

Arkansas INBRE Virtual Research Conference

2020

Nov. 6th – 7th

Arkansas INBRE Research Conference

Arkansas IDeA Network of Biomedical Research Excellence

Schedule of Events

Friday, November 6th, 2020

https://us02web.zoom.us/j/88411214222

1:15 PM – 1:30 PM Zoom opens for audio testing. (Please join us)

1:30 PM – 2:35 PM Keynote Address: Dr. Peter Hotez

3:00 PM – 4:30 PM Student Virtual Presentations: Round 1 (Biology and Chemistry)

Saturday, November 7th, 2020

https://us02web.zoom.us/j/88411214222

- 9:00 AM 10:30 AM Student Virtual Presentations: Round 2 (Biology, Chemistry, and Physics)
- 11:00 AM 12:00 PM Virtual Workshops

For last minute announcements, please follow us on twitter @ARINBRE1

Registration Information

All registered participant will receive a unique registration ID and zoom link with password to join. After you join the meeting, please rename yourself to FirstName LastName RegistrationID.

The 2020 virtual INBRE required Zoom version 5.3.0 or above to participate in all activities. Please **upgrade your zoom** before attending the conference. Zoom on chromebook is not supported. Please use a windows PC or a Mac. Support for a tablet device, such as an ipad, is limited. The presenting author of a virtual presentation should not use a tablet.

For last minute announcements, please follow us on twitter @ARINBRE1

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

Inés Pinto, Christian Tipsmark biological sciences Jingyi Chen, Heather Jorgensen, Josh Sakon, Ying Yuan and Feng Wang; chemistry and biochemistry Reeta Vyas; physics

INBRE Steering Committee

Lawrence Cornett, Ph. D., UAMS, Director Stephen Addison, UCA Traci Abraham, UAMS Program Evaluator Galina Glazko, UAMS Joel Funk, John Brown University Tim Knight, Ouachita Baptist Univ. Richard Morrison, UAMS Mansour Mortazavi, UAPB Liz Pierce, UALR Thomas Risch, Arkansas State Univ. Feng Wang, UAF Jerry Ware, UAMS Ann Wright, Hendrix College

Staff

Diane McKinstry, UAMS, Program Coordinator Caroline Miller Robinson, UAMS, Business Manager

Biotechnology Core Leaders Joshua Sakon, UAF Alan Tackett, UAMS

Participating Institutions

Arkansas State University, Jonesboro Arkansas Tech University, Russellville Central Baptist College, Conway Harding University, Searcy Henderson State University, Arkadelphia Hendrix College, Conway John Brown University, Siloam Springs Lyon College, Batesville Missouri Southern State University, Joplin Missouri State University, Springfield Northeastern State University, Springfield Northeastern State University, Tahlequah Ouachita Baptist University, Arkadelphia Pittsburg State University, Pittsburg Rhodes College, Memphis Southern Arkansas University, Magnolia 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 University of the Ozarks, Clarksville

Featured Speaker

Friday, 1:30 p.m.

For registered participants only https://us02web.zoom.us/j/88411214222

Preventing the Next Pandemic

Peter J. Hotez M.D. Ph. D. Fellow American Academy of Pediatrics Fellow of American Society of Tropical Medicine and Hygiene



Peter J. Hotez, M.D., Ph.D. is Dean of the National School of Tropical Medicine and Professor of Pediatrics and Molecular Virology & Microbiology at Baylor College of Medicine where he is also the Director of the Texas Children's Center for Vaccine Development (CVD) and Texas Children's Hospital Endowed Chair of Tropical Pediatrics. He is also University Professor at Baylor University, Fellow in Disease and Poverty at the James A Baker III Institute for Public Policy, Senior Fellow at the Scowcroft Institute of International Affairs at Texas A&M University, Faculty Fellow with the Hagler Institute for Advanced Studies at Texas A&M University, and Health Policy Scholar in the Baylor Center for Medical Ethics and Health Policy.

Dr. Hotez is an internationally-recognized physician-scientist in neglected tropical diseases and vaccine development. As head of the Texas Children's CVD, he leads a team and product development partnership for developing new vaccines for hookworm infection, schistosomiasis, leishmaniasis, Chagas disease, and SARS/MERS/SARS-2 coronavirus, diseases affecting hundreds of millions of children and adults worldwide, while championing access to vaccines globally and in the United States. In 2006 at the Clinton Global Initiative he co-founded the Global Network for Neglected Tropical Diseases to provide access to essential medicines for hundreds of millions of people

He obtained his undergraduate degree in molecular biophysics from Yale University in 1980 (phi beta kappa), followed by a Ph.D. degree in biochemistry from Rockefeller University in 1986, and an M.D. from Weil Cornell Medical College in 1987. Dr. Hotez has authored more than 500 original papers and is the author of four single-author books, including Forgotten People, Forgotten Diseases (ASM Press); Blue Marble Health: An Innovative Plan to Fight Diseases of the Poor amid Wealth (Johns Hopkins University Press); Vaccines Did Not Cause Rachel's Autism (Johns Hopkins University Press); and a forthcoming 2020 book on vaccine diplomacy in an age of war, political collapse, climate change and antiscience (Johns Hopkins University Press).

Dr. Hotez previously served as President of the American Society of Tropical Medicine and Hygiene and he is founding Editor-in-Chief of PLoS Neglected Tropical Diseases. He is an elected member of the National Academy of Medicine (Public Health Section) and the American Academy of Arts & Sciences (Public Policy Section). In 2011, he was awarded the Abraham Horwitz Award for Excellence in Leadership in Inter-American Health by the Pan American Health Organization of the WHO. In 2014-16, he served in the Obama Administration as US Envoy, focusing on vaccine diplomacy initiatives between the US Government and countries in the Middle East and North Africa. In 2018, he was appointed by the US State Department to serve on the Board of Governors for the US Israel Binational Science Foundation, and is frequently called upon to testify before US Congress. He has served on infectious disease task forces for two consecutive Texas Governors.

In 2017, he was named by FORTUNE Magazine as one of the 34 most influential people in health care, while in 2018 he received the Sustained Leadership Award from Research!America. In 2019 he received the Ronald McDonald House Charities Award for Medical Excellence

Most recently as both a vaccine scientist and autism parent, he has led national efforts to defend vaccines and to serve as an ardent champion of vaccines going up against a growing national "antivax" threat. In 2019, he received the Award for Leadership in Advocacy for Vaccines from the American Society of Tropical Medicine and Hygiene. Dr. Hotez appears frequently on television (including BBC, CNN, Fox News, and MSNBC), radio, and in newspaper interviews (including the New York Times, USA Today, Washington Post, and Wall Street Journal).

Awards

Awards: Prizes will be awarded to the top presentations by undergraduate students in breakout session. The awardees will be informed after the conference at the email address provided during registration. Names of the awardees will be listed on the INBRE website https://inbre.uark.edu

Judging Rules: Each undergraduate virtual presentation will be judged by at least two judges, selected from various institutions. To avoid a possible conflict of interest, a judge from the same institution of the presenting author can not participate in the award discussion of that presentation.

Awards will be given in each of the three disciplines - physics, biology, and chemistry and biology. Only presentation with an undergraduate student being the sole presenter qualify for awards. To be eligible for an award, questions from the audience should be answered only by the presenting author.

Student Live Virtual Presentations

https://us02web.zoom.us/j/88411214222

Round 1 - Friday 3:00 PM to 4:30 PM Biology A/B, Chemistry A/B

Round 2 – Saturday 9:00 AM to 10:30 AM Biology A/B, Chemistry B, Physics/Chemistry C

Biology Session A (Friday)

A1 3:00 PM. Lydia Ostmo Northeastern State University - Broken Arrow Fluorescent Tagging of Replication Proteins to Study Protein-Protein Interactions

A2 3:07 PM. Connor Catron University of Arkansas-Fort Smith

Mating Type Identification and Biology of Sex in Dictyostelium Discoideum

A3 3:15 PM. Emory Malone Harding University Effects of Photocatalysis on Biofilms

A4 3:22 PM. James DuBose

University of Central Arkansas The Overabundance of Paraburkholderia in the Social Amoeba D. discoideum microbiome and its Impact on the Ecological Relevance of the Farming Symbiosis

A5 3:30 PM. Carmela Unnold Cofre Arkansas State University

Engineering Novel Designer Biologics in Plant Cells for Oral Treatment of Inflammatory Bowel Disease (Ibd)

A6 3:37 PM. Victoria Davenport

Missouri State University

Induction of Stress on HeLa Cells from InP/ZnS Quantum Dot Treatment

A7 3:45 PM. Allison Mundy Lyon College

Macroinvertebrate Communities Across A Gradient of New and Existing Poultry Agriculture In Northeast Arkansas

A8 3:52 PM. Chassidy Barnes Ouachita Baptist University

Investigating Gene Interactions in Breast Cancer Liver Metastasis via Cancer Bio Portal Data Analysis Pipeline

A9 4:00 PM. Shelby Kuhnert MSSU

An Exploration of the Sympathetic Component of the Supradiaphragmatic and Abdominal Divisions of the Right Phrenic Nerve

A10 4:07 PM. Sara Ambrocio Paque University of the Ozarks

New Species of The Green Algal Genus Coelastrella from Warren Prairie Natural Area in Southeast Arkansas.

A11 4:15 PM. Lauren Camp

Henderson State University

Further Analysis of a Potentially Ecologically Unique Tennessee Cave System and Future Direction for Study

A12 4:22 PM. Stuti Chatterjee

University of Arkansas at Little Rock

Tunable Sized Combination Nanodrugs Based on Ionic Materials

Biology Session B (Friday)

B1 3:00 PM. Regan Massey University of Arkansas Using CRISPRi-dCas9 to identify nitrogen sources used by a nitrogen-fixing methanogen

B2 3:07 PM. Dominic Dharwadker

UAF - UA Fayetteville Cytosolic and Amylopastic ATP and pH Dynamics in Rice Grains with Contrasting Chalkiness

B3 3:15 PM. Kaylene Reyes Missouri State University

Does Elemental Composition of North American Grapevines Reflect Environmental Adaptation?

B4 3:22 PM. Allison Shildt

University of Arkansas - Fayetteville Evidence from Cnidaria supports an ancient evolutionary origin of FoxP genes in animals

B5 3:30 PM. Michael Uecker Lyon College

Immunolocalization of Osmoregulatory Proteins in Axolotl, Ambystoma mexicanum

B6 3:37 PM. Tessa Watson Ouachita Baptist University Oxygen Production in Spiral and Straight Shaped Arthrospira Platensis

B7 3:45 PM. Nicole Dominguez University of Arkansas- Fayetteville Investigating the Potential Role of Human Herpesvirus 6 (HHV6) Infection in Epileptogenesis

B8 3:52 PM. Charisma Khilling Arkansas Tech University Bacterial Growth Inhibition by Sodium Toxin Na668

B9 4:00 PM. Madeline Richards University of Arkansas Functional Control of the Drosophila Lipin Protein by Phosphorylation

B10 4:07 PM. Gabe Poe Ouachita Baptist University Testing of Novel Photodynamic Agents for Viability and Localization in Photodynamic Therapy

B11 4:15 PM. Alicen Wilcox Harding University Microglia are persistently activated after removal of extracellular TDP-43

Chemistry Session A (Friday)

A1 3:00 PM. Jessica Allred University of Central Arkansas Long chain synthesis of N,N-disquaramides for the treatment of Chagas disease

A2 3:07 PM. Peyton Dodd Ouachita Baptist University Investigation of biomimetic polymers as alternative nanofibrous wound dressings

A3 3:15 PM. Duminduni Hewa Angappulige Arkansas State University Anti-melanoma Studies of Thiazole-androstenone Derivatives

A4 3:22 PM. Hannah Krehbiel UALR Novel FRET-Based Ionic Materials for Bioimaging Application

A5 3:30 PM. Anna Pinson Harding University Metabolism of Halogenated Synthetic Cannabinoid Analogs A6 3:37 PM. Matthew Boston University of Arkansas at Fort Smith Screen Printed Electrodes for the Detection of Active Pharmaceutical Ingredients (APIs) in Drugs

A7 3:45 PM. Harry Jeffrey Ouachita Baptist University Biomimetic Poly (Acrylic Acid) Fiber Scaffolds for Biomedical Applications

A8 3:52 PM. Harmeet Kaur Chohan University of Arkansas Fort Smith Alcohol Unfolded Hemoglobin: Insights from Mass Spectrometry

A9 4:00 PM. Honey Matevia University of Arkansas - Fort Smith Scorpion Venom Peptides as Potential Antiviral Agents against the SARS-CoV-2

A10 4:07 PM. Sarah Friedman University of Central Arkansas Finding a low cost alternative medication for Chagas Disease

A11 4:15 PM. Kayla Whittington Ouachita Baptist University Development of Novel Water-Soluble Porphyrins for Potential Use as Photosensitizers in Photodynamic Therapy

A12 4:22 PM. Anna M. Wolff University of Central Arkansas Synthesis of Espintanol Derivatives for a Cost-effective Treatment of Leishmaniasis

Chemistry Session B (Friday)

B1 3:00 PM. Nikkolette Perkins Lyon College Modified Michael Addition Leads to Biologically Significant Naphthoquinones

B2 3:07 PM. Kaymon Neal Hendrix College Modeling the S100A1 Protein and Developing Drugs to Induce Inhibition

B3 3:15 PM. Nabeel Alwan University of Arkansas - Little Rock Functionalized Ionic Material-based Combination Nanodrug for Treatment of Cancer

B4 3:22 PM. Elizabeth Henry University of Arkansas - Pine Bluff Investigating Peptidic Polymers for Drug Delivery Vehicles Using Computational Methods

B5 3:30 PM. Riley Roper University of Arkansas - Fort Smith Main Protease Peptide Inhibitors for Covid-19 Treatment

B6 3:37 PM. Cladie B. White University of Arkansas - Fort Smith Antimicrobial Peptides against SARS-CoV-2

B7 3:45 PM. Mitch Bandy Hendrix College NO reduction by the repair of iron center enzyme, YtfE

B8 3:52 PM. Mady Rottinghaus Ouachita Baptist University Effects of Temperature & pH on BPA leaching in Oral Hygiene Products using Fluorescence Spectroscopy

B9 4:00 PM. Drake Jackson Harding University BTEX analysis using Raman spectroscopy

B10 4:07 PM. Kameron Klugh Rhodes College Synthesis of Dopamine Analogs to Investigate Enzymatic Function of L-DOPA Dioxygenase

B11 4:15 PM. Darby Mohon Harding University Determination of the Vitamin Content in Oxalis triangularis

Biology Session A (Saturday)

A13 9:00 AM. Izzeldin Ahmed Arkansas State University Effect of Root Biomass on Prenylated Stilbenoid Yield In Hairy Root Cultures Of Peanut

A14 9:07 AM. Devyn Ruiz University of Central Arkansas Investigate the Interactions Between Non-Legume Plants nd Plant Growth-Promoting Bacteria at A Molecular Level

A15 9:15 AM. Hannah Wu Lyon College Osmoregulatory Proteins in the Neotenic Salamander Ambystoma Mexicanum

A16 9:22 AM. Sara Goins Pittsburg State University Surveillance Study on Culex sp. in southeast Kansas and Prevalence of West Nile Virus in the Mosquito Population

A17 9:30 AM. Vanessa Morales Missouri State University How Patterns of Behavioral Flexibility and Diet Breadth Correlate in Bees

A18 9:37 AM. Linh-Chi Ho Arkansas State University Prenylated Stilbenoids from Peanut as Potential Therapeutic Agents for Triple Negative Breast Cancer

A19 9:45 AM. Glory Ehie Missouri State University Myosin 2's effect on Vps10 and Snc1 traffic

A20 9:52 AM. Kengor Nedgee Thermozier University of the Ozarks

A new soil species of the green algal genus Diplosphaera Bialosuknia from Warren Prairie Natural Area in southeast Arkansas

A21 10:00 AM. Olivia Echols Lyon College Nonpoint Source Pollution and Water Quality Under Increasing Pressure from Poultry Agriculture

A22 10:07 AM. Mackenzie Hoogshagen

University of Central Arkansas Dictyostelium Social Amoeba Symbiont Prevalence Across Hardwood Forests of Arkansas

Biology Session B (Saturday)

B12 9:00 AM. Griffin Hopkins Ouachita Baptist University Bioinformatic Analysis of Antibiotic-Producing Soil Bacteria

B13 9:07 AM. Ethan Moore University of Arkansas - Fort Smith Effect of Soil Microbiome Succession on the Prevalence of Antibiotic Resistance

B14 9:15 AM. Samantha Prince Arkansas Tech University Formation and Characterization of Injectable Hydrogel Matrix to Generate Artificial Lymph Node

B15 9:22 AM. Nicole Akers UALR Exploring Connections Between Exosome-Induced Gene Expression and Development in Planaria **B16 9:30 AM. Halie Eastham Arkansas Tech University** Sodium Toxin Na668 Antibiotic Properties

B17 9:37 AM. Karen Morris Hendrix College Collagen Alters Behavior of Thyroid Cancer Tumor Cells

B18 9:45 AM. Taylor Savage Ouachita Baptist University Inhibition of ESKAPE Pathogens by Antibiotic-Producing Soil Bacteria

B19 9:52 AM. Suzette Lopez University of Arkansas - Fayetteville A Comparison of Growth Curve Parameter Estimates Across Parametric and Non-Parametric Approaches in R

B20 10:00 AM. Pratikshya Paudel Arkansas Tech University Efficacy Evaluation of mast cell targeted oral vaccine in generating Influenza A specific antibodies

B21 10:07 AM. Race Karlin Ouachita Baptist University The Effects of Varying Light Wavelengths and Gravity on Phototaxis of Physarum Polycephalum

Chemistry Session B (Saturday)

B12 9:00 AM. Evan Wittig University of Arkansas - Fort Smith Electrochemical drug metabolite synthesis and inhibition assays for preclinical drug screening

B13 9:07 AM. Ryane Thurman Ouachita Baptist University The Photodynamic Therapy Potential of a Novel Water-Soluble Porphyrin

B14 9:15 AM. Jasmine Baughman Ouachita Baptist University The Creation of a Next-Generation Cancer Treatment Using Photodynamic Therapy

B15 9:22 AM. Audrey Lawrence Harding University Chemical Analysis of Man-made Pond Development at Gilliam Research Station

B16 9:30 AM. Macllain R. Edington University of Central Arkansas

Development of novel squaramide drugs to treat Chagas disease in a cost-efficient and environmentally friendly manner

B17 9:37 AM. Kashti Shah Hendrix College EPR Characterization of NO reduction by YtfE

B18 9:45 AM. Dillon Mosman Rhodes College Synthesis of Novel N-based ligands

B19 9:52 AM. McKinley Fox

Lyon College Extraction and Quantification of Polyunsaturated Fats in Rice Bran

B20 10:00 AM. Theresa Thomas Hendrix College

Analyzing Interaction and Structure of Human Cannabinoid Receptor 2-Gi Protein 6PT0 in complex with CB2 Agonist AM1710, GW405833, 9JU, CP55940, and 8D0

B21 10:07 AM. Olivia Crites

Ouachita Baptist Univeristy Determination of BPA in Children's Bamboo Toothbrush Bristles using Fluorescence Spectroscopy

PHCH Session C (Saturday)

C1 9:00 AM. Ethan Taylor Arkansas Tech University Hydrogen Fuel Cell powered drone ambulance

C2 9:07 AM. Adam De Groodt Hendrix College

Cloud condensation nuclei (CCN) activity and water adsorption of model insoluble atmospheric aerosols: Application of Adsorption Activation Theory

C3 9:15 AM. Daryna Safarian Rhodes College

DFT study of ligand binding in the $\beta\mbox{-}1$ adrenergic receptor

C4 9:22 AM. Will Newman

Rhodes College

Backscatter difference analysis of ultrasonic signals measured from brain tissue for possible transcranial applications

C5 9:30 AM. Emma Chavez Hendrix College

Calculating Stability and Structure of the CB1 Receptor Using Computational Methods to design a Positive Allosteric Modulator

C6 9:37 AM. Manling Cheng University of Central Arkansas Comparison of Normal Rat Leg Bone with those under Simulated Microgravity and Cosmic Radiations Conditions

C7 9:45 AM. Melina Reeves

University of Arkansas-Fort Smith Molecular Modelling Approach to Identify Effective Protease Peptides against the Main Protease of SARS-CoV-2

C8 9:52 AM. Rachel Ancar Rhodes College DFT study of the selectivity of Tyrosinase

C9 10:00 AM. Sydney Du University of Arkansas, Fort Smith Clinically Proven Antibacterial Peptides against the Main Protease of SARS-CoV-2: A Molecular Modelling Study

C10 10:07 AM. Abby Bankhead Harding University Photocatalysis As a Means of Purifying Water for Space Flight

Workshops

Saturday, 11:00 a.m. -12:00 p.m.

workshops will be held in breakout rooms of the main conference zoom

https://us02web.zoom.us/j/88411214222

Registration for Workshops is Not Required.

Workshops with enrollment limits will be on a first come first serve basis.

Workshop 1 | Preparing for Graduate School

No Enrollment Limit Colin Heyes, PhD - Department of Chemistry & Biochemistry, University of Arkansas

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:

- Suresh Kumar, Professor of Chemistry and • Biochemistry, UAF
- Adnan Alrubaye, Associate Director of the Cell and Molecular Biology(CEMB) program, UAF
- Yasir Rahmatallah, Assistant Professor of Biomedical Informatics, University of Arkansas Medical School
- Mamello Mohale, Graduate Student, Department of Chemistry and Biochemistry, UAF
- Baronger Bieger, Graduate Student, CEMB, UAF
- Aaron Kemp, Graduate Student in Biomedical Informatics, University of Arkansas Medical School

Workshop 2 | Synthesis of Nanomaterials and their Applications in Cancer Therapy and Chemical Industry

No Enrollment Limit

Hudson Beyzavi, Ph. D. – Department of Chemistry & Biochemistry, University of Arkansas

In this online workshop, the students will learn about new nanoporous materials by attending a 20-minute presentation on nanomaterials and their applications and a 20-minute virtual lab experiment presented by Dr Hassan Beyzavi to learn how nanomaterials are synthesized and learn about their daily life applications. The nanoporous materials will shape beautiful crystals that have very large inner surface areas. The students will see how we use electron microscopes to look at the crystals in nano-meter scale. The nanosized crystals will be utilized in drug delivery systems to encapsulate drugs for diseased cells such as cancer cells. We will also present the application of our nanoporous materials for the capture of toxic contaminants such as iodine from the drinking water.

There is no limitations on the number and the level of attendees. The presentation will take place online on learning about the preparation of nanomaterials and their exciting daily life applications.

Workshop 3 | Making nanomaterials to kill airborne bacteria and viruses

No Enrollment Limit

Susanne Striegler, PhD, Dept. of Chemistry & Biochemistry, UAF

The ongoing COVID-19 pandemic has provoked a global movement to prioritize cleaning and disinfecting. This along with the increasing issue of antimicrobial resistance has driven researchers to develop new classes of antimicrobial agents effective against viruses and bacteria. This workshop will introduce the exciting nanomaterials developed in the Striegler lab that have proven effective at killing Gram positive bacteria with prospects for viruses as well. The discussion will include nanomaterial preparation and characterization as well as an evaluation of their antimicrobial activity. This project is the result of collaboration between synthetic organic and inorganic chemistry, polymer science, and microbiology. An open question and answer session will follow the presentation.

Workshop 4 | Protein Dynamics and Biomolecular Simulations

No Enrollment Limit

Mahmoud Moradi, PhD, Dept. of Chemistry & Biochemistry, UAF

Proteins are workhorses of the cell. What determines the function of a protein is its 3D structure, which is typically determined by experimental techniques such as X-ray crystallography. However, proteins are not static objects. They move and change their structure. To truly understand how a protein functions, one needs to visualize it structural dynamics. In this workshop, you will learn about an interdisciplinary field of science that uses computational power along with physics based models to simulate and visualize protein structural dynamics. The molecular dynamics software NAMD and its accompanying visualization software VMD will be introduced and various applications of molecular dynamics simulations to study realistic biological systems will be discussed.

Workshop 5 | Molecular Modeling

Limited to 8 participants

Peter Pulay, PhD, Dept. of Chemistry & Biochemistry, UAF Methods of molecular modeling on a pers

Methods of molecular modeling on a personal computer will be addressed.

Workshop 6 | Physics: "Super-Resolution Fluroescence Microscopy"

No Enrollment Limit

Yong Wang, PhD, Physics Dept, UAF

This workshop will briefly introduce the basics of super-resolution fluorescence microscopy based on single-molecule localization, which improves the spatial resolution of light microscopy by more than 10 times. Attendees will observe online super-resolution imaging experiments on E. coli bacteria, as well as the related data analysis (i.e., localizing individual proteins molecules inside the bacteria and reconstructing super-resolution images).

Workshop 7 | Physics: "Brain science workshop" No Enrollment Limit

Woodrow Shew, PhD – Physics Department, University of Arkansas

In this online workshop, we will begin with a brief introduction to how large networks of neurons are responsible for our thoughts, perceptions and actions. Then we will have a fun brain trivia match. Hopefully we will debunk a few myths about the brain. And finally, I will lead a lab tour using a mobile camera to show you around and give you a feel for what grad students in our lab do.

Workshop 8 | Physics: "A 2D How-to" No Enrollment Limit

Hugh Churchill, PhD – Physics Department, University of Arkansas

After a brief introduction to the field of 2D material research, I will demonstrate the now-famous "Scotch tape technique" that is used to peel apart atomically thin layers of graphene and many other 2D materials from 3D crystals. Attendees of this remote workshop will have the opportunity to see how this process is done this using tape, tweezers, and silicon chips, followed by "flake hunting" with a microscope.

Workshop 9 | Physics: ""Graduate Application"" No Enrollment Limit

Reeta Vyas, PhD – Physics Department, University of Arkansas

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 | Biology: Visualization of Breast Cancer Metastatic Cells No Enrollment Limit

NO Emonment Emit

Tameka A. Bailey, Ph.D., Biological Sciences, UAF Jodi Simeon, Ph.D. student, Cell and Molecular Biology Program and Department of Biological Sciences, UAF

Our goal is to understand the metastatic biology of triple negative breast cancer (TNBC) metastases. This workshop will highlight the use of ectopically expressed proteins tagged with green fluorescent protein to investigate their cellular localization and effect on stem cell formation in vitro. In vivo investigations include the use of a mouse human tumor xenograft model to visualize metastatic outgrowth and to ascertain whether the proteins promote the development of TNBC metastases. Techniques utilized include cell culture, lentiviral mediated transduction, flow cytometry, ELISA, immunoblot analysis, fluorescent confocal microscopy and stereomicroscopy, as well as subcutaneous and intracardiac injections of athymic mice.

Workshop 11 | Biology: Changes in chemical and electrical signaling in neurotropic virus infection *No Enrollment Limit*

Ruben Michael Ceballos, Ph.D., Biological Sciences, UAF

It is estimated that more than 95% of the world population is infected with Human Herpesvirus-6 (HHV6). Primary infection typically occurs before the age of 3 years old and presents as a rash on the trunk and limbs. This childhood ailment, which includes a fever, is known roseola infantum. After primary infection, HHV6 typically goes into a state of latency. A person can live with infection for their entire life without any subsequent symptomology. However, in some cases, HHV6 can reactivate during adulthood and cause neurological dysfunction. For example, it is suggested that HHV6 reactivation can induce seizure and lead to epilepsy. However, the mechanism by which this occurs is not known. This workshop will introduce the myriad of challenges encountered when attempting to elucidate the mechanisms by which a neurotropic virus causes neurological dysfunction. A cast of undergraduates, graduate students, post-doctoral scholars will put on an interactive short theatrical play that guides the audience through critical thinking steps and experimental methods that could be used to unravel the role of HHV6 in epileptogenesis.

Workshop 12 | Biology: Visualizing embryonic development using fluorescence confocal microscopy

No Enrollment Limit

Adam Pare, Ph.D., Biological Sciences, UAF The ability to "see" specific proteins within living organisms using fluorescence microscopy is one of the most powerful tools in biology, and it has allowed us to understand much about the inner workings of the cell. In this workshop, we will use laser-scanning confocal microscopy to observe cell movements in embryos of the fruit fly Drosophila melanogaster--one of the premier model organisms for biological research. Participants will learn the following: 1) How we collect and mount Drosophila embryos for microscopy; 2) How fluorescent molecules are used to see proteins in living organisms; 3) How laser-scanning confocal microscopy allows us to capture three-dimensional images; and 4) How cell movements establish the basic body plan of the embryo.

Workshop 13 | Biology: Genomics and Bioinformatics using the Arkansas High Performance Computing Center (AHPCC)

No Enrollment Limit

Jeff Pummill, AHPCC, Douglas Rhoads, PhD, Program in Cell and Molecular Biology, UAF

Coverage of tools and resources available to researchers on the AHPCC and beyond. Examples will be presented from assembly of genomes and transcriptomes for the striped bark scorpion (Centruroides vittatus), Timber Rattlesnake Crotalus horridus) and bacterial pathogens. Topics to be covered include accounts, interactive desktops, software tools, and XSEDE resources.

Workshop 14 | Workshop 14 - Biology: Butterflies, Behavior, and Experimental Design No Enrollment Limit

Erica Westerman, Ph.D., Biological Sciences, UAFIn In this workshop, students will learn how to conduct animal behavior research by observing the experimental set up in the University of Arkansas butterfly facility and then conducting a guided field experiment using animals in their local habitats. Dr. Erica Westerman will introduce students to butterfly research via a live streamed tour of the butterfly facility and behavioral assay demonstration. Then, students will learn how to collect behavioral data, and venture outdoors to collect their own data, which will be shared with their fellow workshop-mates and compared to data collected this past spring. Students will then learn how this type of data can be used to inform our understanding of neurobiology, cognitive development, and urban ecology.

Abstracts

Biology Session A

A1. Fluorescent tagging of replication proteins to study protein-protein interactions

<u>Lydia Ostmo</u>, Shwetanshu Das, Michael Smith, Sarah Woller, and Sapna Das-Bradoo

Department of Natural Sciences, Gregg Wadley College of Science and Health Professions, Northeastern State University - Broken Arrow

DNA replication requires an intricate web of interacting proteins. Recent work in our lab with budding yeast has shown that Mcm10 plays an integral role in DNA polymerase functionality. Expanding on this research, we intend to investigate if this role of Mcm10 is conserved in human cells. In the current project, we plan to establish HEK293T cell lines expressing green fluorescent protein (GFP)-tagged Mcm10 and red fluorescent protein (RFP)-tagged PolE to study the dynamics of the interaction during the cell cycle. Using restriction enzyme digestion, ligation, transformation and sequence analysis, we have confirmed successful construction of a GFP-tagged Mcm10 vector. Moving forward, PolE will be labeled with RFP and colocalization studies will be completed using fluorescence microscopy.

A2. Mating Type Identification and Biology of Sex in Dictyostelium discoideum

<u>Connor Catron</u>, Harrison Jenkin, and Sandhya N Baviskar Department of Chemistry and Biology, University of Arkansas-Fort Smith

Dictyostelium discoideum is a unicellular, bactivorous, soil-dwelling amoeba. When food is available, it reproduces asexually. Sexual reproduction occurs under certain conditions, such as darkness and humidity. The sexual cycle in Dictyostelium is uniquely social and has unusual features: one, triparental inheritance is observed, in which gamete fusion involves more than two gametes. Second, Dictyostelium have three mating types (I, II or III) where as most eukaryotes have two sexes or mating types. New natural isolates of Dictyostelium are generally identified and classified based on morphology, but morphological criteria alone could be misleading, as different species of look very similar. Because variation in mating types has genetic basis, researchers agree that mating type identification be used to identify species of new isolates. The goals of this project were 1) to identify the species of OZK11A, a natural isolate from the Ozark region of Arkansas, by identifying its mating type 2) to study sexual interactions of OZK11A by crossing it with strains of known mating types. We hypothesized that OZK11A belongs to Dictyostelium discoideum species and that it would produce macrocyst (sexual stage) when crossed with the other mating types. We performed gene presence/absence assay using polymerase chain reaction (PCR) technique, the amplified gene fragments were sequenced using Sanger's DNA sequencing method and sexual crosses of OZK11A were arranged with known mating types. From PCR, DNA sequencing data and results of sexual crosses, we conclude that OZK11A is a mating type III and therefore, it belongs to Dictyostelium discoideum species.

A3. Effects of Photocatalysis on Biofilms

<u>Emory Malone</u>, Dennis Province, and Sidney Brandon Department of Chemistry, Harding University

Prevention of Staphylococcus aureus Biofilms with Hydroxyl Radicals Produced by TiO2 and UVA Photocatalysis Biofilms in microgravity are more virulent in comparison to biofilms on earth. Astronauts on the International Space Station are at a higher health risk because of the potential for biofilms to form and propagate within their water sanitation system. A more cost and energy efficient system must be in place that prevents the growth of biofilms and kills any bacterial cells in suspension to protect the health of the astronaut crew and maintain the integrity of the water sanitation system. This study examines the effectiveness of photocatalysis with TiO2 surfaces and UVA light in both preventing and eliminating the growth of biofilms. To analyze the effectiveness of photocatalysis in preventing biofilm growth, overnight S. aureus cultures were diluted in tryptic soy broth media supplemented with glucose and NaCl to encourage biofilm growth. The biofilm media was exposed to either TiO2 only, UVA only, or both TiO2 and UVA (365 nm). In addition, half of the treatments were exposed to N-Tert-Butyl-a-Phenylnitrone (PBN), a radical quencher to determine the presence of hydroxyl radicals produced by photocatalysis. The treatment groups were as follows: Control, Control + PBN, TiO2, TiO2 + PBN, UVA, UVA + PBN, and TiO2 + UVA, TiO2 + UVA + PBN. One plate was exposed to UVA with an irradiance of 4 mW/cm². A kinetic reading of the growth curves of S. aureus after treatment revealed that the photocatalytic

treatment delayed the onset of logarithmic growth and significantly reduced the growth rate constant in comparison to the controls (p = 0.006). The UVA treatment alone killed all bacterial cells therefore a growth curve could not be obtained in both the absence and presence of PBN. These results concluded that hydroxyl radicals were present in the photocatalysis treatment and did impair the growth rate of bacterial cells but were unable to completely kill them like the UVA treatment. In order to quantify the biomass of the differently treated biofilms, a crystal violet (CV) stain was performed since there is a direct correlation between absorbance of CV and number of gram-positive bacteria present. The control and TiO2 treatment groups had a significantly larger biomass in comparison to the UVA and TiO2 + UVA treatments. This study assessed the prevention of S. aureus biofilms with TiO2 and UVA photocatalysis. Further research must be done to determine the effectiveness of photocatalysis in eliminating established biofilms.

A4. The Overabundance of Paraburkholderia in the Social Amoeba D. discoideum microbiome and its Impact on the Ecological Relevance of the Farming Symbiosis

<u>James DuBose</u>, Tammy Haselkorn Department of Biology, University of Central Arkansas

D. discoideum is a soil dwelling, bacterivorous, social amoeba that responds to food scarcity by forming spores. Lab experiments suggest that if spores are dispersed to a food-depleted environment, they will die unless the bacterial endosymbiont Paraburkholderia is present and allows for carriage of other food bacteria (farming). If this is an ecologically relevant co-evolved mutualism, we would expect an increase in Paraburkholderia prevalence over time and evidence of host specificity in natural D. discoideum populations. Further, we hypothesized that Paraburkholderia would increase amoeba microbiome diversity. While there was an increase in Paraburkholderia prevalence, Paraburkholderia did not increase the diversity of the microbiome; rather it dominated it, with a greater than 90% Paraburkholderia abundance in most infected samples. Additionally, we identified horizontal transfer of Paraburkholderia, further distinguishing it from the traditional co-evolved mutualist. Future studies will better reveal where Paraburkholderia falls on the parasite-mutualist spectrum in this complicated symbiosis.

A5. Engineering novel designer biologics in plant cells for oral treatment of inflammatory bowel disease (IBD)

<u>Carmela Unnold Cofre</u>, Wenzheng Guo, and Jianfeng Xu Department of Biological Sciences, Arkansas State University

Inflammatory bowel disease (IBD) represents a group of intestinal disorders that cause prolonged inflammation of the digestive tract. The current therapeutic strategies, including the conventional anti-inflammatory medications and the new biologic drugs targeting the pro-inflammatory cytokine tumor necrosis factor alpha (TNF α), have limited therapeutic efficacy and adverse drug reactions resulted from systemic administration. Colon-targeted oral delivery of anti-TNFa agents is highly desirable for the treatment of IBD. Plant cell culture has emerged as a safe and cost-effective bioproduction platform for therapeutic proteins. A unique feature of the plant cells is that they could serve not only as the "bio-factory," but also the oral delivery vehicle for recombinant biologics. This project aims to leverage a unique posttranslational modification – "glycosyl-phosphatidylinositol (GPI) anchor"- to strategically design and engineer novel anti-TNFa biomolecules in plant cells to develop a new class of oral biologic drugs for the treatment of IBD. Specifically, a TNFa inhibitor consisting of a human TNFa receptor (TNFR) fused with the Fc domain of a human IgG1 and a C-terminal GPI anchor (TNFR-Fc-GPI) is designed and expressed in tobacco BY-2 cells. The GPI anchor will facilitate intracellular trafficking of the TNFR-Fc protein, and more importantly, immobilize the protein at the plasma membrane, just like the protein surface display in microbial cells. This will presumably stabilize the recombinant protein during bioproduction and oral administration processes and create a high local concentration of the protein therapeutics after release in colon. The protection, drug release and bioactivity of the plant cell-capsulated TNFR-Fc in gastrointestinal tract will be investigated in vitro in simulated gastric fluids and simulated intestinal fluids. The therapeutic effectiveness of the orally administrated designer anti-TNFa biologic in mitigating the IBD symptom will be assessed in a dextran sulfate sodium (DSS)-induced colitis mouse model.

A6. Induction of Stress on HeLa Cells from InP/ZnS Quantum Dot Treatment

<u>Victoria Davenport</u>, Kyoungtae Kim Department of Biology, Missouri State University

InP/ZnS quantum dots (QDs) are an immerging option in QD technologies for uses of fluorescent imaging as well as targeted drug and anticancer therapies based on their customizable properties. In this study we explored effects of InP/ZnS when treated with HeLa cervical cancer cells. We employed XTT viability assays, reactive oxygen species (ROS) analysis, and apoptosis analysis to better understand cytotoxicity extents at different concentrations of InP/ZnS. In addition, we compared the transcriptome profile from the

QD-treated HeLa cells with that of untreated HeLa cells to identify changes to the transcriptome in response to the QD. RT-qPCR assay was performed to confirm the findings of transcriptome analysis and the QD mode of action was illustrated. Our study determined both IC50 concentration of 69 μ g/mL and MIC concentration of 167 μ g/mL of InP/ZnS. It was observed via XTT assay that cell viability was decreased significantly at the MIC. Production of superoxide, measured by ROS assay and flow cytometry, was decreased, whereas levels of nitrogen radicals increased. Using analysis of apoptosis, we found that induced cell death in the QD-treated samples was shown to be significantly increased when compared to untreated cells. We conclude InP/ZnS QD to decrease cell viability by inducing stress via ROS levels, apoptosis induction, and alteration of transcriptome.

A7. Macroinvertebrate Communities Across A Gradient of New and Existing Poultry Agriculture In Northeast Arkansas

<u>Allison Mundy</u>, Olivia Echols, Eli Kemp, Maryline Bossus, Erik D. Pollock, and Allyn K. Dodd Division of Natural Sciences, Lyon College

Arkansas is currently the nation's second largest producer of poultry. The industry is expanding eastward across the state, with dozens of new farms permitted following the construction of a chicken processing facility in northeast Arkansas in 2016. With the addition of new poultry houses to a pastoral landscape, ecologically sensitive waterbodies are at increased risk of losing sensitive macroinvertebrate taxa due to increased nutrient and sediment pollution. We determined macroinvertebrate community structure of twelve tributaries of the Eleven Point River and Black River along a gradient of poultry house densities (0.04 to 0.57 poultry houses/km2) with various flow path distances to agricultural operations. Our objective was to determine whether relationships exist between agricultural metrics and macroinvertebrate abundance, diversity, and percentage of sensitive taxa in the community. Our preliminary findings from 2 years of summer sampling campaigns suggest that poultry agriculture may be inducing declines in EPT taxa and homogenizing biological communities. Our efforts represent the first intensive monitoring program to address the impact of new poultry operations in eastern Arkansas.

A8. Investigating Gene Interactions in Breast Cancer Liver Metastasis via Cancer Bio Portal Data Analysis Pipeline

Chassidy Barnes Nathan Reyna

Department of Natural Sciences, Ouachita Baptist University

The development of publicly available cancer research databases, such as Caner Bio Portal, has changed the concepts of bioinformatic analysis; as a result, students and researchers alike must be versed in these new databases. Cancer BioPortal is an open-access, collective cancer research resource for the exploration of clinical and genomics data from a wide array of cancer studies. Cancer BioPortal eliminates the barrier of interpreting complex genomic data by providing researchers with easily understandable visualizations that can be interpreted and translated into relevant biological insights on the mutations and genetic alterations involved in the development and progression of cancer and applied in the clinical setting. The portal is used extensively in the research of different cancer types (i.e liver, breast, ovarian, pancreatic, and lymph node); however, efficient workflow for data collection and analysis applicable to researchers of every academic level is not currently available. Therefore an in-depth analysis of the portal to identify shared genes associated with metastasis in both breast and liver cancer was used to develop a pedagogical workflow and video tutorials for Cancer BioPortal. This study demonstrates TP53, CDK12, PTEN, EMSY, and PIK3CA interact to cause Breast Cancer Liver Metastasis. This workflow and associated video tutorials are to be implemented in the classroom and research setting for data collection and analysis using the portal.

A9. An Exploration of the Sympathetic Component of the Supradiaphragmatic and Abdominal Divisions of the Right Phrenic Nerve

<u>Shelby Kuhnert</u> Alla Barry Crystal Lemmons Department of Biology and Environmental Health, MSSU

INTRODUCTION: The phrenic nerve is a mixed nerve that arises from anterior primary rami of C3-C5 bilaterally and is the main motor supply to the diaphragm. The diaphragm muscle has a multifaceted impact on body functions- including breathing, visceral health, CSF flow, and emotional regulation. The phrenic nerve receives catecholaminergic fibers from the middle and lower cervical ganglia. However, previous studies reveal that both phrenic nerves lack the sympathetic component at the level of the diaphragm recovering it in the abdominal region supposedly from communication with a celiac plexus. Despite extensive research efforts, no clear understanding of the autonomic role of the phrenic nerve has been proposed. Thus, the aim of the current study along with investigating the branching pattern of the abdominal portion of the right phrenic nerve was to analyze the constitution of the branches, targeting the presence of sympathetic fibers. METHODS: Six formalin-preserved adult human cadavers were dissected at the MSSU human dissection laboratory. The anatomical course of the supra and subdiaphragmatic portions of the right phrenic

nerve was documented before obtaining tissue samples for histological examination. Samples were collected at the root of the neck, near the inferior vena caval diaphragmatic hiatus, and abdominal communicating branches. All sections were prepared using H&E and Luxol Fast Blue staining. Antibody staining for tyrosine hydroxylase (TH) was used to determine the presence of catecholaminergic fibers. The results were processed with ImageJ software for quantitative analysis. RESULTS: The cervical region displayed no TH activity indicating a lack of catecholaminergic fibers. TH positive fibers were only observed in the posterior trunk and abdominal branches of the right phrenic nerve. CONCLUSION. These findings support previous studies regarding celiac plexus communication with a phrenic nerve and provide a better understanding of the phrenic nerve anatomy and its autonomic function.

A10. New species of the green algal genus Coelastrella from Warren Prairie Natural Area in southeast Arkansas

<u>Sara Ambrocio Paque</u>, Brent Baker*, Marvin Fawley and Karen Fawley Department of Natural Sciences and Mathematics, University of the Ozarks *Arkansas Natural Heritage Commission, Little Rock, Arkansa.

Warren Prairie Natural Area in Bradley and Drew Counties, Arkansas, is a mosaic area of saline slicks that form flat, crusty depressions in a central area with a zone of lichens and a few rare angiosperms, and an outer zone of cyanobacterial mats. The edges of the saline slicks are home to the rare, diminutive vascular plant, Geocarpon minimum Mackenzie (Caryophyllaceae), which is a federally protected threatened species. Because the Warren Prairie slicks are home to many rare and unusual vascular plants, we hypothesized that the soil algae community will also comprise many unusual species. The main objective of our study was to characterize the soil crust eukaryotic algal communities using morphological and molecular techniques. We have characterized strains isolated from soil samples collected in February, 2016 and December, 2017. We generated 18S ribosomal RNA gene sequences for the strains and used BLAST searches of the GenBank database to determine preliminary identifications. Several strains were consistent with the coccoid green algal genera Coelastrella Chodat and Asterarcys Comas (Chlorophyta; Chlorophyceae). Light microscopy showed that cells were uninucleate with an irregular, spherical shape with the presence of autosporic asexual reproduction. In addition, cell wall ribs were observed in some of strains; a definitive characteristic in some species of Coelastrella. Phylogenetic analyses of both the 18S and ribosomal RNA internal transcribed spacer (ITS) regions indicated that some of the strains are a new species of the genus Coelastrella. Other strains are closely related to the recently described species, Coelastrella yingshanensis Qinghua Wang et al., but there is evidence that these strains may also be one or more new species.

A11. Further Analysis of a Potentially Ecologically Unique Tennessee Cave System and Future Direction for Study

<u>Lauren Camp</u>, Kaylie Wheeless, Aspen Huseman, Brianna Horton, James Engman, and Michael Ray Taylor Department of Biology, Henderson State University

Further Analysis of a Potentially Ecologically Unique Tennessee Cave System and Future Directions for Study Lauren Camp1, Kaylie Wheeless1, Aspen Huseman1, Brianna Horton1 Faculty Mentors: James Engman1, Michael Ray Taylor2 1Department of Biological Sciences and 2Department of Communication and Theatre Arts, 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, like Movile and Lechuguilla Cave. In this study, samples of bacterial communities were taken from an incompletely explored cave in central Tennessee, currently mapped to a length of over 13 miles. Samples were collected from a pool in an area called the "Petroleum Passage" because of its strong petroleum smell. The pool has a sandy bottom with scattered patches that give off black droplets of a tar-like substance, and are surrounded by concentric rings of colored sand, suggesting microbial activity. Samples analyzed include the patches and bands, water, and actively growing cave formations. Samples were analyzed with a technique allowing DNA to be removed directly, base sequences read, and matched to a large database to determine the identity of the organisms' present. For nine samples analyzed, 593 different bacteria and Archaea were identified, including many unique species that metabolize sulfur and methane compounds, previously associated with deep sea thermal vents, and others that degrade hydrocarbons. The yellow sand ring in particular had several unique bacteria including some from the order Ardenticatenales, which has been isolated from hydrothermal fields in Japan, and the family Paenibacillaeceae which has previously been found in Lechuguilla Cave. Future plans include retrieving more targeted samples for metagenomic sequencing, salamander identification, standard water chemistry analysis, and hydrocarbon analysis. The results of this survey and future studies could potentially provide insight into how this cave formed and microbial species in extreme environments on Earth, as well as offer a new example of a type of system that has been suggested as a potential model for life in subsurface environments on Mars.

A12. Tunable sized combination nanodrugs based on ionic materials

<u>Stuti Chatterjee</u>, Dr. Noureen Siraj, Dr. Nawab Ali, Samantha Macchi, Robert Griffin, and Amanda Jarman Department of Chemistry/ Department of Biology, University of Arkansas at Little Rock

Cancer is still the second leading cause of death in the US only surpassed by heart disease. Thus, the need for new and more effective treatment methods is of utmost importance. Combination therapy is a technique that involves using one or more methods of treatment simultaneously to avoid the negative side effects of each method. In this work, we combine a photothermal therapy (PTT) drug and chemotherapeutic drug to develop a PTT-chemo combination drug. Aqueous nanoparticles are derived from the combination cancer therapeutic drug using a simple reprecipitation method. Particles of varying sizes were produced to investigate the most optimum size in terms of cytotoxicity in vitro and photothermal effect.

A13. Effect of root biomass on prenylated stilbenoid yield in hairy root cultures of peanut

Izzeldin Ahmed, Krystian Roedel and Fabricio Medina-Bolivar

Arkansas Biosciences Institute and Department of Biological Sciences, Arkansas State University

Stilbenoids are polyphenolic compounds produced in certain plants to combat pathogenic attacks. They have shown to possess antioxidant and anticancer activities with potential benefits to human health. Previously, hairy roots of peanut were established as an inducible bioproduction platform for the non-prenylated stilbenoids resveratrol and piceatannol and the prenylated stilbenoids arachidin-1, arachidin-2, arachidin-3, and arachidin-5. The current procedure involves culturing of the hairy roots in 250 mL flasks with 50 mL of medium containing 3% sucrose. The purpose of this project was to increase the root biomass and consequently the overall yield of stilbenoids in the hairy root cultures. To this end, the hairy roots were grown in various growth conditions which included an increase in sucrose concentration (4 - 6%), flask volume (500 mL), and culture medium volume (100 mL). The highest root biomass was obtained when the hairy roots were cultured in 500 mL flasks with 100 mL of medium. To investigate if this biomass increase would lead to an increase in stilbenoids, hairy roots grown in 500 mL flasks and 100 mL medium were co-treated with the elicitors methyl jasmonate, hydrogen peroxide, cyclodextrin, and magnesium chloride for 168 hours to induce production of prenylated stilbenoids. Upon extraction of the stilbenoids from the culture medium and analyses by high-performance liquid chromatography (HPLC), the yield of stilbenoids (resveratrol, arachidin-1. -2, -3 and -5) was 642.2 mg/L which was almost twice the amount found when the hairy roots were cultured in 250 mL flasks with 50 mL of medium. These findings proved that by increasing root biomass, the yield of stilbenoid can also be increased.

A14. Investigate the interactions between non-legume plants and plant growth-promoting bacteria at a molecular level

<u>Devyn Ruiz</u>, Arijit Mukherjee, Ph.D., John Cook Department of Biology, University of Central Arkansas

Non-legume plants such as rice and maize can form beneficial associations with plant growth-promoting bacteria (PGPB). Several studies have shown that PGPB, such as Azospirillum, Herbaspirillum, Burkholderia, etc. can promote plant growth via nitrogen-fixation and hormone synthesis. Among these, Burkholderia represents an intriguing genus of PGPB whose members are found in various ecosystems, including soil, water, plants, and animals. Burkholderia species are currently classified into two groups, pathogenic species belonging to the Burkholderia cepacia clade (BCC) and plant-beneficial species in the environmental clade (PBE). PBE Burkholderia (e.g., B. unamae, B. silvatlantica, etc.) have a diverse host range (e.g., maize, rice, wheat, etc.) and are considered as one of the most potent PGPB. However, the molecular mechanisms of Burkholderia's association with their host plants (e.g., maize, rice) are mostly unknown. We already established the experimental systems where B. unamae can promote plant growth in rice and maize. Using the same experimental system, our goal is to identify transcriptomic changes in plant roots during their association with the bacteria. Recently, we submitted the different rice RNA samples to the Texas A & M University Genomics facility for RNA sequencing. We expect to identify gene pathways involved in bacterial recognition, crosstalk with the bacteria, successful plant-bacteria association, and transport of essential nutrients. Results from this study will facilitate the identification of potential plant genes that might be involved in pathways leading to plant growth promotion.

A15. Osmoregulatory proteins in the neotenic salamander Ambystoma mexicanum

<u>Hannah Wu</u>, Michael Uecker, Maryline Bossus Department of Biology, Lyon College

Ambystoma mexicanum, most widely known as the Mexican axolotl, is a vertebrate that is extensively used for research to study human diseases, cancer, regeneration, and aging process. Interference against osmoregulation is the cause of health issues and sickness such as cystic fibrosis. Therefore, knowledge of water and ions epithelial transport in axolotl can provide us with new insights on homeostasis mechanisms in vertebrates and potentially have health applications. Little is known about osmoregulation and the proteins involved in this process in amphibians, more specifically, axolotls. This project aims to determine whether osmoregulatory proteins normally found in aquatic vertebrates are also expressed in axolotls and if so, in which organs and at what stage of the development do they appear. Samples were extracted from axolotls at key stages of development and in adults for further molecular analysis. Osmoregulatory proteins were sequenced and real time quantification (qPCR) analysis was used to characterize and localize proteins found in organs known to be involved in osmoregulation. Ongoing research will define the transcellular pathway mechanisms of osmoregulation in Ambystoma mexicanum from embryo stages to adult.

A16. Surveillance Study on Culex sp. in southeast Kansas and Prevalence of West Nile Virus in the Mosquito Population

<u>Sara Goins</u> and Anuradha Ghosh Department of Biology, Pittsburg State University

West Nile virus (WNV) is the most common mosquito-borne disease in Kansas and the United States. Several species of mosquitoes can carry WNV but Culex is the most common in the U.S. The Kansas Department of Health and Environment (KDHE) announced that Kansas and neighboring states are becoming more and more hospitable to the Culex mosquitoes as average temperatures rise. According to the U.S. Centers for Disease Control and Prevention (CDC), 80% of people infected with WNV show no symptoms; but for the remaining 20%, symptoms can include headaches, body aches, joint pains, vomiting, diarrhea, or rash. KDHE reported 600 cases of the worst form of the disease in KS, including 30 deaths (1999-2017). KDHE in recent years has designated different areas of the state at high and moderate risk levels for contracting WNV. Our study aimed at sampling mosquito populations from landscaped vegetation at residential & commercial properties, parks, cemeteries, and wetland habitats in urban and suburban Crawford County and adjacent areas in southeast Kansas. Several water samples have been collected using a long-handled water sampler as well as a triangular dip net. The samples were observed over time for the presence of various life stages of mosquito as well as macroinvertebrates. A CDC light trap was also used to capture mosquitoes from different locations. The mosquitoes were identified using taxonomic keys in the laboratory and sexed. Further, total RNA will be extracted and prevalence of WNV will be determined using real-time reverse transcriptase-PCR (RT-PCR) assays. In addition to the surveillance data available from KDHE, the outcome of this study will provide unique information about viral load in these vectors and host populations as well as early- and late-season testing of the mosquito vectors will detect temporal changes in the viral load.

A17. How Patterns of Behavioral Flexibility and Diet Breadth Correlate in Bees

<u>Vanessa Morales</u>, Abilene Mosher, Avery Russell Biology, Missouri State University

Animal diet breadth varies along a continuum, from extreme specialization (foraging on a few or one food type) to extreme generalization (foraging on many different food types). Greater diet breadth is frequently associated with highly flexible foraging behavior, which is thought to facilitate foraging on diverse food types. Accordingly, increasing specialization (i.e., feeding on fewer and less different food types) should be associated with reduced flexibility in foraging behavior. Bees vary in their pollen diet breadth from being highly specialized on a few flowering plant species, to being highly generalized and foraging on a diverse array of flowering plant species. Likewise, we might expect that bee pollen foraging behavior complexity would correlate with pollen diet breadth. However, we currently lack a consolidated accounting of how pollen diet breadth and foraging behavior vary across the approximately 20,000 bee species. In this study, we are conducting a literature search to determine the pollen diet breadth and number of pollen foraging behaviors (a proxy for behavioral flexibility) of as many bee species as possible. Over 800 bee species and their pollen hosts have been recorded in our database so far. Our records indicate that of these bee species, around 1% are extreme specialists and a further 62% are strongly specialized; only around 37% of the bee species are extreme generalists.

A18. Prenylated Stilbenoids from Peanut as Potential Therapeutic Agents for Triple Negative Breast Cancer

<u>Linh-Chi Ho</u>, Sepideh Mohammadhosseinpour, and Fabricio Medina-Bolivar Department of Biological Sciences, Arkansas State University

Breast cancer is the most common cancer in women worldwide and triple negative breast cancer (TNBC), consisting of 15% of breast cancers, is one of the deadliest types because it does not respond to hormonal treatments. Due to this issue, there is an ongoing search for new treatments to increase its survival rates. Prenylated stilbenoids are phenolic compounds that are produced in plants, such as peanut, pigeon pea, and mulberry, as part of their defense system against stress. These compounds have been shown to exhibit many beneficial properties, one of which is anticancer, and therefore, the overall goal of this study is to evaluate the anticancer activity of prenylated stilbenoids as natural products for the treatment of TNBC. To induce the production of prenylated stilbenoids, peanut hairy root cultures were co-treated with methyl jasmonate, cyclodextrin, hydrogen peroxide, and magnesium chloride, and then the prenylated stilbenoids were separated from extracts of the culture medium via semi-preparative high performance liquid chromatography (HPLC). The anticancer activity of the prenylated stilbenoids was evaluated in different TNBC cell lines. Flow cytometry and MTS assays showed that the prenylated stilbenoids arachidin-1 and arachidin-3 exhibited higher cytotoxicity to the cancer cells than the non-prenylated stilbenoid resveratrol. These studies suggest that prenylated stilbenoids should be further studied as potential therapeutic agents for TNBC.

A19. Myosin 2's effect on Vps10 and Snc1 traffic

<u>Glory Ehie</u>, Vy Nguyen, and Dr. Kyoungtae Kim CNAS, Missouri State University

Alzheimer's disease is very common in America and is partly associated with dysregulation of intracellular trafficking between the endosome and the Golgi. Myosin 2 is involved in intracellular transport among the Golgi, endosome, and transport vacuole. Previously, we identified that Myo2 plays a role in transport of Vps10 and Snc1 to the Golgi. When Myo2 is mutated, localization patterns of these cargoes are found to be significantly disrupted, suggesting Myo2's role in the sorting and delivery of these cargoes. We hypothesize that the majority of Vps10 and Snc1 in myo2 mutant cells won't be retrieved from the endosome and vacuole and that as a result, both cargoes will show high levels of colocalization with endosome and vacuole markers. My findings on this experiment will be presented at the conference. Furthermore, we have worked to see if Myo2 is implicated in Snc1 exocytosis to the plasma membrane, and we found that Snc1 is normally targeted to the plasma membrane even in a myo2 mutant strain. However, we will test this traffic using more myo2 mutants. Our approach to test Snc1's plasma membrane targeting involves the use of Snc1-pm mutant, which is competent in exocytosis and incompetent in endocytosis Taken together, our results will shed new light in activities of myo2 in mediating these cargo trafficking toward the Golgi.

A20. A new soil species of the green algal genus Diplosphaera Bialosuknia from Warren Prairie Natural Area in southeast Arkansas

<u>Kengor N. Thermozier</u>, Brent Baker*, Marvin W. Fawley and Karen P. Fawley Natural Sciences and Mathematics, University of the Ozarks *Arkansas Natural Heritage Commission, Little Rock, AR

Diplosphaera Bialosuknia (Chlorophyta; Trebouxiophyceae) is a very small green alga commonly found as a photobiont in lichens and free-living in many types of soil. Cells of Diplosphaera are spherical or nearly so and are often grouped in short chains. There is essentially no morphological variation among the known species of this genus. In our study of the soil algal community of Warren Prairie Natural Area in southeast Arkansas, we isolated several strains that matched the morphological characteristics of the genus Diplosphaera. BLAST search of the GenBank database using 18S nuclear ribosomal RNA gene sequences from these strains confirmed that the strains are in the genus Diplosphaera. Phylogenetic analysis of DNA sequences from the 18S and ribosomal RNA internal transcribed spacer (ITS) regions confirmed that the Warren Prairie strains are a new species. This conclusion was also supported by analysis of the secondary structure of the ITS2 RNA sequence. All of our results indicate that the Warren Prairie strains are a new species.

A21. Nonpoint Source Pollution and Water Quality Under Increasing Pressure from Poultry Agriculture

<u>Olivia Echols</u>, Linda Fowler, Allison Mundy, Destiny Howell, Tionne Stubblefield, Victoria Prater-Rochier, Erik D. Pollock, Maryline Bossus, and Allyn K. Dodd Division of Natural Sciences, Lyon College

Rapid expansion of new poultry agriculture in Northeast Arkansas since 2016 has increased the likelihood of nutrient enrichment, sediment pollution, and ecological degradation. Despite increasing poultry farm abundance in a landscape already impacted by pastoral agriculture, current water quality monitoring in these watersheds is limited in spatial and temporal coverage. Our objective was to evaluate water quality along a gradient of poultry and pastoral agriculture, thereby identifying areas that may need nonpoint source pollution mitigation. We present results from monthly sampling events from June 2019 to July 2020 in twelve streams along a gradient of subcatchment poultry house densities (e.g. 0.04-0.57 poultry houses/km2), pastoral land cover, and flow path distances from poultry farms. We measured dissolved nitrogen and phosphorus, turbidity, total suspended solids, algal biomass, microcystin, and habitat characteristics at each site. Summer 2019 total suspended solid concentrations increased with greater subcatchment poultry house density. Additionally, summer 2019 total suspended solid concentrations were negatively related to subcatchment pastoral land cover. Our findings suggest that new poultry farms may be enriching headwater streams, while pastures may be reducing sediment loads during the growing season. Our efforts reveal how compounded impacts of animal agriculture influence stream water quality and habitat characteristics.

A22. Dictyostelium Social Amoeba Symbiont Prevalence Across Hardwood Forests of Arkansas

<u>Mackenzie Hoogshagen</u>, James DuBose, and Tammy Haselkorn Department of Biology, University of Central Arkansas

Social amoebae are natural predators of bacteria, digesting them via phagocytosis. Certain bacteria, however, have evolved to resist digestion, leading to the formation of symbioses with the amoeba. This system could be used to answer larger questions on the evolution of symbionts and pathogens that are able to evade macrophages in other organisms. Three bacterial symbionts are known to commonly infect populations of Dictyostelium, but the potential benefit to either the amoeba or the bacteria is largely unknown. These symbionts include Paraburkholderia, Chlamydiae, and Amoebophilus. In lab studies, Paraburkholderia has shown to elicit a farming phenotype when infecting Dictyostelium discoideum, allowing them to carry food bacteria when dispersing. To better understand these symbioses, we collected soil from bottomland and upland hardwood forests across Arkansas. We also measured soil temperature and soil pH. Amoeba fruiting bodies from the soil were then grown and collected in the lab. We then extracted DNA from the fruiting bodies and used PCR screening to determine symbiont presence. We will use the symbiont prevalence to identify environmental conditions that potentially favor the formation of symbiosis.

Biology Session B

B1. Using CRISPRi-dCas9 to identify nitrogen sources used by a nitrogen-fixing methanogen

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

Carbon and nitrogen are required to sustain all life. Bacteria and archaea are critical in the cycling of carbon and nitrogen on earth. For example, methanogens are anaerobic archaea that produce methane, a key intermediate in the global carbon cycle. Methanogens are also the only archaea that possess nitrogenase, the enzyme required to fix dinitrogen (N2) to ammonia (NH3), a critical step in the global nitrogen cycle. Increasing knowledge on the metabolic processes of methanogens can increase their utilization in biotechnological applications, as well as further our understanding of their environmental impact. We are using Methanosarcina acetivorans as a model to understand the synthesis, activity, and regulation of nitrogenase in methanogens. The reduction of N2 by nitrogenase requires significant energy (N2 + 16ATP + 8e- + 8H+ \rightarrow 2NH3 + H2 + 16ADP + 16Pi). Thus, nitrogenase is only used to fix N2 when no other nitrogen source is available. The preferred nitrogen source for methanogens is NH3. The goal of the experiments performed were to discover other possible nitrogen sources for M. acetivorans. This information will aid understanding the regulation of nitrogenase. Using the CRISPRi-dCas9 system, M. acetivorans strain DJL74 was created in which expression of nitrogenase is blocked by dCas9, which abolishes nitrogen fixation. Therefore, strain DJL74 can only grow with nitrogen sources other than N2. The ability of strain DJL74 to grow with organic (amino acids and trimethylamine) and inorganic (e.g. nitrate) nitrogen compounds was tested by adding each compound separately to culture tubes inoculated with strain DJL74. Growth was subsequently monitored by measuring optical density. Ammonium chloride was included as the positive control and water as the negative control. Results showed that, of the amino acids tested, only the addition of glutamine resulted in significant growth of strain DJL74 compared to the controls. DJL74 also exhibited growth with trimethylamine, a known carbon source for M. acetivorans. Addition of inorganic nitrogen sources failed to allow growth of strain DJL74. These results indicate that M. acetivorans has a narrow range of usable nitrogen sources. Therefore, when M. acetivorans is in environments that lack sufficient NH3, glutamine, or trimethylamine it is relegated to the energy intensive process of fixing N2 to provide nitrogen for biosynthesis.

B2. Cytosolic and Amylopastic ATP and pH Dynamics in Rice Grains with Contrasting Chalkiness

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Chalkiness is an undesirable trait in rice that drives down its market value. Previous studies have identified potential molecular markers to breed low chalk rice. A known marker is Chalk5 which codes for vacuolar H+ translocating pyrophosphatase (VPPase), an enzyme hydrolyzing pyrophosphate into inorganic phosphate (Pi) and consequently funneling H+ to the vacuole. Overexpression of Chalk5 has been hypothesized to change the cytosolic pH which accordingly disturbs endomembrane trafficking. The disturbance cascades to starch biosynthesis, leading to the formation of chalky grains. Starch biosynthesis is an energy dependent process that occurs in the cytosol and amyloplast. These suggest that the dynamics of pH in the cytosol, energy in the cytosol and amyloplast, and expression of Chalk5 can partially explain chalkiness. In addition to VPPase, another enzyme which can funnel H+ into the vacuole is the vacuolar ATP Synthase (VATPase). Apart from generating ATP, the H+ translocating nature of vacuolar ATPase indicates that it can also affect cytosolic pH. Thus, genes coding for the subunits of this enzyme such as vacuolar ATPase subunit A (VHA-A2) can be a determinant of chalkiness. To understand the mechanism of these genes in chalkiness, formation of chalk in cultivars with translucent grains under normal condition are induced by heat, a known factor that increases chalkiness. Changes in pH, ATP and Pi levels, gene expression and chalk related traits are observed. Changes in pH are determined using transgenics expressing enhanced green fluorescent protein (eGFP) that are targeted to the cytosol and amyloplast by using Ubiquitin (UBIQ) promoter and Granule Bound Starch Synthase I (GBSSI) signal peptide, respectively. ATP level is estimated by using transgenics with cytosol or amyloplast targeted luciferase expression. The product abundance of these genes, Chalk5 and VHA-A2, is measured through transcript levels at relevant stages. These observations will be correlated with factors which may affect chalkiness including amylose and amylopectin ratio, protein content, and granular morphology.

B3. Does elemental composition of North American grapevines reflect environmental adaptation?

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North American grapevines (Vitis species) are adapted to varied environmental conditions and occupy widely different geographic ranges. This adaptation resulted in a vast biological diversity, which has been exploited by grape breeders over the past 150 years to solve some of the most dire problems of viticulture. We examined if the elemental composition of grape leaves revealed species-specific nutritional features that reflect adaptation to their native environment. We measured the concentration of 19 different ions in leaves of 198 grapevine accessions representing 8 native North American grapevine species. All individuals were well established vines grown in a common garden setting at the USDA National Clonal Germplasm Repository. Multivariate analysis of the resulting ionomics data revealed that a significant percentage of variation could be partitioned among certain species. We found that the concentration of most ions had a significantly greater variability in Vitis cinerea (Englem.) accessions than in other grape species. We were able to demonstrate that linear discriminant analysis could predict the species of native North American grapevine using the concentration of ions found in the leaf as an indicator.

B4. Evidence from Cnidaria supports an ancient evolutionary origin of FoxP genes in animals

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Cnidarians (e.g. jellyfish and sea anemones) can provide valuable insights into the early evolutionary history of animals due to their informative position in the animal phylogeny as a sister group to Bilateria (e.g. vertebrates and insects). By studying the cnidarian N. vectensis, we aim to gain a better understanding of the evolutionary origins of bilaterian traits. The FoxP genes in Bilateria are known to be expressed in the developing central nervous system, but FoxP genes have not been confirmed in Cnidaria. To look at the evolutionary history of this gene, we examined a gene sequence in N. vectensis that had similarities to other FoxP sequences in bilaterian species. In order to determine whether FoxP exists in this species, we used Geneious Prime to import Fox gene sequences

of various families (A-P) in multiple vertebrate and invertebrate species, including the putative N. vectensis FoxP-like gene. Using a maximum likelihood method RAxML, we found that the potential FoxP gene belongs to the FoxP clade. Left and right primers were synthesized with the gene sequence for Reverse Transcriptase PCR to determine whether the gene is expressed in the postembryonic developmental stage. The PCR results were analyzed with gel electrophoresis to confirm the products. With these tests, we concluded that FoxP does exist and is expressed in N. vectensis. This finding indicates that FoxP has an ancient evolutionary origin predating the origins of Cnidaria and Bilateria, and paves the way for further studies examining this gene and its family's role in Cnidaria, and whether it plays a similar neural developmental role in this clade.

B5. Immunolocalization of Osmoregulatory Proteins in Axolotl, Ambystoma mexicanum

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Hydromineral balance regulation is a key physiological process negatively influencing development, growth rate and survival when organisms are subjected to strong environmental stresses. Despite how critical these processes are, the mechanisms of osmoregulation in Ambystoma mexicanum, a vertebrate model extensively used to gain new insights about human physiology and pathology, have yet to be elucidated. This research project aims to use immunohistochemistry to determine which organs are involved in transcellular osmoregulatory mechanisms through the localization of osmoregulation proteins such as Na+/K+-ATPase (NKA), Cystic Fibrosis Transmembrane conductance regulator (CFTR) and Na+/K+/2Cl--cotransporter (NKCC). Organs were sampled from juvenile and adult axolotls, fixed and embedded in paraplast blocks. Sections of 5 µm were performed and used for histological staining and immunolocalization of NKA, the motor of osmoregulation. Ongoing research will determine the immunolocalization of other proteins involved in osmoregulatory transcellular pathway mechanisms in Axolotls at various stages of development.

B6. Oxygen Production In Spiral and Straight Shaped Arthrospira Platensis

<u>Tessa Watson</u>, Jim Taylor, and Race Karlin Department of Biology, Ouachita Baptist University

Space travel is, naturally, not an easy task to accomplish. There is always a drive for becoming faster, more efficient, and more advanced. With missions lasting long periods of time while working with limited supplies of food and oxygen, there is a need for innovation. It may be shocking to some that cyanobacteria could be the answer to these problems. A certain kind of cyanobacteria that has been of particular interest is Arthrospira platensis, otherwise known as Spirulina. Spirulina serves not only as an optimal protein, vitamin, and nutrient food source, but it's also photosynthetic. This means it uses human waste of carbon dioxide to produce oxygen. This experiment worked with two types of Spirulina, including 100% spiral shaped cells and 80% spiral and 20% straight shaped cells. The study focused on examining the difference in oxygen production between them. This was done by growing a culture of each type under similar conditions. From these cultures, about 3 liters of each were placed in plastic tubs designed to measure the amount of oxygen produced. Each tub received a stir bar and were set in light boxes of similar intensities. This way, the experiment mimicked anti-gravity and no natural sunlight such as in space travel. Cell population and the amount of oxygen produced in each tub were measured and recorded after every 24 hours for approximately 72 hours. Although the culture containing 80% spiral shaped and 20% straight shaped cells appeared to produce more oxygen per cubic mL than the 100% spiral shaped Spirulina, it did not produce quite enough to be statistically significant. Despite this, the study did show that Spirulina consistently produced oxygen when cultures are in ideal health. This is yet another example as to why Spirulina could be useful in space travel. Not only would it serve as an excellent food source, but it could also help continuously convert human waste into fresh, breathable oxygen.

B7. Investigating the Potential Role of Human Herpesvirus 6 (HHV6) Infection in Epileptogenesis

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One of the most ubiquitous human herpesviruses is human herpesvirus 6 (HHV6). It is estimated that >95% of the human population is infected with HHV6 by the age of 6. Primary infection manifests as a common childhood ailment known as roseola infantum, which features a rash on the trunks and limbs as well as a short-term fever. After primary infection, HHV6 typically enters into a latent state and can remain that way throughout the life span of the host. However, it can reactivate. Upon reactivation (especially in adulthood), the virus can lead to a host of neurological disorders including multiple sclerosis and, perhaps, epilepsy. However, little information is known about the potential mechanisms by which HHV6 may induce seizure leading to epileptogenesis. Indeed, little is known about nerve cell tropism for the two subtypes HHV6A and HHV6B, especially with regard to susceptibility of distinct

neuronal phenotypes. Furthermore, for those cells that have been shown to be susceptible to one or both of the HHV6 subtypes, cytopathic effects (CPEs) have not been detailed. In this study, differentiated human neural stem cells were challenged with either HHV6A, or alternatively, HHV6B at defined multiplicities of infection (MOIs). We then monitored gross changes in the culture and quantified morphological changes in individual cells to determine if there are differential CPEs between HHV6A- versus HHV6B-infected neurons. Specifically, measures of the number and lengths of neurite projections were recorded at different time points after initial infection. Likewise, soma size was measured for each target neuron and it was noted if HHV6 infection led to syncytia formation. Our data indicates that the HHV-6A and HHV-6B virus has noticeable effects on neuron and glia cells in human neural stem cells. We have created a procedure to find the aforementioned data from light microscopy images of hNSCs. We used a machine learning algorithm plugin via the ImageJ software for light microscopy images of hNSCs, and a separate tool that automatically traces fluorescence microscopy images of neurons called NeuronCytoII. We categorized each cell by their shape: circle, triangle, or square. Our data displayed that the number of cells and the length of the neurites decreased post differentiation for each type of cell.

B8. Bacterial Growth Inhibition by Sodium Toxin Na668

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Antibiotic resistance is a growing problem for the field of medicine, and the only remedy for this problem is the discovery of novel antibiotic compounds. Antibiotic compounds have typically been found in soil samples, but some scientists have been exploring the bodily fluids of animals in search of antibacterial compounds. The same concept is explored here in a study of the antibacterial properties of the venom from Centruroides vittatus, more commonly known as the Striped Bark Scorpion, which can be found in the rural areas of Arkansas. The venom of this scorpion contains a beta sodium toxin which can alter the activity of voltage gated sodium channels. Ion gated channels support chemical gradients in cells that allow them to create electrical potentials across their cellular membranes. Voltage gated channels open and close pores in the membrane that allow specific ions through. Beta sodium toxin Na668, our toxin of interest, attaches to the sodium channels 1.4 and 1.5 and binds to segment 4 of the channel. This causes the energy of activation for sodium ions crossing to be lowered. Since voltage gated sodium channels are essential for the cellular activity, the beta sodium toxin has the potential to kill bacteria by acting on their voltage gated sodium channels. When the activation energy needed for sodium ions to enter the cell is lowered, more sodium can enter the cell than is needed which upsets chemical gradients needed for metabolic activity and may cause the cell to burst if too much fluid enters. In this way, Na668 could be used as an antibacterial compound. The goal of this research project is to determine if Na668 present in the venom of C. vittatus is an effective compound to inhibit bacterial growth, and if so, which bacteria are most effectively inhibited by it. To test this hypothesis, S. aureus and E. coli were cultured then incubated with four different treatments, and later plated to count the colony forming units present in the solution The four treatment solutions are as follows: a positive control, ampicillin to inhibit growth for comparison, Na688 beta sodium toxin, and a negative control.

B9. Functional Control of the Drosophila Lipin Protein by Phosphorylation

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The Lipin protein of Drosophila melanogaster is required for fat storage and fat tissue development. It has a phosphatidate phophatase activity in the cytoplasm that converts phosphatidic acid into diacylglycerol, the direct precursor of neutral storage fats, and a transcriptional co-regulator activity in the nucleus. Whether Lipin acts as an enzyme in the cytoplasm or a transcriptional regulator in the nucleus is regulated by post-translational modifications of the protein. Lipin, and its mammalian counterpart lipin-1, contain a large number of phosphorylation sites located in similar positions within the proteins. Phosphorylation sites in lipin-1 have been shown to be involved in the control of nuclear translocation. They are also thought to be involved in the control of other activities of lipins, such as enzymatic activity. The goal of our project was to generate and characterize a mutant fly stock expressing Lipin in which the serine residue at position 820 of the protein is replaced by a residue of the phosphomimetic amino acid glutamate (LipinS820E). Previous work had shown that rendering this site non-phosphorylatable (LipinS820A) leads to decreased fat stores and increased susceptibility to starvation. We successfully introduced the LipinS820E mutation into the Drosophila genome using CRISPR/Cas9 methodology. Single-stranded oligonucleotides together with a guideRNA-expressing plasmid into early Drosophila embryos, fly lines for individual mutagenized chromosomes were established. These lines were screened for the presence of the mutation through polymerase chain reaction and DNA sequencing. We found that animals homozygous for the mutation were viable. Future work will include a detailed phenotypic characterization of the LipinS820E mutant. Established assays will be used to

examine potential developmental defects of the animals, their starvation resistance, size of trigylceride stores, and fat droplet size and number in the fat tissue.

B10. Testing of Novel Photodynamic Agents for Viability and Localization in Photodynamic Therapy

<u>Gabe Poe</u>, Dr. Joseph Bradshaw, and Dr. Timothy Hayes Department of Biology, Ouachita Baptist University

Design of novel cancer drugs and treatments is an always present need. One of these treatments is photodynamic therapy (PDT). It involves the use of a light sensitive compound, called a photodynamic agent (PDA), and light exposure to kill cancerous cells. PDAs can include a porphyrin, chlorin, or bacteriochlorin backbone with varying substituents. Our experiment sought to test the effectiveness of three porphyrins, H2TTP-DIPA, ZnTTP-DIPA, and GaNO31- TTP-DIPA, at different concentrations. All three porphyrins had the same substituents. They were distinguished by the exclusion or inclusion of a metal chelated in the center of the porphyrin rather than the typical hydrogens. They were compared to the PDA Foscan, which works at a very low concentration. They were tested on the A549 non-small cell lung cancer cell line using MTT viability assays. Of the three porphyrins only ZnTTP-DIPA effectively killed cells at a low enough concentration for further testing. Confocal Microscopy was undertaken to determine possible localization of the ZnTTP-DIPA and Foscan, which was once again used as a control. Three organelle trackers (mitochondria, endoplasmic reticulum, and golgi apparatus) were used as comparisons for the compounds. Correlations were found between Foscan and an ER tracker, suggesting Foscan localizes to the ER. No correlations were found between ZnTTP-DIPA and the trackers used.

B11. Microglia are persistently activated after removal of extracellular TDP-43

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

The proper response to protein signals is necessary for a healthy central nervous system, and protein dysregulation is a feature of neurodegenerative diseases. Transactive response DNA-binding protein-43 (TDP-43) is an intranuclear protein in motor neurons and dysregulation is associated with amyotrophic lateral sclerosis (ALS). Cerebrospinal fluid and blood plasma of ALS patients contain TDP-43, demonstrating its release into the extracellular space. Our previous research and the literature suggest that TDP-43 is a pro-inflammatory stimulus. The goal of this study was to determine the impact of TDP-43 on microglial function and recovery. To study this, cultured microglia were stimulated for 24 hours with TDP-43 or a vehicle; then the media was changed to remove the stimuli. This model allowed us to measure microglial activation after a recovery period following TDP-43 stimulation. The results show that activation of microglia remains persistent throughout the recovery period. These data demonstrate that TDP-43 shifts the balance of signaling pathways toward an inflammatory phenotype and alters the ability of microglia to appropriately recover after removal of the inflammatory stimuli.

B12. Bioinformatic Analysis of Antibiotic-Producing Soil Bacteria

<u>Griffin Hopkins</u>, Taylor Savage, and Dr. Ruth Plymale Department of Biology, Ouachita Baptist University

The ESKAPE pathogens, a group of six multidrug-resistant bacteria associated with nosocomial infections, have led to a search for new treatments able to combat antibiotic-resistant infections. Soil bacteria in the genera Burkholderia (strain name Hargis) and Pseudomonas (strain name DL-A23) were previously found to produce antibiotics capable of inhibiting growth of several Gram negative ESKAPE pathogens. Whole-genome sequencing was performed on both Hargis and DL-A23 using a PacBio Sequel instrument, with sequencing and assembly done at MOgene. QUAST was used to verify that reconstruction of each chromosome into a single contig, with Hargis assembling into three contigs and DL-A23 assembling into one. BUSCO further verified complete genome assembly; Hargis contained 92% of expected bacterial BUSCOs and DL-A23 contained 96%. FastANI was then used to classify each bacterium to species; at least a 95% FastANI identity is required to identify a bacterium to species. Hargis had a 95.12% similarity to Burkholderia pyrrocinia, and DL-A23 had a 97.83% similarity to Pseudomonas rhodesiae. Prokka was used for preliminary genome annotation, finding 7,579 coding sequences in the 8.5 Mbp Hargis genome and 5,424 coding sequences in the 6.1 Mpb DL-A23 genome. Finally, the programs BAGEL, AntiSMASH, and Prism were run to find genes that may contribute to antibiotic production.

B13. Effect of Soil Microbiome Succession on the Prevalence of Antibiotic Resistance

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Antibiotic resistance is a major threat to human health, with more than 2.8 million antibiotic-resistant infections per year in the U.S. alone. To better understand antibiotic resistance in natural environments, the long-term goal of this project is to determine how bacterial-fungal interactions impact the prevalence of antibiotic resistance genes (ARGs) in soil microbial communities undergoing tallgrass prairie restoration. We are currently investigating the abundance and diversity of bacteriome and mycobiome communities in soils from virgin (Massard Prairie); and remnant, developed, and tallgrass prairie undergoing restoration since 2016/2017 in Ben Geren Park (Fort Smith, AR). We sampled 12 bacteriomes from these sites in February 2019 (Shaver et al. 2020), and 16S rRNA (bacteriome) and 18S-ITS1-ITS2 (mycobiome) gene sequencing of samples collected at the same sites for a second (February 2020) and third (September 2020) timepoint are currently underway. In addition, the determination of prevalence and abundance of 87 ARGs in our initial 12 soil samples from February 2019 has just begun. ARGs in each sample will be profiled using the Antibiotic Resistance Genes Microbial DNA qPCR array available from Qiagen (Valencia, CA; Cat. no. 330261 BAID-1901ZRA) and compared to results from Kirby-Bauer antibiotic disk diffusion analysis of soil isolates. The qPCR assay targets ARGs representing all major classes of antibiotics used extensively for medical and veterinary applications. We predict higher abundance of ARGs in turfgrass and earlier restorations and decrease in abundance over time as fungi become more dominant in soils (Ritsema 2020). The qPCR assays, and 16S rRNA and 18S-ITS1-ITS2 sequencing are being carried out at UAMS in the Genomics Core Lab. This project is supported by the Research Technology Core of the Arkansas INBRE program, supported by a grant from the National Institute of General Medical Sciences, (NIGMS), P20 GM103429 from the National Institutes of Health.

14. Formation and Characterization Of Injectable Hydrogel Matrix To Generate Artificial Lymph Node

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Department of Biological Sciences, Arkansas Tech University, Russellville, AR, 72801 Breast cancer is one of the most commonly diagnosed cancer among women. A woman living in the United States has a 12.3% lifetime risk of being diagnosed with breast cancer. Lymph node (LN) excision, in combination with radiation and chemotherapy, is widely recommended to treat early breast cancer cases. These treatments generally result in secondary lymphedema. Secondary lymphedema develops due to insufficient drainage of interstitial fluid by lymphatics. Protein-rich interstitial fluid in secondary lymphedema may serve as a portal of infection. Therefore, secondary lymphedema is considered as one of the most dreaded complication following breast cancer treatment. Current approach to reduced secondary lymphedema rely on medications like diuretics or compression therapies with temporary and limited success. Previous studies in sheep animal model showed that the autologous LN translation significantly reduced secondary lymphedema. In the current study, we investigated the feasibility to generate artificial LN like structure by injecting LN reticular stromal cells in hydrogel matrix (sodium hyaluronate with 0.5% poly-ethylene glycol-diacrylate and vesicular growth factors) after LN excision in mice. Our study showed that injection of LN reticular stromal cells with hydrogel matrix re-established the lymphatics. Which further need to be studies for its effect in reducing secondary lymphedema and safety

B15. Exploring connections between exosome-induced gene expression and development in planaria

<u>Nicole Akers</u>, and Stefanie Leacock Department of Biology, UALR

Exploring connections between exosome-induced gene expression and development in planaria Exosomes are membrane-bound extracellular vesicles that are secreted by nearly all eukaryotic cell types and contain DNA, RNAs, lipids, and proteins. Exosomes secreted by cancer cells may play a key role in cancer pathways by acting as intercellular messengers capable of altering the gene expression of recipient cells. Recently, glioma-derived cancer exosomes were shown to influence the transcription of genes associated with cell proliferation and astrocyte differentiation in human mesenchymal stem cells (Sharma et al. 2020). The specific functions of genes identified as upregulated in response to glioma-derived exosome exposure in glioma pathways, and in cancer pathways in general, are still not clear. In order to disentangle the specific functions of genes upregulated in response to glioma-derived exosome exposure in differentiation, proliferation, or other biological functions, we plan to examine the role of these genes in planaria. We are screening the data by using Gene Ontology categories including positive regulation of cell proliferation, astrocyte differentiation, and regulation of endothelial cell proliferation. We propose that comparative study of the selected genes using planarians as an in vivo model could help to distinguish between potential candidates that might be contributing to cell proliferation or tissue differentiation. Therefore, we will select candidate genes with a known, yet uncharacterized, planarian homolog. Based on

the predicted roles of selected genes in human glioma studies, we predict that these genes may play roles in planarian stem cell differentiation or proliferation. These predictions could be tested using RNAi techniques in regeneration studies in combination with in situ hybridization and microscopy. This work may lead to new hypotheses and experiments to test the roles of genes targeted by glioma exosomes. Sharma, K. D., Schaal, D., Kore, R. A., Hamzah, R. N., Pandanaboina, S. C., Hayar, A., Griffin, R. J., Srivatsan, M., Reyna, N. S., & Xie, J. Y. (2020). Glioma-derived exosomes drive the differentiation of neural stem cells to astrocytes. PloS one, 15(7), e0234614. https://doi.org/10.1371/journal.pone.0234614

B16. Sodium Toxin Na668 Antibiotic Properties

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Antibiotics are used to prevent and treat bacterial infections; however antibiotic resistance occurs when bacteria become resistant and change in response to the use of these medications. Antibiotic resistance has become an increasingly serious problem in recent years. The first, and still most common, antibiotics come from fungi and soil bacteria. In order to combat the growing issue of antibiotic resistance, researchers have begun to study the bodily fluids of animals for antibiotic properties. This research is designed to study the antibacterial properties of the venom from Centruroides vittatus, also referred to as the Striped Bark Scorpion, which can be found in the rural areas of Arkansas. Neurotoxins, such as sodium \u03b2-toxin protein present in the Striped Bark Scorpion, alter the kinetic activity of the sodium channel gating in cells where they have been injected. Beta sodium toxin Na668 is the specific toxin being observed in this experiment. It attaches to the sodium channels and causes a lowering of the activation energy required for sodium ions crossing the channel. This allows more sodium to enter the cell than necessary and can cause disruption of the chemical gradients needed for metabolic activity. It can also cause the cell to undergo osmotic lysis, which occurs when a cell bursts due to the imbalance that has caused excess water to diffuse into the cell. Because of this, the beta sodium toxin Na668 can act as an antibacterial compound. This project focuses on the antibiotic effects of the Na668 toxin against E. coli compared to other standard antibiotics such as ampicillin and kanamycin. To test this, E. coli was cultured then incubated with five different treatments, and later plated to count the colony forming units in the solution. The five different treatments included a positive control, ampicillin to inhibit growth for comparison, kanamycin to inhibit growth for comparison, Na688 beta sodium toxin, and a negative control.

B17. Collagen alters behavior of thyroid cancer tumor cells

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Thyroid cancer is the most common endocrine malignancy to date and is expected to surpass colon cancer as the most common cancer by 2030. The most common classification of thyroid cancer is well-differentiated, and it makes up 95% of cases. Well-differentiated has two sub-types, papillary thyroid cancer (PTC) and follicular thyroid carcinoma (FTC). It also has a relatively good prognosis and can be treated with radioactive iodine treatments and/or surgery. Poorly-differentiated disease makes up 5% of cases and is extremely aggressive. Even though poorly-differentiated cancers only make up a small percentage of cases, it is has a high moratlity rate. Despite the good prognosis of well-differentiated cases, 85% of PTC cases progress into poorly-differentiated. For this reason, our research focused on what causes progression. We investigated how elements of the tumor microenvironment (TME) alter how the tumor cell behaves using western blotting, three-dimensional cell culturing, next-generation sequencing, and noted substantial differences between thyroid cancer cells grown in the presence of collagen.

B18. Inhibition of ESKAPE Pathogens by Antibiotic-Producing Soil Bacteria

<u>Taylor Savage</u>, Griffin Hopkins, and Dr. Ruth Plymale Department of Biology, Ouachita Baptist University

The pathogenic ESKAPE bacteria are listed on the CDC's list of urgent antibiotic resistance threats in the United States. An estimated 35,000 Americans die from nosocomial infections by ESKAPE pathogens each year. Thirty-nine different soil bacteria for antibiotic production against these ESKAPE pathogens was performed using swab patches on glucose starved and protein starved M9 salts agar plates. In this technique, an antibiotic-susceptible strain of each ESKAPE pathogen was swabbed on a starvation plate and the soil bacterium was plated on top of the pathogen. Antibiotic production was determined by pathogen growth inhibition following incubation. We identified seven different soil bacteria producing antibiotics against Enterococcus faecium, 16 against Staphylococcus aureus, 20 against Klebsiella pneumoniae, four against each Acinetobacter baumannii and Pseudomonas aeruginosa, and 13 against Enterobacter aerogenes. The antibiotic-producing soil bacteria were ranked by the number of ESKAPE pathogens each inhibited, and high-ranking soil bacteria were selected for whole genome sequencing.

B19. A Comparison of Growth Curve Parameter Estimates Across Parametric and Non-Parametric Approaches in R

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A desire to better understand and compare microbial growth patterns required the introduction of quantitative approaches or "growth curve analysis". Several primary models, including the Gompertz, logistic, Baranyi, and Richards models were developed and later modified to extract biologically significant parameters such as the maximum specific growth rate, asymptotic growth level, and lag time to compare growth. An alternative measure sensitive to variations in parametric values is the area under the curve. Several open source and proprietary software packages exist for estimating these growth parameters from cell count data (as a function of time in culture). The R packages growthcurver, grofit, and growthrates allow estimation of growth curve parameters through nonlinear least-squares fitting or estimation via splines. Using these R packages, estimates for A, μ _max, and AUC from two sets of microbial growth data were extracted to determine the reliability of each package and approach. Statistical analysis of one data set comprised of an array of virally infected Sulfolobales crenarchaea hosts indicates a significant difference between growth parameters estimates across packages, especially for the growth parameters μ_max and AUC. Of the 288 pair-wise comparisons of growth parameter differences across packages from the Sulfolobales dataset, 40% were found to be statistically significant (p < 0.05). These findings suggest that growth parameter estimates obtained from many available software differ in a statistically and biologically significant manner. Furthermore, estimates within individual software packages can vary significantly. Therefore, caution is warranted when analyzing growth parameter estimates available in the literature. It is necessary to consider the impact of software package used as well as model chosen when making comparisons of quantitative growth curve data.

B20. Efficacy Evaluation of mast cell targeted oral vaccine in generating Influenza A specific antibodies

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The mucous membrane covers a large surface of the body lining. Majority of pathogens enter the host through these surfaces. Therefore, it is critical to develop an effective immune response on these sites to neutralize pathogens before their entry. The main challenge in developing an effective mucosal immune response is that the mucosal immune system is biased for immune tolerance. There are number of vaccine adjuvants used to break this tolerance with their own limitations. In the current study, we evaluated the gut mast cells mediator as natural vaccine adjuvant to generate an effective mucosal immune response. Vaccine formulation containing nanoscale-liposome encapsulating mast cell activator, compound 48/80 (C48/80: 285 µg) and antigen, Influenza A-nucleocapsid peptide (InfANC: 20 µg) were fed to mice at day 0 followed by booster (oral) at 7 day. The weekly body weight was measure in all mice while blood was collected at 0, 7 and 35 days post vaccination and analyzed for InfANC specific antibody. Results showed that mice fed with C48/80 had higher body weight (~20% more) gain as compare to non-C48/80 fed mice. The mice fed with InfANC and C48/80 also had higher (~4 times higher) InfANC specify serum immunoglobulin G (IgG). The evaluation of mucosal IgA and other parameters are in progress. Therefore, for it can be conclusion that C48/80 can be used as an effective mucosal vaccine adjuvant, however, its safety still need to be studied.

B21. The Effects of Varying Light Wavelengths and Gravity on Phototaxis of Physarum Polycephalum

<u>Race Karlin</u>, Tessa Watson, and Jim Taylor Department of Biology, Ouachita Baptist University

Background Physarum polycephalum is a multinucleated unicellular organism that does not fall into the animal, plant, or fungi kingdoms. It is a slime mold and has a unique life cycle that includes a mobile plasmodial stage where the slime mold expands its membrane by pushing cytoplasmic fluid back and forth to travel in search of food. The plasmodia are well known for navigating and responding to environmental stimuli while also self-organizing to optimize food consumption and exploration. Purpose Examine the effects of the visible light spectrum on Physarum polycephalum as well as the effects of anti-gravity conditions. Methods In this experiment, expansion or total growth of the Physarum polycephalum was studied under red, green, blue, and white light. Total growth was also analyzed in anti-gravity conditions which are produced by a clinostat. Results Findings indicate that the effects of visible light and anti-gravity did not influence the expansion or total growth of Physarum polycephalum. Plasmodial expansion in red, green, blue, and white light groups were similar to dark environmental control groups. The total growth of the plasmodia in anti-gravity conditions was also statistically indifferent to groups in stationary conditions.

Chemistry Session A

A1. Long chain synthesis of N,N-disquaramides for the treatment of Chagas disease

<u>Jessica Allred</u>, and Gregory Naumiec Department of Chemistry, University of Central Arkansas

Chagas disease is caused by the parasite Trypanosoma Cruzi and plagues nearly 10 million people in the Americas. While this disease is not widely researched, it is an epidemic that is ravaging the desolate nations of Central and South America. Unfortunately for patients diagnosed with this disease, the two cures available are expensive, harmful to the patient, and are becoming alarmingly more ineffective due to drug resistances. Because of this, it is crucial that new chemical entities can be identified, created, and tested in search of a novel cure. In this research, viable drug targets from the squaramides class of compound are created from diethyl squarate in two high yielding and quick synthetic steps. Two classes of compounds have been synthesized: 1) those with two squarate cores and 2) those with one squarate core but using large amino side chains. These compounds are designed to interact with the parasite that causes Chagas disease, by puncturing holes within the membrane, killing the T. cruzi, thus ultimately curing the infected individual of this parasitic infection. This experimentation has found that the double squarate core and large amino side chains have an average percent yield of 68.8%, which is larger than the average percent yield of 40.7 for the eight compounds with two squarate cores. In future experimentation, the compounds created will be sent to the Drugs for Neglected Disease Initiative to test their efficiency against the parasite itself, giving insight into the most effective compounds in each class.

A2. Investigation of biomimetic polymers as alternative nanofibrous wound dressings

<u>Peyton Dodd</u>, Dr. Sharon K. Hamilton Abigail Walker Alexis Summerford Chemistry Department, Ouachita Baptist University

For several decades, scientists have been developing a variety of biomolecules to promote cell adhesion, proliferation, migration, coagulation, hemostasis, and prevent infections in a wound healing environment. Through the electrospinning process, polymers including biomolecules can be spun to create non-woven nanofibrous scaffolds for wound healing. Biopolymers such as dermatan sulfate (DS), hyaluronic acid (HA), collagen, and the polysaccharide chitosan, are frequently utilized in wound healing to promote the cellular responses listed above. Given that these biopolymers are expensive to purchase or synthesize in short chains, research in our lab has focused on producing cost-effective biomimics of these polymers. Due to the role that natural polymers play in wound healing and the extracellular matrix, functional groups have been added to a poly(vinyl alcohol) (PVA) backbone to mimic the most prominent moieties found in HA and DS to create a biomimetic PVA (bPVA) polymer. Our lab has prepared collagen and DS/HA biomimics via organic modifications on commercially available polymer backbones. The goal of this research is to improve upon the previous synthesis of the DS/HA biomimetic polymer and to test the effectiveness of these biomimics compared to the biopolymers mentioned above. In this project, we have optimized the parameters of the DS/HA biomimic synthesis to ensure an efficient addition of functional groups. Additionally, the response of cells to our collagen analog, biomimetic poly(acrylic acid), was compared to that of chitosan and collagen. Each of these polymers was electrospun with PVA as a copolymer as well as a cross-linking molecule to produce cross-linked unwoven mats. These mats as well as a commercially available collagen-based dressing were analyzed via a scratch assay, degradation study, and cell viability and proliferation test. In the future, bPVA will be electrospun as a copolymer instead of commercial PVA to further increase cellular responses. It is anticipated that constructs made from these biomimetic polymers could provide low-cost materials for use in a variety of biomedical applications.

A3. Anti-melanoma Studies of Thiazole-androstenone Derivatives

<u>Duminduni Hewa Angappulige</u>, and Mohammad A. Alam Department of Chemistry and Physics, Arkansas State University

Anti-melanoma Studies of Thiazole-androstenone Derivatives Duminduni Hewa Angappulige, Mohammad A. Alam* Department of Chemistry and Physics, Arkansas State University Jonesboro Steroidal hormones involved in many biological signaling processes in the human body are chemically oriented molecules isolated from different microorganisms and plants. The major role of assorted synthetic derivatives is widely used as therapeutics in pursuit of drugs, drug-candidates and other useful entities such as herbicides. Steroidal derivatives comprise one of the broadest spectra of therapeutic class of compounds hence used extensively in modern medicine to discover beneficial treatments for different anomalies including cancer. Moreover, the therapeutic properties of both natural and synthetic derivatives of androstenone are agonists of cell-surface G-protein coupled bile acid receptor 1 (GP-BAR1),

anticancer, neuroactive, anti-alzheimer and several other medicinal properties. The thiazole derivatives hold another category of compounds in which are associated in several important drugs including dasatinib and ritonavir. Several steroidal-based drugs that are comprised with heterocyclic rings have recently been validated for therapeutic applications such as Emflaza (deflazacort) to treat Duchenne muscular dystrophy (DMD) and Zytiga (abiraterone acetate) to treat metastatic castration-resistant prostate cancer. With the use of readily available thiourea, thioamide and enone derivatives, one new methodology has been developed to synthesize novel fused thiazole- androstenone derivatives. The objective of this research is to assess the differential activity of thiazole- androstenones against several melanoma cell lines and the mode of action of potent compounds.

A4. Novel FRET-Based Ionic Materials for Bioimaging Application

<u>Hannah Krehbiel</u>, Caroline Kornelsen, Amanda Jalihal, and Dr. Noureen Siraj Department of Chemistry, UALR

Bioimaging is crucial for the noninvasive visualization of biological processes in the body. The process of bioimaging requires the use of a fluorescent probe to label molecular structures and processes. Commonly used NIR probes have many disadvantages including fragility and having costly and difficult syntheses. Herein, we introduce novel, FRET-based ionic materials and nanomaterials for bioimaging application. These materials are composed of both donor and acceptor ions and thus have a simple, low-cost, high-yield synthesis and highly tunable photophysical properties.

A5. Metabolism of Halogenated Synthetic Cannabinoid Analogs

<u>Anna Pinson</u>, Dennis Province, and Grover P Miller Department of Chemistry and Biochemistry, Harding University

Synthetic cannabinoid (SCB) abuse has become the center of a drug crisis in the past decade. SCBs are a group of compounds that were originally synthesized to mimic the psychoactive effects of Δ^9 -tetrahydrocannabinol, the most active molecule in the plant Cannabis sativa. Over time, these designer drugs have evolved into highly-toxic compounds that induce a plethora of harmful side effects. One newly-observed theme among SCBs is the inclusion of a halogen somewhere in their structure. Because this halogen increases the distribution and retention of the drug in vivo, it is vital that the metabolism is fully understood. Many sources in the literature, including our lab, report that a fluorine is removed from some SCBs via an oxidative defluorination step that is not dependent upon NADPH, the essential cofactor for many drug-metabolizing enzymes. The study of this novel enzymatic activity would normally require the use of legitimate SCB samples, which is illegal without a costly license from the Drug Enforcement Administration. To circumvent this problem, we have proposed a plan to synthesize an SCB analogue with varying halogen attachments. This analogue base, N-(pentyl)-1-methyl-1H-indole-3-carboxamide, will contain a halogen at the end of the pentyl chain as observed in many SCBS. From this research, we hope to gain knowledge that will aid in the characterization of the previously-unknown oxidative dehalogenation enzyme activity and more fully comprehend SCB metabolism in the human body.

A6. Screen Printed Electrodes for the Detection of Active Pharmaceutical Ingredients (APIs) in Drugs

Matthew Boston, and Charuksha Walgama

Department of Physical Sciences, University of Arkansas at Fort Smith

Quality control analysis of pharmaceuticals is an essential process in pharmaceutical industry. Various chromatographic, spectroscopic, titrimetric, and electrochemical methods have been used in quality assurance process to estimate the active pharmaceutical ingredients (APIs) in drugs. In this study, we propose a convenient, rapid, and cost-effective electroanalysis technique to detect oxidative pharmaceuticals as a single droplet on screen printed electrodes (SPEs) modified with carbon nanotubes. For this pilot study, we will be including over-the-counter medications like Acetaminophen (an analgesics) and Ibuprofen (a nonsteroidal anti-inflammatory drug). We are planning to optimize our electrochemical assay parameters and develop dose-response plots for those selected drugs. We will also investigate how chemical structure, molecular size, and polar/nonpolar features of the electrode surface contribute to the interaction of the analyte with the electrode surface to facilitate interfacial charge transport, and thus the oxidation current signals. We hope our findings will provide more insights on applicability of single drop electroanalysis as a cost-effective and instant analytical tool for the quality assurance (QA) of APIs.

A7. Biomimetic Poly(Acrylic Acid) Fiber Scaffolds for Biomedical Applications

<u>Harry Jeffrey</u>, Dr. Sharon K. Hamilton, Abby Walker Madeline Wauters Department of Chemistry, Ouachita Baptist University

Current biomaterials used in wound treatment include collagen, a naturally occurring protein found in the body, and chitosan, a deactylated derivative of chitin. Gauze, which are the common method of wound treatment, are known to create a secondary injury upon removal from the wound. The products of a collagen and chitosan based electrospun materials have exhibited favorable conditions for prevention of infection, stimulation of cell growth, and a lower probability of secondary injury. Electrospun materials are able to conform to many different shapes and sizes due to its non-woven scaffold like structure. Collagen has many advantages in biomedical applications as it is biocompatible, biodegradable, and weakly antigenic. Collagen has also been known to stimulate new tissue growth, promote angiogenesis, and epithelization. Chitosan is an excellent natural polymer to utilize in new wound dressing, as its cationic nature destabilizes the outer membrane of Gram-negative bacteria. While chitosan is a cost-effective material, collagen is very expensive. The main objective of this project is to develop a cost-effective synthetic collagen analog and electrospin an alternative wound dressing. Our lab modified poly(acrylic acid) (PAA) with different substituents to mimic collagen. Substituents were added through amide coupling and examined using NMR spectroscopy to confirm attachment and percent modification of each reaction. Biomimetic poly(acrylic acid) (bPAA), was electrospun in different solutions to make a fiber mat and used in vitro cell studies. NIH 3T3 cells were cultured in DMEM with 10% CBS and 1% pen-strep. Each mat was then analyzed via a scratch assay, degradation study, and a cell viability and proliferation test. In future studies, these results will be compared to the cellular responses of collagen containing mats. It is anticipated that these results and products will help develop a wound dressing similar to the extracellular matrix in a more cost effective manner.

A8. Alcohol Unfolded Hemoglobin: Insights from Mass Spectrometry

Harmeet Kaur Chohan, and Mohammad A. Halim

Department of Chemistry, University of Arkansas - Fort Smith

Hemoglobin is a protein found in red blood cells that originates from deoxyribonucleic acid (DNA) which carry out the oxygen from lungs and transport to the tissues and organs all over the body. Heme is part of hemoglobin that contains iron and gives the ability for hemoglobin to bind with oxygen and transfer it throughout the body. Using Thermo LTQ mass spectrometry, we explored the structure of hemoglobin in different environment specifically in water, 1% acetic acid, 1% NH4OH, and 50% methanol. The mass spectra give different charge states, which indicate whether the protein is folded or unfolded in different environment. When the protein is folded, it means that the protein is in native conformation and can function normally but when the protein is unfolded the protein losses the heme and creates malfunctioning. In this study, the results showed that in neutral state, it has charge state distribution from +7 up to +12, where +10 was the most intense peak. In basic solution, similar pattern was observed. However, with methanol solution, the charge state was spread from +6 to +14 with the most intense peak of +10. On the other hand, in acetic acid solution, the charge state showed from +8 up to +15 with +11 being the intense peak. Thus, hemoglobin with acetic acid and methanol showed more charge states, which indicates that the protein was unfolded while hemoglobin with water and NH4OH showed that the protein was folded. We hypothesize that the drinking alcohol may unfold Blood's hemoglobin and responsible for impairments including slowed reflexes and slurred speech and other side effects

A9. Scorpion Venom Peptides as Potential Antiviral Agents against the SARS-CoV-2

<u>Honey Matevia</u>, Harmeet Chohan, Archana Mishra, and Mohammad A. Halim Department of Physical Sciences, University of Arkansas - Fort Smith

The corona virus began a worldwide pandemic in the beginning of 2020, infecting over 30 million and killing over 950 thousand people worldwide in the last nine months. Serious efforts to produce vaccines against the virus has led the identification of novel lead molecules that are currently undergoing clinical trials, however, no vaccine has been approved by FDA so far. Repurposing of drugs such as Remdesivir, Favipiravir and others exhibit some therapeutic efficacy against Covid-19. Therefore, development of new effective and specific antiviral agents and strategies are urgently needed to provide alternate therapeutic molecule to treat SARS-CoV-2. Antimicrobial peptides, isolated from living species, are potential broad-spectrum antiviral agents. Scorpion's venom contains a mixture of peptides and proteins with varied bioactivities and receives a great attention due to their potential application in peptide drug design and development. In this study, we have selected twelve scorpion venom peptides that have already shown antiviral activity against different viruses. The focus of this study is to identify the binding affinities and interactions of these peptides against the main protease, 3-C like protease (3CLpro), of SARS-CoV-2. The 3CLpro protein received great attention because of its important role in post-translational processing of replicase polyproteins and viral replication. Using computational chemistry,

binding affinity and interaction between the protein and the peptide were identified using Patchdock and Firedock. Peptides with highest binding affinity and interaction with the active site residues, His41 and Cys145, were chosen. Among these peptides, AVP1700, AVP1701, AVP1820, AVP2053, and AVP2054 showed the highest binding affinity ranging from -67.16 to -57.94 kcal/mol. All selected peptides interact with the active site amino acids. Various noncovalent interactions such as hydrogen bonding and hydrophobic interactions are detected in peptide–3CLpro complexes. MD simulation is performed for the best peptides. Structural stability and compactness are observed for the peptide–3CLpro complexes.

A10. Finding a low cost alternative medication for Chagas Disease

Sarah Friedman, and Gregory Naumiec

Department of Chemistry, University of Central Arkansas

A single bite from a kissing bug that carries the parasite Trypanosoma cruzi can lead to death. Known as Chagas disease, this neglected tropical ailment affects millions of people, primarily in Central and South America, every year. Concern about the disease is continually increasing, as the insect vectors are moving north into the United States. Kissing bugs have been sighted as far north as Delaware. Only one medication, benznidazole, is approved by the U.S. Food and Drug Administration (FDA) to treat Chagas disease. This one therapeutic is not enough to combat Chagas disease. Not only does benznidazole have harsh side effects, it is very expensive and is only FDA-approved for children. Additionally, there are alarmingly increasing accounts of treatment failures due to mutations in T. cruzi's TcNTR gene, leading to drug resistance. Since the kissing bug is steadily moving north and medications are limited, more treatment options are needed. This research focuses on disqauramides, small molecule antiparasitic compounds that are anti-Chagastic. Disquaramides require low-cost reagents, can be created through a simple two-step organic synthesis, and are able to infiltrate the parasite's membrane, causing parasitic death. In order to make vital treatment options for Chagas disease available, this study focuses on creating a drug library of disquaramides. This study has created and confirmed 21 compounds by 1H and 13C Nuclear Magnetic Resonance (NMR) spectroscopy with moderate percent yields. Future work includes sending these compounds to the Drugs for Neglected Disease Initiative (DNDi) to test them against the parasite in vitro. While one kissing bug bite can lead to death, one compound can save a person's life.

A11. Development of Novel Water-Soluble Porphyrins for Potential Use as Photosensitizers in Photodynamic Therapy

<u>Kayla Whittington</u>, and Joseph Bradshaw Department of Chemistry, Ouachita Baptist University

Photodynamic therapy (PDT) is a treatment modality for various illnesses including some types of cancer. This research focused on synthesizing novel water-soluble porphyrin compounds for use as photosensitive agents in PDT. The outside of the porphyrin core can be modified with various substituents to assist with water-solubility and cytotoxicity. In this research, the core of 5, 10, 15, 20-tetrakis(4-carboxyphenyl)porphyrin, H2TPPC, was modified with the attachment of L-threoninol to create the novel H2TPP-LT. The core was also modified with tris(hydroxymethyl)aminomethane, TRIS, to synthesize H2TPP-TRIS. Additionally, ZnTPPC was modified using TRIS to form the novel ZnTPP-TRIS. Each compound was filtered prior to purification by column chromatography using both Sephadex LH-20 and Sephadex G-50. Additionally, nuclear magnetic resonance (NMR), infrared (IR), and UV-visible spectroscopies (UV-vis) were used to characterize each compound. Purity of the final products was determined using high performance liquid chromatography (HPLC). Finally, compounds were tested using MTT assays to determine cell viability in both light and dark conditions on an A549 non-small cell lung cancer cell line.

A12. Synthesis of Espintanol Derivatives for a Cost-effective Treatment of Leishmaniasis

<u>Anna M. Wolff</u> and Gregory Naumiec Department of Chemistry, University of Central Arkansas

Leishmaniasis, a parasitic disease commonly found in tropical and subtropical areas, is classified into a group of diseases known as Neglected Tropical Diseases (NTDs). These illnesses are most commonly found in underdeveloped regions of South America and Africa, as well as Asia and the Pacific Islands and, more recently, the Southern United States. Leishmaniasis, which affects over 12 million people worldwide, is spread through the bite of sand flies, primarily in South America and Africa. It can manifest itself in three general forms: cutaneous, visceral, or mucosal. Unfortunately, current medication is not efficient at eradicating the parasite from its host. While treatment options exist, these antimony-based drugs are often inefficient, expensive, or toxic. In addition, lack of treatment diversity has led to drug resistance in leishmania parasites. Over the years, cases in underdeveloped regions continue to be left untreated while researchers and scientists in developed countries show little effort in developing new treatment plans. The research I am conducting consists of the synthesis and study of compounds derived from espintanol, a natural product with antileishmanial properties found in Bolivian spruce trees. However, despite these properties, espintanol is quickly metabolized in the body, making it an inefficient method of treatment. The purpose of this research is to develop a library of espintanol-based compounds that efficiently and inexpensively treat cases of leishmaniasis. By optimizing the synthesis of espintanol and modifying the steps needed to alter the compound, our goal is to produce a derivative with a slower metabolism that will remain in the body long enough to effectively eradicate the parasite. Currently, we are focused on investigating a safer synthesis of espintanol by adjusting the first step of the synthesis to obtain new squarate compounds. Several failed synthesis attempts resulted in a greater understanding of the conditions needed for each reaction step to take place. A series of reflux reactions using alcohol reagents like diisopropyl alcohol and diisobutyl alcohol allow for substitutions on C-3 of espintanol, one area we are focused on making bulkier. We expect this to result in a much slower metabolism when used as a treatment for Leishmaniasis, making it much more effective than espintanol. Several other steps of the synthesis allow for substitutions to be made on espintanol, including using a variety of grignard reagents for step two of the synthesis. Future work includes continuing to alter these steps of the synthesis in order to develop a drug bank which will ultimately be tested in vitro and in vivo to evaluate their effectiveness.

Chemistry Session B

B1. Modified Michael Addition Leads to Biologically Significant Naphthoquinones

<u>Perkins, N</u>., Ho, K., Humphrey, M., Smith, E., Jenkins, S. V., Dings, R. P., and Nawarathne, I. N. Department of Chemistry, Lyon College

Modified Michael Addition Leads to Biologically Significant Naphthoquinones Perkins, N.1; Ho, K.1; Humphrey, M.1; Smith, E. 1; Jenkins, S. V.2; Dings, R. P.2; Nawarathne, I. N.1 1Mathematics and Science Division, Lyon College, Batesville, AR, 72501 2College of Medicine, University of Arkansas for Medical Sciences, Little Rock, AR, 72205 New therapeutics are essential to improve 5-year lung cancer survival rate (16% for men and 23% for women; 24% for non-small cell; and 6% for small cell tumors). Naturally occurring and synthetically derived naphthoquinones show a wide range of pharmacological uses; naphthoquinone scaffold is present in some of the widely used antineoplastics such as Doxorubicin, Napabucasin, Streptonigrin, and Actinomycin; it is known to selectively target cancer cells acting as ROS-inducing agents and inhibit enzymes such as STAT3, DNA topoisomerase I and II, and AKT kinases; have demonstrated activity against multi drug resistant cancer cell lines; they can be exploited as multitarget drugs toward a broad spectrum of cancers. Taking advantage of modified Michael Addition reactions, we have incorporated functional groups such as azido, amino, amino acid, and peptide to the napthoquinone core to create multitudes of biologically significant naphthoquinones. The modifications are further extended by utilizing copper-catalyzed azide-alkyne cycloaddition reactions (premier example of click chemistry) to generate triazoles and by using peptide chemistry. We are constantly testing the novel naphthoquinones for their lung anticancer activities and also for antimicrobial properties.

B2. Modeling the S100A1 Protein and Developing Drugs to Induce Inhibition

<u>Kaymon Neal,</u> and Dr. Caitlin Scott Department of Biology, Hendrix College

Proteins are responsible for many reactions within the body and are essential to human health. Overabundance or minimal amounts of necessary proteins can lead to harmful diseases, some even fatal. The S100A1 protein, for example, is responsible for serving as a modulator and integrator of calcium signaling in the heart and is an integral to its overall function. Insignificant levels of the S100A1 protein can lead to diseases such as cardiomyopathy. This project assesses the virtual modeling of the S100A1 protein and later creating or finding drugs that bind to its exposed binding site that would help inhibit the activity of the protein. The structure of the S100A1 protein in this research is activated so that a possible binding site, represented by a hydrophobic pocket on an inner portion of the protein, is exposed through introduction of calcium ions. Even though this is seen as a possible site for drug-protein interactions, there is no experimental structure of how the drugs bind to the S100A1 protein. The drug-protein complexes were generated with DockThor software, which simulates the protein-drug interactions and predicts the binding affinity of said interactions. Four drugs that have been known to inhibit other S100 proteins were used in this research. These drugs include Propranolol, Cromolyn (or cromoglicic acid), Olopatadine, and Amlexanox. After successfully creating a drug-protein complex with DockThor, we see that Glu-91, Asp-50, and Asp-46 are all residues that could possibly be involved with facilitating drug inhibition due to their prevalence in all simulated drug-protein complexes. Examining which drugs have the ability to inhibit the function of the

S100A1 protein in the body could lead to new avenues of therapies for diseases, such as cardiomyopathy, in humans and give more understanding on how proteins interact with drugs.

B3. Functionalized Ionic Material-based Combination Nanodrug for Treatment of Cancer

Samantha Macchi, <u>Nabeel Alwan</u>, Mohd Zubair, Noureen Siraj PhD, and Nawab Ali PhD Department of Chemistry, University of Arkansas - Little Rock

Herein, we present a novel approach to develop an ionic nanoparticle-based combination drug for cancer therapy. Chemotherapeutic and photodynamic therapeutic (PDT) drugs were combined to develop chemo-PDT combination drugs using single-step ion exchange reactions. The combination therapy drugs and nanodrugs were characterized using various techniques to investigate their purity and morphology of the nanoparticles. The surface of nanoparticles were functionalized to improve the selective toxicity towards cancer cells. Photophysical properties are studied in detail to investigate the PDT performance of the combination drug. The cytotoxicity of the combination therapy drugs and their respective parent materials were also tested in vitro using MCF-7 (cancer cells) and MCF 10 (non-cancerous) cell lines. The combination nanodrugs showed selective toxicity towards cancer cells after surface functionalization.

B4. Investigating Peptidic Polymers for Drug Delivery Vehicles Using Computational Methods

<u>Elizabeth Henry</u>, and Dr. Zeeshan Habeeb Department of Chemistry, University of Arkansas - Pine Bluff

Biocompatible polymers made from unnatural amino acids used as drug delivery vehicles are presented in this poster. For biomaterials to be biocompatible, they cannot incite any form of adverse reaction when subjected to the tissues they contact. Such polymers can be used to encapsulate small molecule therapeutics and functionalized to target specific binding sites. Peptide polymers constructed from beta and gamma amino acids are constructed and investigated for their stability using computational methods.

B5. Main Protease Peptide Inhibitors for Covid-19 Treatment

Riley Roper, and Mohammad A. Halim

Department of Physical Sciences, University of Arkansas - Fort Smith

Severe acute respiratory syndrome (SARS) is caused by a newly emerged coronavirus (CoV-2) which infected more than 30 million individuals and resulted in more than 970 thousand fatalities in 2020. In the United States, this virus has killed over 205,000 people and infected at least 7million people. The main protease of SARS-CoV-2 has been exhibited to be important for viral replication and has hence been documented as an effective drug target for coronavirus infection. Despite the intensive research around the globe, still there is no effective treatment available for this pandemic. Protease inhibitors are special types of therapeutics, which are extensively used to treat HIV/AIDS and hepatitis C stopping the viral replication by selectively binding to viral proteases and blocking proteolytic cleavage of protein. In this study, we have selected eight protease peptide inhibitors containing 8-16 amino acids to assess their binding affinity and interaction with the main protease. Among them, peptide HIP310 shows the highest binding affinity of -65.58 kcal/mol. Two other peptides including HIP125 and HIP377 also exhibit strong binding affinity with both being over -60.00 kcal/mol. The selected best candidates are further assessed through MD simulations, which show that these peptides form stable interactions with hot-spot residues.

B6. Antimicrobial Peptides against SARS-CoV-2

<u>Cladie B. White</u>, Archana Mishra, and Mohammad A. Halim Department of Physical Sciences, University of Arkansas - Fort Smith

SARS-CoV-2, known to infect humans, is responsible for COVID-19 and declared as a global pandemic. Various symptoms include fever, coughing, breathing difficulties, and in severe cases pneumonia, and multiple organ failure are reported. It resulted in killing over 981 thousand people worldwide as of September 2020. There is no specific drug or vaccine has been recognized by FDA as proven treatment against this virus. Antimicrobial peptides, which can be isolated from bacteria, fungi, animals and plants, and other species, are abundant in nature. They are known as host defense peptides, which can generally kill microbial pathogens directly. There are several antimicrobial peptides in clinical trials and have shown to be very effective. Herein, we have designed

eight clinically proven antimicrobial peptides and tested their binding activity against the main protease, Mpro, of SARS-CoV-2. CABS-fold server was used to model these peptides in de novo fashions from its amino acid sequence. Molecular docking between peptides and main protease protein is performed by Patchdock and subsequent refinement is conducted by Firedock. The most of the peptides show a binding affinity over -50 kcal/mol where the highest binding affinity is detected for DRAMP18160 peptide (-59.9 kcal/mol). This peptide also shows strong interactions with His41 and Cys145 residues of protease. To explore the dynamic nature of the interaction between peptide and protein, all atoms molecular dynamics (MD) simulation was performed that revealed selected peptide remain in the binding pocket of Mpro protein without altering protein structures.

B7. NO reduction by the repair of iron center enzyme, YtfE

<u>Mitch Bandy</u>, Michael Miller, Kashti Shah, and Dr. Bill Gunderson Department of Chemistry, Hendrix College

To protect against bacterial infections, mammalian cells produce high concentrations of reactive oxygen species (ROS) and reactive nitrogen species (RNS). ROS and RNS kill the bacterial pathogens by damaging proteins, lipids, and DNA. Proteins that contain iron-sulfur (FeS) clusters are particularly susceptible to damage by nitric oxide (NO), a common RNS. FeS clusters are found ubiquitously in nature and have a wide range of functions that underlie essential biological processes including transcriptional and translational regulation, DNA replication genome maintenance, and metabolism. Disruption of FeS activity leads to inactivation of proteins and eventually cell death. However, bacteria have evolved systems that protect against damage from NO and can restore function to damaged FeS clusters, thus it is essential to understand the mechanisms by which bacteria protect against damage from NO. One essential bacterial response system utilizes non-heme diiron enzymes that facilitate the direct repair of FeS centers following exposure to oxidative or nitrosative stress. Genes for the repair of iron cluster (RIC) class of metalloproteins have been identified in several pathogenic bacteria and are upregulated upon exposure to NO and hydrogen peroxide. Of this class of proteins, the RIC-protein from E. coli (YtfE) is the best characterized, and two functions have been identified: (1) YtfE reduces NO to N2O, protecting the bacteria from nitrosative stress, and (2) YtfE repairs damaged FeS clusters, restoring function to the protein. Here, we explore the mechanism of NO reduction by YtfE using electron paramagnetic resonance spectroscopy and enzyme kinetic studies. Kinetic rates indicate that YtfE does not reduce NO efficiently, suggesting that this may not be the primary function for the enzyme.

B8. Effects of Temperature & pH on BPA leaching in Oral Hygiene Products using Fluorescence Spectroscopy

Mady Rottinghaus, and Dr. Sara Hubbard

Department of Chemistry, Ouachita Baptist University

Bisphenol-A (BPA) is found in many hard plastics and has been linked to health concerns such as cardiovascular disease, reproductive issues, and effects on endocrine development. BPA binds to estrogen receptors because the structure is similar to estradiol. These health effects are of particular concern in infants and young children. As a result, BPA is regulated in many products; however, BPA is not regulated in oral hygiene products, specifically children's toothbrushes. Past research was conducted to examine the presence of BPA in infant toothbrushes and compare the levels in labeled and not labeled toothbrushes. This research was continued by analyzing the effects of temperature and pH on BPA leaching from plastic toothbrushes. Fluorescence spectroscopy was used to monitor BPA leaching from several plastic toothbrushes that were previously determined to contain BPA using an FS5 Spectrofluorometer from Edinburg Instruments with excitation peaks at 278 nm and emission peaks at 304 nm. Fluorescence calibration curves and analytical figures of merit under various conditions solutions were obtained. Temperature tests were run using body temperature (37°C) and room temperature (20°C) and pH tests were run at pH 3, pH 6, and pH 10. These temperature and pH values were selected to mimic the oral cavity based on what foods and/or beverages have been consumed before brushing may affect the amount of BPA leached from the children's toothbrushes. Infant toothbrushes that had been previously tested and confirmed to have BPA in them were each placed in a 1:1 (methanol:water) solution for time increments varying from five minutes to 1440 minutes. Aliquots of 5-mL were collected from the solutions as the toothbrushes soaked for each time interval and measured using fluorescence. These values were compared using statistical analysis to determine the effects of oral temperature and oral pH on the release of BPA from the toothbrushes.

B9. BTEX analysis using Raman spectroscopy

<u>Drake Jackson</u>, and Edmond Wilson Department of Chemistry and Biochemistry, Harding University

Analysis of most environmental and biological samples is best carried out by hyphenated methods involving liquid chromatography or gas chromatography and mass spectrometry such as GC/MS or LC/MS. These methods are very powerful and sensitive. The drawback is that GC/MS or LC/MS methods require samples to be brought to the instrument's location. Many times an adequate analysis can be developed that employs a portable instrument with less resolution and sensitivity and with substantially less cost. Recently, several portable Raman spectrographs, designed for field use have been brought to market. They are rugged because they have no moving parts, are easy to use, and are inexpensive. Our team has designed a compact Raman spectrograph and applied it to analysis of BTEX (benzene, toluene, ethylbenzene, o-xylene, m-xylene and p-xylene) a group of substances hostile to the environment and found in too many places. We report progress in developing methods to analyze the BTEX in a matrix of motor fuels: kerosene, gasoline and diesel. GCMS was used to validate the results obtained from the Raman spectrograph.

B10. Synthesis of Dopamine Analogs to Investigate Enzymatic Function of L-DOPA Dioxygenase

<u>Kameron L. Klugh</u>, Ryan Marasco, and Larryn W. Peterson Department of Chemistry, Rhodes College

The goal of this research project was to design and synthesize dopamine analogues in order to create specific substrates for L-DOPA dioxygenase, an extradiol enzyme that cleaves the aromatic ring of catechols (figure 1). L-DOPA is part of the structural family of vicinal oxygen chelate (VOC) dioxygenases. This superfamily is composed of structurally related proteins that provide a metal coordination environment with two or more open sites to promote direct electrophilic participation of the metal ion in catalysis1. L-DOPA contains an iron-bound center. The aim of the project was to create a variety of dopamine and L-DOPA analogs that will help us identify the catalytic rate and function of the L-DOPA dioxygenase. This project focuses on the synthesis of the dopamine analog 6-carboxydopamine. Figure 1(unable to be submitted in this format): Proposed mechanism for the cleavage of a catechol ring by L-DOPA dioxygenase.

B11. Determination of the Vitamin Content in Oxalis triangularis

<u>Darby Mohon</u>, Dennis Province, PhD, and Michael Nicodemus, PhD. 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. The Oxalis genus of plants have been reported to have high concentrations of Vitamins C and E. 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 Oxalis 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, research was also conducted on the ability of Oxalis triangularis to grow in Martian regolith. Oxalis was determined to be viable in Martian regolith, with growth between 0.2-0.4g of fresh weight. At this time, only standards have been established in these methods. Estimated daily amounts are 1000 mg of Vitamin C and 15 mg of Vitamin E, 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.

B12. Electrochemical drug metabolite synthesis and inhibition assays for preclinical drug screening

Dr. Charuksha Walgama, and <u>Evan Wittig</u> Department of Biology, University of Arkansas - Fort Smith

The time to develop a pharmaceutical drug and bring it to the market takes on average 12.5 years and billions of dollars. Examining the metabolic fate of drugs inside the human body is an essential part of this drug development process. Such metabolic reactions are mainly governed by membrane bound liver enzymes such as cytochrome P450s (CYPs), cytochrome P450 reductases (CPRs), carboxyl esterases, and UDP- glucuronosyltransferases (UGTs)). Presently, these in-vitro studies are conducted using hepatic (liver) or purified liver enzyme-based biological assays. Longer incubation times, lower yield of drug metabolites, use of expensive NADPH cofactor and purified enzymes, and tedious purification protocols are some practical issues integrated with these conventional

biological assays. In this study we are proposing a simple liver tissue based electrochemical bioreactor technology to perform drug activity assays. The CYP-specific bioactivity of the liver tissue film on the electrode will be confirmed by monitoring the electrocatalytic conversion of testosterone to 6β - hydroxytestosterone and its inhibition by the CYP-specific ketoconazole inhibitor. We hope our findings will have successful implications in the design of a one-step, electrochemical bioelectrode to perform drug activity and inhibition assays in preclinical drug development process.

B13. The Photodynamic Therapy Potential of a Novel Water-Soluble Porphyrin

<u>Ryane Thurman</u>, and Joseph Bradshaw Department of Chemistry, Ouachita Baptist University

Photodynamic therapy (PDT) has potential use in the treatment of cancer and other health disorders. PDT utilizes light and a photosensitive agent that once activated by light, generates singlet oxygen that affects surrounding cells. The goal of this research was to synthesize and characterize the novel photosensitive agent, H2TPP-3-Amino-1,2-Propanediol. The H2TPP-3A12P was purified using column chromatography and characterized using IR, UV-Vis, and NMR spectroscopies. Purity was determined using high-performance liquid chromatography. Cytotoxicity testing of the H2TPP-3A12P using A549 lung cancer cells in light and dark conditions determined that this novel material has potential as a next generation PDT agent.

B14. The Creation of a Next-Generation Cancer Treatment Using Photodynamic Therapy

<u>Jasmine Bauqhman</u>, and Dr. Joseph Bradshaw Chemistry Department, Ouachita Baptist University

Photodynamic therapy (PDT) is a treatment for various health disorders, including cancer, that uses a photosensitive agent and light. Unlike other cancer treatments, PDT is a focused treatment that kills cancerous cells without harming the surrounding tissues. When a photosensitive agent is administered, it accumulates in the tumor as it binds to low density lipoproteins. When the tumor is exposed to a specific wavelength of light, the photosensitive agent is activated; this results in the release singlet oxygen, which kills the tumor. The objective of this research was to synthesize and characterize a novel photosensitive agent, H2TPP-2A2E. Purification of the novel material was achieved using column chromatography. In addition, IR, UV-vis, and NMR spectroscopies were used to characterize the product, and purity was determined using HPLC. After determining that our product was refined, cytotoxicity testing in light and dark conditions revealed that the novel H2TPP-2A2E, could potentially be used in the next generation of photodynamic therapy.

B15. Chemical Analysis of Man-made Pond Development at Gilliam Research Station

<u>Audrey Lawrence</u>, Dr. Dennis Province, and Dr. Steven Cooper Department of Chemistry and Biochemistry, Harding University

Little research has been done on the chemical development of ponds, though there is much information on the conditions of water that are ideal for different types of life. In the spring of 2019, three pits were dug to make way for a gravel road and they subsequently filled with water, making them ideal for testing to see how water quality changes over time, specifically in relation to ecological succession. Baseline tests measuring oxygen content, ammonium and nitrate content, salinity, pH, temperature, and turbidity were conducted at varying depths. The measurements were continued, taken once a week to see how the water quality changed over time. It is hoped that the research conducted will be useful in providing guidelines for the chemical development of ponds.

B16. Development of novel squaramide drugs to treat Chagas disease in a cost-efficient and environmentally friendly manner

Macllain R. Edington and Gregory R. Naumiec

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Neglected tropical diseases (NTDs) include a wide array of diseases that are caused by a variety of pathogenic parasites, viruses, and bacteria that over one billion individuals around the world are infected by. Although not exclusively, NTDs are most prevalent among some of the world's poorest populations in primarily tropical and subtropical nations. There are currently 20 NTDs identified by the World Health Organization, one of which being Chagas disease, which is caused by the parasite trypanosoma cruzi and currently affects over ten million people worldwide. Chagas disease is endemic in many Latin American countries, including Mexico and a

majority of countries in South and Central America. In the acute phase of Chagas disease, individuals experience minor flu-like symptoms including, but not limited to, fever, fatigue, vomiting, and body aches. In the chronic phase, people infected by Chagas disease may experience severe complications in the cardiovascular and gastrointestinal systems. Chagas disease is the leading cause of chronic cardiovascular disease in Latin America and kills more people annually than any other parasite-borne disease. The overall objective of this research is to optimize the synthesis of squaramide drug candidates to treat Chagas disease in a time and cost-efficient manner, while also attempting to make these reactions more environmentally friendly. Using diethyl squarate as a precursor, it is possible to synthesize the desired drug candidates using a straightforward one-step synthetic process conducted at room temperature using concentrations of ethanol varying from 0-100% as a solvent, with zero percent being pure water. By diluting the ethanol used in this reaction, this contributes to the overall goal of not only making this synthetic process more cost-efficient, but also making this process less harmful to the environment. This one step reaction involves a substitution reaction in which one of the ethoxy substituents on diethyl squarate is replaced by an amine-based compound. Using twelve different concentrations of ethanol ranging from 0-100%, this reaction has been carried out successfully within a timeframe of less than an hour, while also achieving moderate to high yields even in 100% water. This project is a step in the right direction towards the development of a novel drug to effectively treat Chagas disease in a cost-efficient manner, while also minimizing environmental risks.

B17. EPR Characterization of NO reduction by YtfE

<u>Kashti Shah</u>, Mitch Bandy, Michael Miller, and Dr. William Gunderson Department of Chemistry, Hendrix College

The repair of iron cluster enzyme from E. coli, YtfE, has been shown to reduce NO to N2O, suggesting that it plays an important role in the bacterial response system. Crystal structures of YtfE reveal a diiron site at the active site. Thus, it is hypothesized that the reduction of NO depends on the oxidation state and local coordination geometry of the two iron ions. To characterize the interaction of YtfE with NO electron paramagnetic resonance (EPR) spectroscopy is utilized as a site-specific probe for the diiron cluster. Here we demonstrate that 2 mol of NO are consumed per diiron site of YtfE. These results suggest that NO reduction does occur at the diiron site.

B18. Synthesis of Novel N-based ligands

<u>Dillon Mosman</u>, and Dr. Kimberly Brien Department of Chemistry, Rhodes College

2,6-bis-hydrazinopyridine (BHP) has been prepared and is presently being used in preparation of chelating ligands that are more difficult to generate through other means. Previous research has implicated BHP as a useful reactant in the preparation of larger chelating ligands, but further research has indicated that it can be reacted with 1,2-dibromoethane to form a nitrogen-based hexadentate ligand.

B19. Extraction and Quantification of Polyunsaturated Fats in Rice Bran

<u>Fox, McKinley</u>, Newcomb, K., Oliveira, C., Shakiba. E., and Nawarathne, I. N. Mathematics and Science Division, Lyon College

Rice bran oil has many unique properties and a wide range of health benefits that can be utilized in food, pharmaceutical, and chemical industries. These desirable benefits can be attributed to the polyunsaturated fats found within the oil. We have extracted rice bran oil from both parent and hybrid lines of rice bran using an organic extraction that involves hexane as the solvent following vacuum filtration. Then we used High Pressure Liquid Chromatography (HPLC) to quantify the different types of polyunsaturated fats in the rice bran lines in order to determine the success of genetic modifications in generating the hybrid lines. The aforementioned systematic HPLC analysis of bran oil from various rice lines has allowed us to efficiently extract, quantify, and compare the polyunsaturated fats in each line. Further development and validation of our analytical method shows the potential to allow scientists to determine which rice bran lines can be used to produce the healthiest overall rice bran oil for public consumption.

B20. Analyzing Interaction and Structure of Human Cannabinoid Receptor 2-Gi Protein 6PT0 in complex with CB2 Agonist AM1710, GW405833, 9JU, CP55940, and 8D0

<u>Theresa Thomas</u>, and Caitlin Scott Department of Economics, Hendrix College

Within the endocannabinoid system, the cannabinoid type 1 (CB1) and type 2 (CB2) receptors are both targets for pain mediation; however, activation of the CB2 receptor lacks the undesirable physiological responses accompanying the CB1 receptor activation. Agonists, such as tetrahydrocannabinol (THC) found in marijuana, leads to the beneficial effects like pain relief due to activation of the CB1 receptor. However, psychoactive side effects associated with this substance make it federally illegal and uncovered by health insurance. Using the CB2 receptor as a potential therapeutic target for relieving pain can be a promising treatment for inflammatory diseases while avoiding the adverse psychotropic effects that can accompany CB1 receptor activation. Our goal is to use computational drug design to develop safe and effective pain medication that targets the CB2 receptor and eliminates the side effects caused by CB1. To confirm that the software could accurately reproduce crystallized binding poses, we used the webserver DockThor to dock WIN552122, and AM12033 to the crystal structure of a human CB2 receptor, which was crystallized in complex with the activating Gi protein and the agonist WIN55,2122 (PDB ID: 6PT0). Then, we docked experimentally known CB2 agonists like AM1710, GW405, CP-55,940 to the CB2 receptor. These drugs have never been crystallized with CB2, so we determined the best binding affinity and predicted the binding sites. We recognized specific residues that the agonist bound to through non-covalent interactions like hydrogen bonding as well as aromatic interactions. Using Protein Prep Wizard, the protein ligand structure was optimized and minimized by aligning the protein structure and deleting unnecessary residues, leaving the receptor of the protein bound to the ligand. This process allowed us to find structural conformation with minimum energy. After minimization, we discovered that all the structures had favorable interaction stability due to the low protein energy values. For future analysis, we will determine the stability by calculating the proteins' RMSD values of these structures within a lipid bilayer, which would mimic a realistic cellular environment. These optimized structures provide a template for designing agonists and drugs that selectively target the CB2 receptor, which holds a promising treatment for various pathologies, and other beneficial effects that THC would present while avoiding psychotropic effects mediated by the CB1 receptor.

B21. Determination of BPA in Children's Bamboo Toothbrush Bristles using Fluorescence Spectroscopy

Olivia Crites, and Dr. Sara Hubbard

Department of Biology / Department of Chemistry, Ouachita Baptist University

Determination of BPA in Children's Bamboo Toothbrush Bristles using Fluorescence Spectroscopy Bisphenol A (BPA) is a compound used in many every day plastics and resins. Because BPA is similar in chemical composition to estrogen/estradiol, it can bind to estrogen receptors, acting as both an agonist and antagonist for estrogen mechanisms within the human body. BPA has been linked to endocrine, reproductive, and neurological harm and to health problems such as cardiovascular disease, diabetes, and Alzheimer's disease. Children can be more susceptible than adults to the negative side effects of BPA because their endocrine systems are not fully developed. Although BPA has recently been removed from many children products and other everyday plastics, there are currently no regulations for BPA in toothbrushes. Previous research in our lab indicated some plastic toothbrushes contain BPA, and that there is a significant amount of BPA in the nylon bristles of these plastic toothbrushes when compared to the handle. Bamboo toothbrushes are quickly becoming as popular as traditional plastic toothbrushes, and are being advertised as a "safer, non-toxic alternative to plastic toothbrushes" and are more "eco-friendly" than their plastic counterpart. The purpose of this project was to determine if the nylon bristles in bamboo toothbrushes also contain BPA. The children's bamboo toothbrush bristles were analyzed for BPA, using the FS-5 Spectrofluorometer from Edinburgh Instruments. A calibration curve and analytical figures of merit were used to determine if BPA had leached from the nylon bristles of the children's bamboo toothbrushes. The nylon bristles from bamboo toothbrushes were placed in 100 ml of 50% methanol/water and 5 ml aliguots were collected over a 24-hour timespan to monitor the leaching of BPA. Fluorescence intensities were measured at an excitation wavelength of 278 nm and an emission wavelength of 304 nm to determine if BPA was present within the bamboo toothbrushes' nylon bristles. Bamboo toothbrushes labeled as "BPA-Free" were then compared using statistical analysis to other bamboo toothbrushes not labeled as "BPA-Free", as well as to plastic toothbrushes used in previous research, to determine which (if any) of the bamboo toothbrushes contained BPA.

PHCH Session C

C1. Hydrogen Fuel Cell powered drone ambulance

Ethan Tylor, and Seyed Ehsan Hosseini

Department of Mechanical Engineering, Arkansas Tech University

As technological innovations continue to shape the modern world, there has been an observable trend in human life expectancy. From 1800 to 2019, human life expectancy has doubled in major first world countries and even tripled or quadrupled in second or third world countries. There seems to be no plateau with this trend, and the rate at which human life expectancy increases remains positive. Research in quicker response times by emergency medical personnel shows a promising lead for further advancement with medical technology, found that reducing ambulance response time during cardiac arrest cases to 8 minutes increased the predicted survival to 8% and reducing it to 5 minutes increased survival to 10-11%. In fact, reducing ambulance response rates to 5 minutes could double survival rate. In this context, using drone ambulances would be helpful in situations where a typical manned ground ambulance cannot efficiently perform. The objective of this research is to investigate the performance of a drone ambulance in tactical and time sensitive situations. Existing drones are not able to meet the flight time requirements in most of the ambulance missions because the energy density of the employed conventional batteries is extremely low. Therefore, Hydrogen Fuel Cell powered drone ambulances have been proposed to significantly increase flight time and transfer up to 10 pounds of first aid medical equipment and medicines at speeds of up to 60 mph. The drone ambulances have the potential to lower the rate at which people die of cardiac arrests and strokes and could even provide situational analysis for other first responders such as firefighters.

C2. Cloud condensation nuclei (CCN) activity and water adsorption of model insoluble atmospheric aerosols: Application of Adsorption Activation Theory

<u>Adam De Groodt</u>, Julia Dick, Olivia Eddings, Hanna Detar, Aubrey Brink, Rebecca Parham, Bang-Gaio Nguyen, and Courtney D. Hatch Department of Chemistry, Hendrix College

The aerosol indirect climate effect remains the most uncertain factor that contributes to climate change. Cloud condensation nuclei (CCN) activity measurements and our theoretical understanding of cloud formation are important for quantifying the role of atmospheric aerosol on cloud formation and the resulting indirect climate effect. However, discrepancies exist in the literature between theoretical adsorption parameters measured from CCN activation and water adsorption of insoluble atmospheric aerosols, likely due to aerosol surface microstructure and fractality. The goal of the work presented is to demonstrate experimental closure between theoretical adsorption parameters measured from CCN activation and water adsorption measurements in the absence of surface microstructure, using polyhydroxylated nanospheres (PHS) as spherical model insoluble atmospheric aerosols. Adsorption model parameters were measured by applying Frenkel Halsey Hill Adsorption Activation Theory (FHH) to bulk water adsorption and direct CCN activation measurements of size-selected PHS spheres. Results suggest that, in the absence of surface microstructure, climate model parameters determined from CCN activity and bulk water adsorption measurements are in agreement, further supporting the hypothesis that the source of experimental discrepancies in the literature arise from aerosol surface microstructure and fractality.

C3. DFT study of ligand binding in the β -1 adrenergic receptor

<u>Daryna Safarian</u>, Megan Simons, Larryn Peterson, and Mauricio Cafiero Department of Chemistry, Rhodes College

The β 2-adrenergic receptor, which binds noradrenaline in the prostate region is integral for the activation of an angiogenic switch which induces exponential growth of prostate tumors. The removal of Adrb2, a gene encoding the β 2-adrenergic receptor, inhibits angiogenesis. This causes the endothelial cells to rely on their own nutrients and energy, halting tumor growth. Therefore, the removal of Adrb2 can slow down the progression of prostate cancer and can serve as an alternative to chemotherapy for cancer treatment. Comparison of a β -2-adrenergic receptor (PDB ID: 5X7D) and a β -1-adrenergic receptor (PDB ID: 2Y04) structures showed a conserved binding region on Chain A offset by approximately 8 amino acids between the two receptors. Hence, the structure of the β -1-adrenergic receptor with a bound partial agonist of salbutamol was used to create a model of the active site of the β -2adrenergic receptor. The adrenergic receptor was optimized in the active site using M062X/6-31G with relaxed amino acid sidechains. Interaction energies between the ligands and the receptor were calculated using M062X with the 6-311+G* basis set. From the tested molecules, positively charged inhibitors show greater interaction energies as compared to neutral and negatively charged inhibitors.

C4. Backscatter difference analysis of ultrasonic signals measured from brain tissue for possible transcranial applications

<u>Will R. Newman</u>, Cecille Labuda, and Brent K. Hoffmeister Department of Physics, Rhodes College

Transcranial ultrasonic backscatter can, in principle, be used to analyze brain tissue properties non-invasively. The main challenge involves errors associated with ultrasonic attenuation and distortion of the ultrasonic wave front by the skull. A newly developed backscatter difference technique may be relatively insensitive to these errors. The goal of this study was to generate parametric images of brain tissue based on a backscatter difference parameter called the normalized mean of the backscatter difference (nMBD). nMBD measures the power difference (in dB) between two different portions of a backscatter signal adjusted for the time difference (in us) between the two portions. Tissue specimens used in the study were 1 cm thick slices of preserved sheep brain prepared from the coronal, sagittal and transverse anatomic planes. Ultrasonic measurements were performed using a broadband transducer with a center frequency of 10 MHz. The transducer was mechanically scanned to acquire signals from all locations on each slice. Values of nMBD measured at each location were used to produce parametric images of the brain specimens. Structures visible in the parametric images were consistent with the known morphologic features of the brain. Measured values for the spatial mean and standard deviation of nMBD was 1.33 +/- 1.09 dB/us for the coronal slice, 1.04 +/- 1.54 dB/us for the transverse slice and 1.34 +/- 1.56 dB/us for the sagittal slice. These results lay the groundwork for transcranial ultrasonic backscatter measurements of the brain by providing baseline measurements of nMBD for brain tissue. Future work will compare these results to measurements made through skull bone.

C5. Calculating Stability and Structure of the CB1 Receptor Using Computational Methods to design a Positive Allosteric Modulator

<u>Emma Chavez</u>, and Dr. Caitlin Scott Department of Chemistry, 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. Positive allosteric modulators modify the duration and location of the agonist's affect within the body by binding to a distinct site than the agonist does, which make PAMs attractive to drug design. Our objective is to use molecular dynamics and computational chemistry to monitor the CB1 receptor's structure over time in a cellular environment as it samples conformations until finding a stable structure. For molecular dynamics, we used CHARMM-GUI to generate a physiological system consisting of POPC lipids, TIP3P water molecules, 0.15 M NaCl and protonated residues. We performed molecular dynamic simulations using Amber software on Marcy computers at Furman University provided by MERCURY. We performed minimization of lipids, waters and counter ions, a minimization on the entire system and an equilibration of the lipids and counter ions at a temperature of 300 K. In the future we will continue to run molecular dynamic simulations to find a stable conformation of the CB1 receptor and design a positive allosteric modulator that will interact with the predicted receptor structure.

C6. Comparison of Normal Rat Leg Bone with those under Simulated Microgravity and Cosmic Radiations Conditions

Manling Cheng, Rahul Mehta, and Brent Hill

Department of Physics and Astronomy, University of Central Arkansas

Abstract Presentation (Virtual) INBRE Annual meeting University of Arkansas Fayetteville Nov 6,7, 2020 Comparison of Normal Rat Leg Bone with those under Simulated Microgravity and Cosmic Radiations Conditions Manling Cheng1, Rahul. Mehta1 and Brent Hill2 1Department of Physics & Astronomy, University of Central Arkansas, Conway, AR 72035 2Department of Biology, University of Central Arkansas, Conway, AR 72035 In space, microgravity conditions and cosmic radiation have detrimental effects on the skeletal system of humans such as weakened bones, lowered elastic moduli and abnormal concentrations of calcium and phosphorus, as compared to bones not subject to these conditions. The hypothesis for this research is that under the simulated space conditions, bone compositions would be degraded due to loss of mechanical stimulation. There are three experimental groups: control, HLS (hind limb suspension), and radiation exposure. The rat bones (tibia and femur) were subjected to the three-point bending technique to measure the stress, strain, and elastic modulus. The three-point bending method fixes the bones at both ends while a force transducer exerts a known force upwards at a known speed, acting perpendicular to the bone. At the middle of each bone, force was induced on the posterior, medial, lateral, and anterior sides. After the 3-point bending experiments, the bones were cut in thin cross-section with a diamond tip saw. Then, the bone cross-sections were imaged using a Leica MZ6 microscope (IL, USA) equipped with an OptixCam digital camera. The image analysis program, ImageJ (NIH, USA), was used to measure the cortical and cavity areas. Finally, the bone sections were sputter coated with gold for analysis using the SEM (Scanning Electron Microscope). In addition to imaging the bone, an energy dispersive analysis (EDA) quantifies the relative percentages of carbon, oxygen, phosphorus, and calcium present. As previous studies have shown that microgravity could decrease the elasticity and the ratio elements of composition of the bone. Radiation exposure has been shown to damage osteoblast precursors within the irradiated volume but the specific mechanisms and potential influences on bone elasticity are still unknown. Acknowledgment: This work is supported by the Arkansas Space Grant Consortium (ASGC). The authors also acknowledge the assistance of Natalie King and Parimal Chowdhury (University of Arkansas for Medical Sciences)

C7. Molecular Modelling Approach to Identify Effective Protease Peptides against the Main Protease of SARS-CoV-2

Melina Reeves, and Mohammad A. Halim

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In late November of 2019, Wuhan, China experienced an outbreak of a pulmonary disease now referred to as coronavirus disease 2019 (COVID-19). What started in China, quickly spread to the rest of the world, resulting in the World Health Organization declaring it a global pandemic on March 11, 2020. COVID-19 was caused by a novel coronavirus called severe acute respiratory syndrome-coronavirus 2 (SARS-CoV2). Among 16 non-structural and 4 structural proteins, the main protease (3CLpro) has been identified as being one of the key structures responsible for the viral replication of COVID-19. One of the most important drug targets among coronaviruses is the main protease, which includes a Cys145-His41 catalytic dyad. In this study, nine proteases peptides were modelled to find out the potential inhibitors against the main protease (3CLpro). The 3D structure of the peptides was conducted by PEP-FOLD. It is a de novo method, which predicts and models peptide structures from amino acid sequences using coarse-grained force field. The modelled peptides are subjected to molecular docking against the main protease using Patchdock and Firedock. Based on the binding affinity and interactions, the best candidate were selected. Peptide with VHIPLGDA sequence exhibits the highest binding affinity of -55.57 kcal/mol whereas EWRKKRYS peptide shows the lowest binding affinity. Molecular dynamics simulation showed that the best peptides could strongly bind with the catalytic site of the main protease.

C8. DFT study of the selectivity of Tyrosinase

<u>Rachel Ancar</u>, Elise Moix, Danielle Wilson, Larryn Peterson, and Mauricio Cafiero Department of Neuroscience, Rhodes College

L-DOPA, a commonly used treatment for patients with Parkinson's disease, is converted into dopamine by DOPA-Decarboxylase. Before this can occur, Tyrosinase can convert L-DOPA into DOPAquione. By using targeted inhibition of Tyrosinase, this may lead to an increase in overall dopamine production. The effectiveness of L-DOPA can be prolonged by regulating dopamine's metabolism through the creation of a suite of dopaminergic derivatives that are designed to inhibit Tyrosinase. The interaction strength between the enzymatic active site and this suite of derivatives were compared and analyzed for its effectiveness as a Tyrosinase inhibitor. The model of the active site was created from a crystal-structure of the Tyrosinase enzyme bound with L-DOPA in its active site (PDB ID: 4P6S). Previously, new dopaminergic derivatives were optimized in the active site using M062X/6-31G with implicit solvation and relaxed amino acid side-chains. Interaction energies between the protein and the ligands were calculated using M062X with 6-311+G* basis set. Some of those molecules studied showed promise for being competitive inhibitors. Based on this early work, a new suite of molecules called the EM molecules were developed and also show promise for being competitive inhibitor. By creating and utilizing these novel ligands, it allows more effective treatments that will inhibit enzymes that break down L-DOPA and dopamine, while not inhibiting enzymes that promote dopamine synthesis.

C9. Clinically Proven Antibacterial Peptides against the Main Protease of SARS-CoV-2: A Molecular Modelling Study

<u>Sydney Du</u>, Archana Mishra, and Mohammad A. Halim Department of Physical Sciences, University of Arkansas - Fort Smith

In December 2019, an outbreak of pulmonary disease erupted in Wuhan, China. This disease, COVID-19, was caused by a new coronavirus named severe acute respiratory syndrome-coronavirus 2 (SARS-CoV-2). This disease spread rapidly, and the outbreak was soon declared a global pandemic on March 11, 2020 by the World Health Organization. The main protease (3CLpro) of SARS-CoV-2 is one of the key structures responsible for the viral replication of COVID-19. This makes it an ideal target for drug design research. The main protease signals for the cleavage of viral peptides into functional units which are then used for virus replication and packaging within the host cells. The functional units are dimers and each subunit of the dimer includes a Cys145-His41 catalytic dyad. In this study, six antibacterial peptides in the clinical trial were modelled to test as potential inhibitors against the main

protease. CABS-fold was used to model the selected peptides. These peptides were docked to 3CLpro using Patchdock and initial 1,000 peptide-3CLcomplexes obtained from Patchdock were then refined by Firedock. The best candidates were chosen based on the highest binding affinity and strong interactions of the peptide with Cys145 and His41 residues. 100 ns molecular dynamics simulations were then performed on the best candidates, which demonstrated that IMX942 strongly interacted with the catalytic sites. These results can assist the rational design of selective peptide inhibitors targeting the main protease of SARS-CoV-2.

C10. Photocatalysis As a Means of Purifying Water for Space Flight

<u>Abby Bankhead</u>, Dr. Dennis Province, and Dr. Jeffrey Massey Department of Engineering and Physics, Harding University

A way to purify water for use in water sanitation systems in space stations is Photocatalytic Oxidation. The use of surface-mount LEDs to emit UV radiation in correlation with Titanium Dioxide will affect a chemical reaction which forms Reactive Oxygen Species (ROS). These reactive oxygen series will kill the bacteria, compounds the bacteria feed on, and other substances left in the water on the ISS like chemicals from shampoos such as DMSD and things of the sort. Photocatalytic Oxidation is a good solution to what is currently being used on the ISS because substances like iodine and silver that have been used to flush the system are time consuming expensive, and although this keeps microbe levels down, it does nothing to get rid of DMSD, a chemical left behind by substances like deodorant and soap. This new method relies on the production of ROS and, consequently, does not introduce harmful substances into the water. Current testing has focused on the efficacy of UV-LED's in static fluid samples with good success. Use of the LED's in correlation with the catalyst Titanium Dioxide was much more effective in killing microbes than using those assets separately. To compare the two types of LED's they were both tested with the surrogate molecule methyl orange which simulates the presence of bacteria. As the orange pigment of the solution goes away, the figurative bacteria levels would be going away, so to test the effectiveness of the LED's, we measured the absorbance of the solution over time. After graphing and reviewing the data, it was seen that the absorbance of the system using the surface mount LEDs after an hour was about where the canned LED system was after two hours. Thus, the new LEDs were roughly twice as powerful as the 10 canned UV LEDs put together. This was promising data for our proof of concept. The goal of this work is to deliver a test system that simulates the fluid conditions that the UV-LED purification system will need to operate in. The International Space Station uses a closed fluid purification system to produce potable water from the crew's urine (which is first processed through the Urine Processor Assembly), latent crew moisture, and Sabatier product water. To test the efficacy of photocatalysis in this environment, a closed fluid flow system is needed to house more powerful surface mount UV-LEDs, pump the surrogate waste water, and (in the future) allow a place where we can introduce bacteria (which cause biofilms). This flow system needs to be able to pump water through at a constant flow rate, have a reaction chamber for the surface mount LED's and TiO2 substrate, be chemically inert, and have access to the fluid for sampling. The work for this specific proposal is focused on the design and fabrication of the reaction chamber. Other Harding researchers are building the fluid flow system and developing the sampling process. Additional to the reaction chamber, there is work to be finished with regard to the UV-LED electronics. The UV-LED's will self-heat and require cooling. Therefore, another objective of this work is to finish fabricating the electrical board, including a cooling system, for the UV-LED's. The approach is to cool the UV-LED's by a heat sink which will increase their light output and extend their lifetime. The UV-LED's electronics have been designed to be controlled by an Arduino (or other controller board) to supply alternating current to the lights or turn them on and off with sequences if needed. Another team is working on the Arduino control system. The final objective of this pilot work for the flow system will include a system integration of the flow system, reaction chamber, and the UVLED electronics board. System level tests will be run to characterize the flow systems effect on the test fluid. The last objective of this work will be to run a methyl orange and water solution test to compare to static fluid test results. The results will be analyzed and presented in preparation for future testing of the efficacy of the UVLED system with DMSD and biofilms. This is an ongoing research project. Last year, a test board with the new surface mount LED's was created for a proof of concept to compare the efficacy of these new LED's to the canned UV LED's that were being used by the chemistry students. As mentioned before, the results of these preliminary tests were extremely promising and indicated that I was ready to begin designing a more final board with these new LED's. What was completed last year was a design for a multi-LED circuit board that will be able to be programmed by an Arduino pr other kind of controller. The purpose of being able to control the circuit board in this manner is to allow programming of the board to turn the lights on and off when needed to conserve energy and deliver the most efficient way of destroying bacterial. Fabrication of this board is ongoing currently. The design for the reaction chamber to house the catalyst is currently being finalized from last year, and will be fabricated in the near future to be integrated with the multi-LED board and closed flow system for testing. Other students at Harding University are developing this flow system.

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