyme 5'methylthioadenosine/S-adenosylhomocysteine nucleosidase (MTAN) has been discovered to be a part of the quorum-sensing pathway regulates gene expression in response to an increase in cell population density and essential for bacterial growth. The enzyme, MTAN, has been recognized as an antibiotic target because it is vital for the metabolism of MTA and SAH in several microbes, one being S. aureus. Production of recombinant proteins is essential for drug development, and the refolding process could significantly increase the production.

116A. Inhibitor activity characterization of MTA nucleosidase mutants from S. aureus

<u>Lauv Patel</u>, Tripti Shukla, and Shanzhi Wang, Chemistry, University of Arkansas - Little Rock

The bacterial enzyme 5'-methylthioadenosine/Sadenosylhomocysteine nucleosidase (MTAN) is known to be a critical factor in bacterial survival, communication, and growth due to its function as a component in the quorum sensing pathway of some bacteria. MTAN was discovered to be an antibiotic target for some microbes. The reason MTAN is significant is due to its function in the metabolism of MTA and SAH in microbes. Our study is to focus on mutant MTANs from Staphylococcus aureus (S. aureus). S. aureus is a gram positive bacteria that is capable of growing aerobically or anaerobically. Tight-binding transition-states have already been developed for the wild-type and have shown to be extremely effective. The effect of the inhibitor on all of the potential active sites of MTAN is still not completely understood; for this purpose, the activity of the inhibitors on mutant MTAN will be accessed.

116B. Nanomaterial effects on degradation of polymer biomaterials

<u>Ruby D. Trotter</u>, Amanda G. Murphy, Christopher D. Griffin, Shawn E. Bourdo, and Alexandru S.

Biris, Center for Integrative Nanotechnology Sciences, University of Arkansas - Little Rock

Polyurethanes (PU) are a class of materials that have shown suitable biocompatibility, and as a result are becoming increasingly applied to biomedical materials such as prosthetics, drug delivery devices, and biomedical scaffolds. Due to this wide range of uses and applications, it is necessary to examine the long term behavior and stability of these biomaterials in vitro and after implantation in vivo. Many nanomaterials are utilized in biomedical applications and may also be incorporated into polyurethane depending on a specific application. These nanomaterials may modify the stability of these resulting composites and contribute to the understanding of polymerbased biomaterial stability. Two polyurethane films were produced, one with graphene and one without any additive as a control, to compare their inherent stability. The films were subjected to oxidative environments in vitro using hydrogen peroxide solution. In this one year longitudinal study, graphene was shown to impact the polymer stability in such environments indicating interactions between the polymer structure and the graphene filler. Additionally, molecular weight and spectroscopic analysis will be presented to determine any structural changes in the polymer after degradation.

117A. Value added product by catalytic electrochemical reduction of carbon dioxide

<u>Sadie Goss</u>, and Anindya Ghosh, Department of Chemistry, University of Arkansas - Little Rock

We synthesized CoFe₂O₄/C nanocomposite for carbon dioxide (CO₂) reduction reaction (CO₂ RR) using nanocellulose and metal salts of Co and Fe via co-precipitation and pyrolysis methods. The morphology, elemental composition, and chemical bonding of the nanocomposite were studied by different analytical techniques. The results showed the presence of mixed oxide nanoparticles on the carbon surface which are spherical in shape and nanometer in size. The presence of Fe, Co, O, and C elements in CoFe₂O₄/C was confirmed by XPS. The CO₂ RR was performed electrochemically using an H-type electrochemical cell in 0.1 M KHCO₃ solution by bubbling CO₂ and Ar gases. A significantly high current density and reduction potential were observed in the CO₂ -saturated electrolyte compared to Ar-saturated, which is due to CO₂ RR catalyzed by the nanocomposite. We also tested the electrocatalytic activity of nanocomposite toward CO₂ RR via other electrochemical techniques (LSV, CA) at different pH, scan rates, and potentials. The reduced products formed after CO₂ reduction electrolysis were alcohol and hydrocarbon gases, as confirmed by GC-MS analysis.

117B. Ionic material based phthalocyanine photosensitizers: A potential photodynamic therapy nanomedicine

<u>Haris Atif</u>, Samantha Macchi, and Noureen Siraj, Biology, University of Arkansas - Little Rock

Phthalocyanines (Pcs) are a class of dye molecules that are often applied as photosensitizers in photodynamic therapy (PDT). An optimal PDT's photosensitizer possesses certain characteristics such as high molar absorptivity at clinically relevant wavelength (600-850 nm) and high singlet oxygen quantum yield. Herein, a simple ion-exchange reaction has been applied to tune the spectral properties of two Pcs using bulky phosphonium counterions. Further, aqueous ionic nanomaterials are synthesized via simple reprecipitation method. Their absorbance and emission properties have been studied in detail. It has been found that these materials show a red-shift in absorbance and enhancement of molar absorptivity compared to parent Pcs. Additionally, singlet oxygen quantum vield is enhanced upon conversion to ionic materials making these compounds highly promising for PDT applications. This project highlights a simple and inexpensive methodology to enhance the photophysical properties of photosensitizing dyes. In vitro cytotoxicity will be determined for these Pcs ionic materials.

118A. Novel FRET-Based ionic materials for bioimaging application

<u>Hannah Krehbiel</u>, Caroline Kornelson, Amanda Jalihal, and Dr. Noureen Siraj, Department of Chemistry, University of Arkansas - Little Rock

Bioimaging is crucial for the noninvasive visualization of biological processes in the body and requires the use of a fluorescent probe to label molecular structures and processes. Clear and accurate images are essential in order for physicians to make proper diagnoses and treat patients effectively. Currently used probes tend to have complicated organic syntheses, degrade easily, and do not absorb well in the NIR (near infrared region), which is important for visualization of deeper tissues within the body. Herein, we seek to synthesize and characterize novel FRET-based ionic materials and nanomaterials for use in bioimaging. These materials contain both donor and acceptor moieties and thus are highly tunable and have a simple, low-cost, high-yield synthesis.

118B. Chemotherapy-photothermal therapy (chemo-PTT) ionic nanomedicines for combination cancer treatment

<u>Arisha Ishtiaq</u>¹, Samantha Macchi¹, Dr. Nawab Ali², Dr. Robert Griffin³, and Dr. Noureen Siraj¹ ¹Department of Chemistry, University of Arkansas -Little Rock ²Department of Biology, University of Arkansas -

Little Rock

³Winthrop P. Rockefeller Cancer Institute, Arkansas Nanomedicine Center, Department of Radiation Oncology, University of Arkansas for Medical Sciences

Cancer is still the second leading cause of death in the US only surpassed by heart disease. Nanotechnology has made great strides in improving treatment for the disease. Specifically, combination nanodrugs are gaining attention due to lessened side effects and tumor targeting ability of nanoparticles. In this work, we combined photothermal therapy (PTT) drugs with a chemotherapeutic drug to develop chemo-PTT combination drugs. Aqueous nanoparticles are derived from the therapeutic drugs using a simple reprecipitation method. The photophysical properties which influence the PTT performance and the light to heat conversion efficiencies are investigated in detail to determine the most promising combination for further in vitro studies. Acknowledgement: Arkansas INBRE NSF

119A. Molecular dynamic investigation of the pH-dependent influenza hemagglutinin protein conformational changes

<u>Nada Tolba</u>, Shadi Badiee, Vivek Govind Kumar, and Mahmoud Moradi, Department of Chemistry and Biochemistry, University of Arkansas -Fayetteville

Hemagglutinin (HA) is an antigenic glycoprotein found on the surface of the influenza viruses. HA is a homotrimer that mediates the binding of the virus to the host cell and the subsequent membrane fusion. The HA trimer is synthesized as inactive HA0 to prevent any unwanted fusion activity. Prior to membrane fusion, HA0 must be cleaved to HA1 and HA2 by host proteases. HA binds to the monosaccharide sialic acid present on the surface of the target host cells. The cell membrane then engulfs the virus through endocytosis and formsendosome. The cell then attempts to begin digesting the contents of the endosome by acidifying its interior and transforming it into a lysosome. When the pH within the endosome drops, the HA2 molecule becomes partially unfolded and moves away from HA1, releasing a hydrophobic portion of the peptide chain named fusion peptide that was previously hidden within the protein. The loop-to-helix secondary structural transition of HA2 moves the fusion peptide away from the virion surface and facilitates its insertion into the target membrane. We separated HA2 chains from HA1 chains in the membrane protein structure to investigate the conformational changes of HA2s with and without the HA1 using computer modeling and molecular dynamics simulations under various pH conditions. The simulations revealed the mechanistic details of pH-dependent conformational changes of HA protein.

119B. A virtual screening campaign targeting dihydrofolate reductase to identify small molecule antibacterial agents.

<u>Zane Neal</u>, Harmeet Cohan, Kairy Galvez, Sayo. O. Fakayode, and Souvik Banerjee, biochemistry, university of Arkansas - fort smith

Antibiotic resistance is one of the most severe public health concerns of the twenty-first century resulting from the rise of multidrug-resistant (MDR) bacteria, which lead to infections not treatable by conventional therapeutics. A group of multi drug resistant bacteria, namely ESCAPE, are often isolated from the hospital settings, and considered to cause majority of the nosocomial infections. In this current study, a structure-based pharmacophore, developed based on the dihydrofolate reductase cocrystal structure (DHFR) from Streptococcus aureus S1 (PDB: 2W9S), was employed to identify small molecules with potential inhibitory activity. Pharmacophore hits underwent molecular docking mediated screening to identify a group of candidates with very low binding affinities towards the DHFR active site. Top five leading candidates with one of the lowest binding affinities were further analyzed for ADMET to identify two ideal candidates with wide therapeutic windows. Further research is needed to biologically evaluate top two hits.

120A. Antibiotic removal from wastewater by carbon-based materials

<u>Shiraz Atif</u>, Amanda Jarman, Zane Alsebai, and Noureen Siraj, Chemistry Department, University of Arkansas -Little Rock

Antibiotic removal from wastewater by carbonbased materials, University of Arkansas Little Rock Doxycycline is widely prescribed antibiotic thus are likely found in waste water. This abundance of doxycycline can lead to the proliferation of antibiotic resistant bacteria, making the removal from waste water of paramount importance. Carbonized materials have emerged as a low cost and environmentally friendly materials in a variety of applications. In this work, carbonized soy protein (Profam) is doped with ammonium polyphosphate for use as an antibiotic adsorbent. This carbonized Profam is synthesized using a facile and prompt microwave method to achieve a high surface area carbon material. The carbonized material is physically characterized using XPS, SEM and BET to investigate the elemental composition at the surface, surface morphology and surface area with porosity characteristics respectively. The doxycycline removal efficiency of the carbonized Profam is evaluated using absorption spectrophotometer. The synthesized carbonized material showed efficient removal of doxycycline form water with the added benefit of simple, low cost synthesis.

120B. Purification of staphylococcus aureus major extracellular proteases

<u>Sahana Bettadapura</u>, and Shanzhi Wang, Biology, University of Arkansas - Little Rock

Major bacterial pathogen Staphylococcus aureus rapidly acquires resistance to traditionallydeveloped antibiotics, making it urgent to develop long-lasting inhibition of S. aureus infection. Extracellular proteases Aur, SspA, SspB, and ScpA have recently been suggested to have therapeutic potential by significantly reducing biofilm and surface adherence of S. aureus. This provides a possible target for the design of inhibitors. However, further investigation is inhibited in part by their limited availability in significant purified quantities. Here, we plan to express the proteases in their pro-forms with the activation/proteolysis sites mutated to a TEV protease cutting site and a 6xHis tag added to the N-termini to ensure high expression levels and minimize glycine residue formation at the N-termini after activation.

121A. Immunosuppressant Targeting within the Islet Microenvironment

<u>Olivia Allen</u>, Sean Quinnell, and Arturo Vegas, Chemistry, University of Arkansas - Pine Bluff

Immunosuppressant Targeting within the Islet Microenvironment Authors: Olivia Allen, Sean Quinnell, Arturo Vegas Type 1 diabetes is an autoimmune disease that is characterized by the destruction of insulin producing Beta Cells. The current treatment for type 1 diabetes is exogeneous insulin that sometimes leads to limb amputation, blindness and kidney failure. Scientists and doctors alike have been looking into other ways to treat type 1 diabetes outside of glycemic management. Immunosuppressants have successfully been used to treat type 1 diabetes but the drawback with using immunosuppressants to treat type 1 diabetes is that there are adverse side effects. We have come up with a novel approach to use islet-targeted conjugates to localize immunosuppressive agents to the islet microenvironment which will consist of a structure that has a targeting ligand, a linker, a cleavable bridge and a therapeutic warhead. We first synthesized a PEG linker with a dye attached and then conjugated exenatide analogs to the molecule to act as our targeting ligand. Exenatide is a sugar level reducer used to treat type 2 diabetes. We used a confocal microscope to examine the uptake and localization of our conjugates within the cells. If the labeling can be replicated on a constant basis the next step for this project will be to add a cleavable bridge to allow for drug release. If effective and successful, this islet targeted conjugation will go from in vitro studies to in vivo within non obese diabetic mice.

121B. Characterization of a Ras-related protein in the presence and absence of a small molecule inhibitor

<u>Alexia Lo</u>, and Dr. Paul Adams, Chemistry and Biochemistry department, University of Arkansas-Fayetteville

Cell division cycle protein 42 (Cdc42) is a Rho subfamily protein from the RAS superfamily that has been a potential candidate for regulating cell proliferation, cytokinesis, and cell growth in cancer. These cellular activities happen because of how Cdc42 is overexpressed through growth factor receptors in which guanine nucleotide exchange factors (GEFs) regulate GDP/GTP exchange.1 The GDP/GTP exchange involves an inactive GDP and an active GTP in which Cdc42 circles between to activate downstream effectors. Cdc42 is also a potential candidate for drug therapies to treat malignancies. The purpose of this research was to further understand the protein interactions of Cdc42 and its variant T35A with the presence and absence of AZA197 while performing a time-dependent denaturation experiment using urea. Fluorescence spectroscopy will also be used to identify protein interactions between Cdc42 and the small molecule. Applications of biochemical techniques and methods will be done for protein production.

122A. QSAR analysis of drug-like therapeutic candidates against resistant bacterial infections

<u>Harmeet Chohan</u>, Kairy Galvez, Neal Zane, Joshua Thammathong, Zain Rana, Souvik Banerjee, and Sayo Fakayode, Department of Physical Sciences, University of Arkansas - Fort Smith

Rapid screening of potential drug candidates is a challenge in rational drug design. Quantitative structural activity relationship (QSAR) analysis and computational studies have proven efficient and low-cost for fast screening and pattern recognitions of drug-like therapeutic candidates (DLTC) with remarkable accuracy. This study utilized QSAR, Principal Component Analysis (PCA), PLSregression, and computational studies to evaluate the binding affinity of a set of DLTCs on dihydrofolate reductase (DHFR) from Streptococcus aureus S1 and penicillin binding protein 2x (PBP 2X) from Streptococcus pneumoniae co-crystal structures. The result of the analysis showed interesting pattern recognition based on DLTC's QSAR and binding affinities with DHFR and PBP 2X binding sites. DLTCs binding energies with DHFR and PBP 2X were modeled and predicted with good accuracy. Future study includes molecular dynamic simulation and biological evaluation of top leading DLTCs against resistant bacterial infections.

122B. The synthesis of a low cost disquaramide drug library for chagas disease

<u>Psalm Dang</u>, and Dr. Gregory Naumiec, Chemistry, University of Central Arkansas Neglected tropical diseases, or NTDs, are a category of infectious diseases that impact approximately 1.7 billion people around the world, especially in tropical areas with no access to clean water or sanitation. An example of a potentially fatal NTD is Chagas disease, or American trypanosomiasis. Chagas disease results from the parasite Trypanosoma cruzi, which resides in insect vectors (most commonly infected triatomine bugs or "kissing bugs"). Previous treatments, benznidazole or nifurtimox, were discontinued because of adverse side effects, such as digestive system irritation, skin disorders, and neurological symptoms. As a result, new drugs are currently being researched and developed. Our investigation was launched in order to create a disquaramide drug library, in the interest of creating a safer treatment for Chagas disease with less side effects. So far, we have created 15 drugs in search of that goal in moderate to high yields. Once the library is complete, we will send them for testing against the T. cruzi parasite with the help of the DNDi.

123A. Investigating the conformational ensemble of calmodulin-binding protein PEP-19

<u>Mattie Gordon</u>, Macllain Edington, Tori B. Dunlap, Department of Chemistry and Biochemistry, University of Central Arkansas

PEP-19 is a small, intrinsically disordered protein (IDP) that regulates the binding kinetics of the protein calmodulin (CaM) to calcium. Calmodulin is a calcium signal messenger, responding to changes in intracellular calcium levels to regulate hundreds of different pathways. PEP-19's role is crucial, with inappropriate expression leading to calcium signaling disruption that can contribute to neurodegenerative diseases, cardiac hypertrophy, and cancers. In the brain, its presence helps to protect against calcium overload, with increased concentrations found in areas spared from Alzheimer's disease, and decreased concentrations found in Huntington's disease. Despite playing such an essential role. little is known about the conformational ensemble of PEP-19 and how it affects calmodulin binding to its target proteins. Our goal is to study this conformational ensemble using

fluorescence resonance energy transfer (FRET) fluorometry, labeling with the organic fluorophore IAEDANS. This allows us to measure the end-toend distance of PEP-19 in order to look for changes in its compaction or expansion. By measuring FRET in the presence and absence of different crowding agents, denaturants, and osmolytes, we can observe the effect of the local environment on the PEP-19 conformational ensemble.

123B. Investigation of calmodulin and PEP-19 surfaces in biological systems

<u>Adrian N. Brown</u>, and Tori B. Dunlap, Department of Chemistry and Biochemistry, University of Central Arkansas

Calmodulin (CaM) is a calcium sensing protein that plays a vital role in regulating within cell signaling pathways. CaM binds to its targets while also bound to calcium, which allows for it to have an altered conformation. When it is bound to four calcium ions it can cause disordered regions of its ligands to form a helical structure. This altered structure allows CaM to bind to many different targets. Disruptions of calcium signaling pathways CaM is involved in are also associated with several different neurological diseases, such as Alzheimer's Disease. PEP-19 is a disordered protein that binds to CaM and alters its calcium binding kinetics and target protein binding. Along with understanding how CaM and PEP-19 behave when binding, it is vital to understand how the protein surfaces of CaM and PEP-19 behave in the biological setting. The behavior of the surface is normally observed in vitro, which might not represent how it behaves in a living organism. We plan to observe the physiological role played by the surface of CaM and PEP-19 by measuring the equilibrium thermodynamics and kinetics in living E. coli. This will be done by labeling CaM and PEP-19 with fluorine and then using NMR to observe the behavior of the folded and unfolded states of the proteins.

124A. An inexpensive and efficient approach to cure chagas disease

<u>M. Johanna Lasiter</u>, and Gregory R. Naumiec, University of Central Arkansas

Neglected Tropical Diseases (NTDs) pose an enormous threat to those in poverty-stricken regions of the world such as Central and South America. NTDs have affected the lives of nearly 2 billion people worldwide. With limited funds and resources, research on NTDs is lacking. Chagas disease, one such NTD, is a parasitic infection that is now becoming increasingly common throughout the southwest United States. Chagas disease is caused by the parasite Trypanosoma cruzi, carried by an insect known as the "kissing bug". Once infected, the insect passes parasites through their feces and can eventually cause "Chagas heart disease," resulting in death. There are currently two drugs in the market for treating Chagas, benznidazole and nifurtimox. Benznidazole is the only drug of the two that is FDA-approved (only in children), and both drugs have severe side effects along with alarming reports of treatment failures due to drug resistance in T. cruzi. We aim to make a new class of anti-Chagastic compounds using disquaramide structural motifs. Disquaramides have shown to have anti-parasitic activity and are facile and cost-efficient to synthesize. Our research has incorporated the use of diamines in order to make cyclic disquaramides. To date, we have successfully synthesized three of these compounds with moderate to high yield (21-96%). The main focus of this research is to create inexpensive drugs to aid in the fight against Chagas disease.

124B. The optimizations of N,N'-diarylurea: repurposing failed antimalaria drugs for snail fever

<u>Rachel Barnhardt</u>, and Gregory Naumiec, Department of Chemistry and Biochemistry, University of Central Arkansas

Neglected tropical diseases (NTDs) are a group of diseases mostly caused by parasites that widely affect poorer regions of the globe. Snail Fever (Schistosomiasis), one of the most common NTDs, affects 200 million people globally mainly in underdeveloped nations. No vaccine currently exists

for Schistosmiasis, though evidence leads us to believe a vaccine is possible. Alongside investigation into a vaccine, new drugs are being examined and tested for activity, selectivity, toxicity, and chemical attractiveness. One of the most active chemical moieties are the diarylureas. These compounds are relatively nontoxic and have shown a reduction rate of parasitic flatworms by as much as 52.5%, which means no only is this group of compounds highly active, they can be explored more for improvement. We are investigating the effects of a broad range of aniline compounds to produce a small library of diarylureas to increase the reduction rate of the Schistosoma parasites closer to 100%. The bulk of the current progress is in optimizing the reactions to produce the diarylureas. Literature sources indicated the synthesis of diarylureas required overnight heating at 55°C for roughly 80% yield. Initially, we heated the reaction at 55°C and analyzed using thin-layer chromatography (TLC) to monitor reaction time and reduced the waiting period to 2 hours for completion of the reaction. We are currently changing the reaction temperature for optimization of reaction conditions. Additionally, we are exploring both microwaving and sonicating the same reaction. Each reaction to produce a diarylurea is run in all three conditions and results compared to determine the best method of production.

125A. N,N'-disquaramide synthesis to combat chagas disease and human african trypanosomiasis

<u>Jamie Chen</u>, and Dr. Gregory Naumiec, Department of Chemistry and Biochemistry, University of Central Arkansas

At least one billion people around the world are infected with a neglected tropical disease (NTD), and these people are usually in underdeveloped countries that either cannot afford funding for cures or the pharmaceutical companies do not have incentives to work with those countries. NTDs such as Chagas disease (CD) and Human African Trypanosomiasis (HAT) are caused by a parasite which affects work and health development along with possible damage to the nervous system and heart. This research project aims to synthesize a cost efficient compound drug to combat both CD and HAT through synthesis of N,N'-disquaramides. Commercially available diethyl squarate (DES) has been reacted with one equivalent of Nmethylpropargylamine in ethanol solution at room temperature to attach an amino group via a substitution reaction with 53% yield. One equivalent of propargylamine was also substituted onto DES with 77% yield. Future work on N,N'disquaramides will include the use of a nickel catalyst NiCl2(PPh3)2 in a Sonogashira coupling of the product from N-methylpropargylamine substitution to add an aromatic carboxylic acid group with known anti-parasitic properties.

Poster Abstracts Physics

201A. Tellurium dioxide nanoparticles synthesized by pulsed laser ablation in liquids

<u>Tina Hesabizadeh</u>, and Dr. Gregory Guisbiers, Physics and Astronomy, University of Arkansas -Little Rock

Tellurium (Te) is a chemical element that is exceptionally rare in the Earth's crust. Nonetheless, Te produces compounds that are of considerable interest to scientists, owing to their optoelectronic characteristics as well as a wide range of biological features whose study has grown in popularity in recent decades. This project describes the production of TeO₂ nanoparticles in liquids using pulsed laser ablation. In biology and optoelectronics, tellurium dioxide (TeO₂) is an essential nanomaterial. The advantage of this synthesis method is that it gives nanoparticles a clean surface, allowing them to interact with bacteria more effectively. One Gram-positive and one Gram-negative bacteria were examined in this experiment. At concentrations of less than approximately 10 parts per million (ppm), TeO₂ proved effective in annihilating both kinds of bacteria.

202A. An analysis of Monte Carlo tunneling for high energy barrier problems

Juan de la Cruz, and Feng Wang, Mathematics and Chemistry, University of the Ozarks

A study to compare the subspace sampling method (SSM) and the Metropolis Monte Carlo algorithm is presented. Simulations were performed under the canonical ensemble in a single-particle system under a double well potential with large energy barrier at the center. The SSM shows to have better performance sampling various regions among discontinuities and high energy barriers by adding a transfer move between subspaces. Hence, the SSM provides better performance when calculating free energy differences of complex system such as protein-ligand binding.

203A. Using Raman Spectroscopy to determine composition of our growth of germanium-Tin Nano Structures

<u>Christopher Hocevar II</u>, and Dr. Gregory Salamo, Physics, Oklahoma State University

A Nano-material containing the alloy Germanium-Tin was grown on layers of Indium Gallium Arsenide through MBE (Molecular Beam Epitaxy. This Nanoscale material was examined through Raman Scattering, sending a specific frequency of light in and receiving the change in frequency of the light back out. This data was evaluated to describe material composition of the grown layer. These materials are separately evaluated by XRD and data from both can be used to understand the grown sample. The samples in this experiment did not supply sufficient information through XRD, but through Raman gave a better understanding of the material composition of our surface layers. Separate samples of Germanium-Tin grown by CVD on a silicon layer were examined by Raman before and after annealing and that data was examined similarly to the first samples. These experiments gave a better view on the grown samples as well as the effects on annealing on Germanium-Tin samples. This research was supported by the NSF-REU (NSF Award 1851919)

204A. What is friction at the atomic level? Adhesion and shear force

Zach Kauffman, Dr. Greg Salamo Mohammad, and Zamani Alavijeh, Physics, Missouri State University

Atomic force microscopy (AFM) is a hallmark of scanning probe technology; it uses nanoscale contact to map the surface's morphology, but the mechanism can also be used to investigate the friction qualities of the material. This series of experimentation focused on analyzing three facets of atomic-scale friction: First, this study analyzed the relationship between tip surface area and adhesion force. Second, this study produced a relationship between tip surface area and overall lateral friction. Lastly, this study analyzed the wear process on AFM tips as a function of normal forces are applied over time on different surfaces. Investigating each of these aspects of friction will improve our understanding of surface-to-surface interactions absent confounding variables such as interlocking asperities or surface roughness. It was found through these results that surface area and elasticity had notable implications for friction measurements which deviates from traditional understandings of friction.

205A. Field programmable gate array for correlation measurements and data acquisition system

<u>Apoorva Bisht</u>, and Hiro Nakamura, Physics, University of Arkansas - Fayetteville

A photon correlation measurement system has been developed using field programmable gate array (FPGA). This has been tested for classical light sources like coherent and bunched light. These were generated via unmodulated and modulated laser respectively. We will further use FPGA for advanced photon manipulations such as temporal multiplexing of single photons. FPGA specifically will be used for implementing the routing logic for the single photons to generate a regular sequence of single photons.

206A. Two-dimensional mapping of the ultrasonic properties of brain at 2.25 MHz

<u>Shona Harbert</u>, Will R Newman, *Cecille Labuda, and Brent Hoffmeister, Physics, Rhodes College, *Department of Physics and Astronomy, University of Mississippi

Transcranial ultrasound may be used to detect changes in brain tissue caused by disease or injury. The goal of this study was to characterize the ultrasonic attenuation and speed of sound of brain tissue. 1-cm thick slices of brain tissue were prepared from 12 preserved sheep brains. Slices were oriented along the transverse, sagittal and coronal planes. Ultrasonic measurements were performed in a water tank at room temperature using a 2.25 MHz transducer. The transducer was mechanically scanned to acquire measurements from multiple locations on the specimens. Twodimensional maps of attenuation and speed of sound were constructed from the data. Measured values (mean \pm standard deviation) were (0.87 \pm 0.29) dB/cm/MHz for the frequency slope of attenuation and (1538 ± 7) m/s for the speed of sound. This study represents the first two-dimensional mapping of the ultrasonic properties of brain at 2.25 MHz.

207A. Motility dynamics of E. coli in dense environments using differential dynamic microscopy

<u>Seth Williams</u>, and Pradeep Kumar, Department of Physics, Arkansas Tech University

Motility of bacteria has traditionally been studied by having a sparse population of bacteria moving in a quasi-2D environment whereas positions of cells can be tracked in real time under a microscope. Such methods fail to work for a dense population of bacteria where tracking single cells become difficult, and in some cases impossible. Dynamics of dense bacterial environments can be studied by using a method coined Differential Dynamic Microscopy (DDM). In this talk, I will describe the method and its implementation with bright field microscopy using colloidal beads as an example. Furthermore, I will discuss the dynamics of Escherichia coli cells at various concentrations of magnesium sulfate. This research was supported by the NSF-REU (NSF Award 1851919)

208A. Effects of metal ions on DNA bendability measured by Fluorescence Resonance Energy Transfer (FRET)

<u>Kaitlin Callies</u>, and Yong Wang, Department of Physics, University of Arkansas- Fayetteville

Sharp bending and looping of double-stranded DNA is of great importance due to their ubiquitous presence in cellular processes in eukaryotic cells, bacteria, and virus. For example, to package doublestranded DNA of a linear contour length of 1 m into a eukaryotic cell with a size of 10 µm, most of the eukaryotic genomic DNA is wrapped around histone proteins and sharply bent. In addition, it is important to understand how the bendability of DNA depends on metal ions, which are essential for various fundamental processes in cells, including the formation of secondary and higher-order structures of nucleotides, DNA repair, and genomic stability. In this work, we investigated the effects of silver and magnesium ions on the bending flexibility of double-stranded DNA using selfassembled bent DNA molecules and FRET. We measured that the FRET efficiency decreased as the concentration of silver ions increased but increased at higher concentrations of magnesium ions. These observations suggested that silver ions destabilized the bent DNA, while magnesium ions increased the stability of the bent DNA molecules. Compared to our previous work with gel electrophoresis, the FRET measurements were quicker, simpler, and more efficient. This work is expected to contribute to a better understanding of the biophysical properties of double-stranded DNA, which will benefit DNA-related medical research and treatment development.

209A. Effects of microgravity and radiation on rat bone strength and composition

<u>Hypatia Meraviglia</u>, Rahul Mehta, and Brent Hill, Department of Physics and Astronomy, University of Central Arkansas

The effect of prolonged exposure to microgravity and cosmic radiation on bone strength has long been of critical pertinence to human spaceflight. Previous studies have shown that these deep space conditions reduce bone strength and elasticity and increase levels of calcium and phosphorus. We investigate these effects in male Sprague-Dawley rats, divided into four groups: a control group, a group exposed to cumulative 2.4 Gy radiation, a group suspended with hind legs up to simulate low-gravity conditions, and a group subjected to both 2.4 Gy radiation and simulated low gravity. The strength and chemical composition of right-side tibias and femurs of sacrificed rats were tested through threepoint bending and a scanning electron microscope (SEM). We applied force to the center of each of the four anatomical sides of each bone with a force transducer. We measured the cortical area of slices from the center of each bone and the relative percentages of carbon, oxygen, phosphorus, and calcium under a scanning electron microscope (SEM). Hind-leg suspension reduced bone strength statistically significantly, while radiation had no significant impact in either test (three-point bending and spectroscopy via SEM). We present additional findings, discuss implications for bone health in deep space conditions, and propose future research. Acknowledgement: This work is supported by the Arkansas Space Grant Consortium (ASGC). The authors also acknowledge the assistance of Manling Cheng, Natalie King, and Parimal Chowdhury (University of Arkansas for Medical Sciences).

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Hutchison, Chloe	113B
Ishtiaq, Arisha	118B
Ivers, Alaina	4B
John, Eliana	2B
Johnson, Faith	18A
Jones, Ganell	23A
Jones, Nicholas	104B
Kauffman, Zach	204A
Kauffman, Zach	03:15PM
Kaur, Harmeet	114B
Kaur, Harmeet	122A
Kim, Daniel	1A
Kockaya, Lara	102B
Krehbiel, Hannah	118A
Krisanic, Gabriella	110A
Lasiter, M. Johanna	124A
Lasiter, M. Johanna	04:15PM
Lawrence, Audrey	101A
Le, Nhi	6A
Le, Nhi	03:30PM
Lee, Davis	113A
Lo, Alexia	121B
Massey, Regan	03:15PM
McCann, Lauren	11A
Meraviglia, Hypatia	209A
Meraviglia, Hypatia	03:00PM
Mohon, Darby	101B
Neal, Reagan	106B
Neal, Zane	119B
Nyamkondiwa, Kudzai	110B
Ostmo, Lydia	03:45PM

Parker, Olivia	1B
Patel, Lauv	116A
Paternoster, Nickolas	23B
Paxton, Bethany	3A
Pelley, Megan	104A
Pickering, Emily	103B
Pigott, Sidney	108A
Pope, John	15B
Ralston, Kaili	9A
Randolph, Danielle	19A
Roberts, Gabrielle	14B
Rouse, Emma	107B
Say, Ty	17B
Schad, Mary	106A
Shukla, Tripti	115B
Skinner, Bailey	22A
Smith, Jake	105A
Spiva, Joshua	03:30PM
Steiner, Jessica	111B
Strickland, M.Will	3:15
Tarlton, Andrew	107A
Taylor, Lauren	112B
Thammathong, Joshua	03:00PM
Thomas, Theresa	102A
Tidwell, Grace	10B
Tidwell, Grace	03:00PM
Tolba, Nada	119A
Tran, Amy	24A
Trotter, Ruby	116B
Tyler, Syan	18B
Villalobos, Alexis	22B
Vue, Sarah	4A
Wilcox, Alicen	2A
Williams, Seth	207A
Williams, Seth	03:45PM
Woller, Sarah	7B
Xhafkollari, Gisela	109B
Xhafkollari, Gisela	04:00PM



May 15-20: INBRE Sponsored Health Sciences Entrepreneurship Boot Camp.

A week long educational program held on the campus of UCA where students will learn the fundamentals of entrepreneurship and formulate new health science ventures.

• Website: https://inbre.uams.edu/



The week of May 23rd (exact date TBA): A one-day workshop focusing on obesity and diabetes.

Spend a day with clinicians and scientists exploring the current research involving obesity.

• Website: https://inbre.uams.edu/



Intensive 10-week research program. Competitive

stipend included. Applications now being accepted.

• Website: https://inbre.uams.edu/

