53rd Annual
ACS Southeast Undergraduate Research Conference

February 16-17, 2024

Clinton, MS

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Michigan State University

Professor of Chemistry

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2022 ACS President

Angela K. Wilson is the John A. Hannah Distinguished Professor of Chemistry at Michigan State University, Associate Dean for Strategic Initiatives in the MSU College of Natural Sciences and Director of the MSU Center for Quantum Computing, Science, and Engineering.

Angela earned a Ph.D. in chemical physics from the University of Minnesota and a B.S. in chemistry from Eastern Washington University. She was a postdoctoral fellow at the Environmental Molecular Sciences Laboratory (EMSL) at Pacific Northwest National Laboratory in theoretical physical chemistry.

In 2000, she joined the faculty at the University of North Texas where she became a Regents Professor and the Associate Vice Provost for Faculty and head of UNT's Office of Faculty Success. She was also the founder and Director of the Center for Advanced Scientific Computing and Modeling.

Angela was the 2022 President of the American Chemical Society. She has served as the Division Director (head) of the Division of Chemistry at the U.S. National Science Foundation where she was responsible for nearly $1B investments in chemistry nationwide, and led the strategic direction and national priorities in chemistry for NSF. Her honors include Fellow of the American Chemical Society, Fellow of the American Physical Society, Fellow of the American Association for the Advancement of Science, Francis P. Garvan-John M. Olin Medal, the International Union of Pure and Applied Chemistry Distinguished Woman in Chemistry Award, 2023 Iota Sigma Pi National Honorary Member, and the 2023 AWIS Zenith Award. In 2018, she was inducted into the Michigan Women's Hall of Fame. She is a National Associate of the U.S. National Academies of Science, Engineering, and Medicine (NASEM).

She is on the editorial advisory board of the Journal of Physical Chemistry and Cell Reports Physical Chemistry, the editorial board of Scientific Reports, and on the board of Chemical & Engineering News. She has served as President of the Division of Physical and Biophysical

Chemistry of the International Union of Pure and Applied Chemistry (IUPAC), Chair of the Chemistry Section of the American Association for the Advancement of Science (AAAS), and as Editor for Computational and Theoretical Chemistry. She has served as editor of six books including "Pioneers of Quantum Chemistry". She is Vice President of the non-profit QuSTEAM, and serves on the advisory board of EeroQ, a quantum computer hardware company. Angela's physical (computational and theoretical) chemistry research spans quantum mechanical and quantum dynamical method development, transition metal and heavy element chemistry, drug discovery, environmental chemistry, catalysis, thermodynamics, and sustainability. Her computational chemistry methodologies are utilized worldwide. She has published ~200 papers and has mentored ~200 students in her research group.

for 6 years before becoming chairman of the board. He joined the chemistry faculty at Mississippi State University in 2009. His current research is focused on water remediation and soil amendment using byproducts from the biofuel generation industry.

Titles by Session

Oral Session 1

9:00 a.m. in President's Dining Room B

Sponsored by CF Industries Yazoo Complex

Moderated by David H. Magers of Mississippi College

O1-1 **In Silico Strategy for Modelling of SARS-CoV-2 Immune Escape.**
Allyson McGowan, Jordhan D. Booth, Karina Kapusta
Department of Chemistry and Physics, Tougaloo College, Tougaloo, MS

O1-2 **Better safe than sorry: Preventing the next pandemic by studying newly emerging coronaviruses**
Misa Meadows, Uttara Jayashankar, Sydney Beechboard, Emma Lendy, Arun K. Ghosh, Andrew D. Mesecar
Department of Chemistry, Belhaven University, Jackson, MS
Department of Biological Sciences, Purdue University, West Lafayette, IN
Department of Biochemistry, Purdue University, West Lafayette, IN
Department of Chemistry, Purdue University, West Lafayette, IN

O1-3 **Natural Chemical Compounds as Potential Inhibitors Of an Omicron SARS-CoV-2 Mutants' Spike Glycoprotein. Computational Approach**
Jordhan D. Booth, Karina Kapusta
Department of Chemistry and Physics, Tougaloo College, Tougaloo, MS

O1-4 **CRISPR-mediated genome editing tool development for targeting and addressing USH2A mutation for patients with Usher syndrome type II**
Katerina Anamisis, Piyush K. Jain, and Noah Rakestraw
Department of Molecular Genetics and Microbiology, University of Florida
Department of Chemical Engineering, University of Florida

Oral Session 2

9:00 a.m. in Meeting Room B

Moderated by CJ Stephenson

O2-1 **Synthesis of Densely Functionalized Pyrroles from Alpha-Aminoketones and Alkynes**
Andrew J. Rowell, Matthew G. Donahue
Department of Chemistry, University of Southern Mississippi

O2-2 **Synthesis of Terminal Methylidyne Ligands by a Novel "C-H" Transfer Reagent**

Chandler Woo, Rajesh Mukkera, Sidney Creutz
Department of Chemistry, Mississippi State University, Starkville, MS

O2-3 **Photochemical Key Steps in the Synthesis of Isoindolone Piperidines As Kinase Inhibitors: Asymmetric Photochemical Cyclization**

Zoe O. Elder[1], Tynai J. Bridges[1], Caroline A. McKinney[1], Mariam R. Bhatti[1], Hayley T. Allen[2], Matthew G. Donahue[2], Wolfgang H. Kramer*[1]
[1]Department of Chemistry and Biochemistry, Millsaps College, Jackson, MS, E-mail: kramewh@millsaps.edu
[2]Department of Chemistry and Biochemistry, The University of Southern Mississippi, Hattiesburg, MS

Poster Session 1

10:45 a.m. in Anderson Hall

P1-AE1 **Analysis of Toxic Metal Contamination in Cosmetic Beauty Products**

Alison Cevallos, Caroline McCaleb, Ashley Basset, Pazia Kingma, Miles Taylor Leverette, ArKayla Martin, Maha Obaid, and Scoty Hearst
The Department of Chemistry and Biochemistry, Mississippi College, Clinton, MS

P1-AE2 **Emergent Methods for Isomer Differentiation using Mass Spectrometry**

Andie L.M. Nanney, Matthew J. Carlo, Amanda L. Patrick
Department of Chemistry, Mississippi State University, Mississippi State, Mississippi, USA 39762

P1-AE3 **Absorption of Lithium in Various Organs of Crayfish: A Laboratory Study**

Andrew Doubert, Javian Ervin, Jacob Garteiser, Scoty Hearst, Joseph Kazery
Department of Biological Sciences, Mississippi College, Clinton, MS

P1-AE4 **Characterization of Commercially Available Delta-8-THC Products from Martin, TN**

Austin Vest, Amanda Burkhart
Department of Chemistry & Physics, University of Tennessee at Martin, Martin, TN

P1-AE5 **River Monsters: Predatory Fish as Sentinel Species for Toxic Metals in Aquatic Environments**

Chinaza Nwaiwu, James Lock, Alexandria Harris, Mohammad Ibrahim, Martha Hollowell, Jose Alfonso Xavier, Takaye Farmer, Lillian Sisson, Joseph Kazery, Trent Selby, and Scoty Hearst

Department of Chemistry and Biochemistry, Department of Biology, Mississippi College, Clinton, MS

P1-AE6 **Bottle stir vs. Soxhlet extraction of parthenolide from *Magnolia grandiflora*, followed by flash chromatography separation**

Erin Timm, Dr. Sven Eklund

Department of Chemistry, Louisiana Tech University, Ruston, LA

P1-AE7 **Loblolly Pine Needles as a Template for aluminosilicate Xerogels.**

Ian Misiak, Dr Sven Eklund

Louisiana Tech Chemistry Department

P1-AE8 **Temperature Effects on Adsorption and Absorption of a New Pollutant in Crayfish**

Javian Ervin, Andrew Doubert, Jacob Garteiser, Scoty Hearst, Joseph Kazery

Department of Biological Sciences, Mississippi College, Clinton, MS

P1-BM1 **Women Chemists Who Won the Nobel Prizes in Chemistry: A Brief Overview**

Jordan Smith, Ganna Lyubartseva

Department of Biochemistry and Chemistry, College of Science and Engineering, Southern Arkansas University, Magnolia AR 71753

P1-BM2 **Impact of Lemongrass Extract Citral on Mouse Motor Coordination, Fear, and Anxiety**

Selah Roberts, Gracie Bassett, Ashley Carter, Jameson Cook, Mitchel Creel, Addie Jolly, Alana Latorre, ArKayla Martin, Stephen Mills, Analee Rios, Sukhbir Sohal, Hinaben Patanvadia, Harsh Patel, Anuradha Ragila, Pinalba Zala, Nilay Kantibhai Zalavadiya, Trent Selby, and Scoty Hearst

Mississippi College Chemistry and Biochemistry Dept, Clinton, MS

P1-BM3 **Evidence of SARS-CoV-2 antibodies in Mississippi White-tailed Deer**

Stephen Mills[1], Pedro Palermo[2], Doug Watts[2], Kamen Campbell[4], John Bates[3], Scoty Hearst[1]

1. Chemistry and Biochemistry, Mississippi College, Clinton, MS, United States.
2. Department of Biological Sciences and Border Biomedical Research Center, The University of Texas at El Paso, El Paso, TX, United States.
3. Department of Cell and Molecular Biology, University of Mississippi School of Medicine, Jackson, MS, United States.
4. Deer Program, Mississippi Department of Wildlife Fisheries and Parks, Jackson, MS, United States.

P1-BM4 **Isolation of Bioactive Secondary Metabolites from Mangrove Fungal Endophyte**

Emma Burdick, Ezequiel Cruz Rosa, Bill Baker

Department of Chemistry, University of South Florida, Tampa, Fl

P1-IM1 **Understanding the formation, reactivity, and physical properties of anionic lanthanide complexes**

Ben Willis, Elisabeth Fatila

Louisiana Tech Department of Chemistry

P1-IM2 **Investigations into Light-Activated Ruthenium-Ligand Complexes as Potential Anti-Cancer Compounds**

Caleb Buell, Aditya Kuppravalli, Chandni Bhat, Olaitan Oladipupo, Elizabeth Papish

Department of Chemistry & Biochemistry, The University of Alabama, Tuscaloosa, AL

P1-IM3 **Effects of Selenium Doping on BaZrS3 Nanocrystals**

Paul Gramelspacher, Vaishali Kshirsagar, Sidney Creutz

Department of Chemistry Mississippi State University,

P1-OP1 **Photochemical Key Steps in Cyclization Reactions: Synthesis of Isoindolone Piperidines As Kinase Inhibitors**

Caroline A. McKinney[1], Tynai J. Bridges[1], Mariam R. Bhatti[1], Hayley T. Allen[2], Matthew G. Donahue[2], Wolfgang H. Kramer*[1]

[1]Department of Chemistry and Biochemistry, Millsaps College, Jackson, MS, E-mail:kramewh@millsaps.edu

[2]Department of Chemistry and Biochemistry, The University of Southern Mississippi, Hattiesburg, MS

P1-OP2 **Progress Towards the Synthesis of the Cannabichromene**
Jimenez Xavier, Baron Verna B.
University of Tennessee at Martin

P1-OP3 **A Novel Approach to Incorporating Multiple 6F Groups for Enhanced Properties of Polycondensation Polymers**
Kari M. Chamberlain, Gustavo Munoz, Charles U. Pittman, Dennis W. Smith
Department of Chemistry, Mississippi State University, Mississippi State, MS

P1-OP4 **Developing an Environmentally Conscious Method to Synthesize N-nitrosodicyclohexylamine for its Utilization in Co-crystallization**
McKenzee Henson, Kylie Carruth, S. Ariel Kelley
Department of Chemistry, Belhaven University, Jackson, MS

P1-OP5 **Carbazole Derivatives as Photocatalysts in the C—H Arylation of *N*-Methylpyrrole**
Natalie A. Reece, Ashley R. Longstreet
Department of Chemistry, Biochemistry, and Physics, The University of Tampa, Tampa, FL

P1-OP6 **Synthesis of diaminopyridinylethynylarene macrocycles**
Sydney Watts, Samantha J. Schwartz, Trent D. Selby
Department of Chemistry & Biochemistry, Mississippi College, Clinton, MS

P1-PC1 **High Accuracy Potential Energy Surfaces and Spectroscopic Properties for the Magnesium Monocarbide Radical**
Caleb Joshua Culler, Donatus Atsu Agbaglo, Nathan J. DeYonker
Department of Chemistry, University of Memphis, Memphis, TN 38152, U.S.A.

P1-PC2 **Theoretical NMR Analysis of Nitrosamines**
Desmond Simms, S. Ariel Kelley, and D. Brandon Magers
Department of Chemistry & Physics, Belhaven University, Clinton, MS

P1-PC3 **Stabilization Factors in Fluoro and Chloro Derivatives of the Cyclopropyl Carbinyl Cation**
Hanna K. Bynum and David H. Magers
Computational Chemistry Group, Department of Chemistry & Biochemistry, Mississippi College, Clinton, MS

P1-PC4 **Investigating the effects of linker substitution on hydrogen adsorption between two isostructural Metal-organic Frameworks**
Herrera, Louis; Pham, Tony
University of South Florida

P1-PC5 **Computational Characterization of Aluminum Nitride Clusters for Interstellar Chemistry**
Jonathan Dotson, Charles Palmer, Ryan Fortenberry
Department of Chemistry, University of Mississippi, Oxford, Mississippi

P1-PC6 **Computational Investigation of Vitamin C and Vitamin E on Basal Cell Carcinoma**
Katia Gonzalez-Adame, Patricia M. Todebush
Department of Chemistry and Biochemistry, University of North Georgia, Oakwood, GA 30566

P1-PC7 **Conventional Strain Energies of Cyclopropylborane, Borirane, Boretane, the Diboretanes, Borolane, the Diborolanes, Borinane, and the Diborinanes**
Kaylee E. Hood, Rachel M. Rocray, and David H. Magers
Computational Chemistry Group, Department of Chemistry & Biochemistry, Mississippi College, Clinton, MS

P1-PC8 **Enthalpies of Formation of Quinoline Derivatives by Homodesmotic Reactions**
Ryleigh G. Borbash, Caitlin E. McCormick, and David H. Magers
Computational Chemistry Group, Department of Chemistry & Biochemistry, Mississippi College, Jackson, MS

Oral Session 3

1:00 p.m. in President's Dining Room B

Sponsored by the Vinyl Intitute

Moderated by D. Brandon Magers of Belhaven University

O3-1 **Performance of a hybrid explicitly correlated coupled cluster method for the use in anharmonic vibrational frequency computations**
Alexandria Watrous, Brent Westbrook, and Ryan Fortenberry
Department of Chemistry and Biochemistry, University of Mississippi, University, MS

O3-2 **Single Molecule Spectroscopy and Super-resolution Microscopy Imaging**

James Ethan Batey, Geun Wan Kim, Meek Yang, Darby Heffer, Elric Pott, Hannah Giang, and Bin Dong*

Department of Chemistry and Biochemistry, University of Arkansas

O3-3 **Predicting F-SAPT Interaction Energies from MM/GBSA Analysis for the Chorismate Mutase Enzyme**

Nathan DeYonker, Jose Bachega, Khawlah Almurisi

Department of Chemistry, University of Memphis, Memphis, TN

Oral Session 4

1:00 p.m. in Meeting Room B

Moderated by S. Ariel Kelley of Belhaven University

O4-1 **The Synthesis of Piperidines via the Intramolecular Prins Cyclization of N-Sulfonyl Alpha-Aminoacetals**

Damien D. Cooper, Matthew G. Donahue

Department of Chemistry, University of Southern Mississippi

O4-2 **Pyridine-based HIV Integrase Inhibitors: Side-Chain Development**

Tyler D. Twedt[1], Brenna R. Macaluso[1], A. Margaret Miller[1], Hannah J. N. Mattke[1], Christopher T. Bruni[1], Sharon E. Suffern[1], R. Victor Mishoe[1], Gavisha Mugon[1], Sarah J. Hayek[1], Jacques J. Kessl[2], Julie A. Pigza[2], Matthew G. Donahue[2], Wolfgang H. Kramer[1*]

[1]Department of Chemistry and Biochemistry, Millsaps College, Jackson, MS, E-mail: kramewh@millsaps.edu

[2]Department of Chemistry and Biochemistry, The University of Southern Mississippi, Hattiesburg, MS

O4-3 **Synthetic Efforts Toward Halofuginone as a Therapeutic for Tick-Borne Diseases**

Oussama Errida, Matthew G. Donahue

Department of Chemistry, University of Southern Mississippi

Poster Session 2

2:30 p.m. in Anderson Hall

P2-AE9 **Degrading Organic Pollutants via the Generation of Radical Oxygen Species from Piezoelectric Materials**

Nathan Holley

Department of Chemistry, Louisiana Tech University

P2-AE10 **Revealing molecular mechanism in heterogeneous catalysis under nanoconfinement at single molecule level**

Darby Heffer, Geunwan Kim, Bin Dong

Department of Chemistry and Biochemistry-- University of Arkansas, Fayetteville AR

P2-AE11 **Analysis of Toxic Metals in Bigmouth and Smallmouth Buffalo Fish of the Mississippi River**

Jose Alfonso Xavier Fernandez, Ella Bailey, Javian Ervin, Stephen Mills, Chinaza Nwaiwu, Fritz Valerio, Wilson Hooker, Caroline Armstrong, Christian Leach, Alison Cevallos, Trent Selby, and Scoty Hearst

Mississippi College Chemistry and Biochemistry Dept, Clinton, MS

P2-AE12 **Usage of Lab-Built Solution-Cathode Glow-Discharge Atomic Emission Spectrometer to Determine Concentration of Lithium in Brines.**

Gracen R. Andres

Department of Chemistry, Louisiana Tech University, Ruston, LA

P2-AE13 **Osteo-deer-porosis: Nutrient and heavy metal analysis of weak antlers in Mississippi white-tailed deer**

Caroline Armstrong, Jose Alfonso Xavier, Lee Yelverton, Marguerite Yelverton, Megan Malone, Trent Selby, and Scoty Hearst

The Department of Chemistry and Biochemistry, Mississippi College, Clinton, MS; The Highland Veterinary Clinic, Ridgeland, MS

P2-AE14 **Comparison of Methods for Determining Stress in a Crayfish Model and Environmental Application**

Jacob Garteiser, Javian Ervin, Andrew Doubert, Joseph Kazery

Department of Biological Sciences, Mississippi College, Clinton, MS

P2-AE15 **Assessing Storage Conditions of Ignitable Liquids on Carbon Strips for Applications in Forensic Fire Debris**

Imani Peat, Amanda Burkhart
Department of Chemistry & Physics, University of Tennessee at Martin, Martin, TN

P2-AE16 **A multigenerational study of insect larvae that consume expanded polystyrene**

Madison Ely, Nellie Massey, Miles Taylor Leverette, Scoty Hearst, Trent D. Selby
Department of Chemistry & Biochemistry, Mississippi College, Clinton, MS

P2-BM5 **Surveillance for Zoonotic Parasites in Mississippi Raccoons**

Javian Ervin, Stephen Mills, Chinaza Nwaiwu, Fritz Valerio, Wilson Hooker, Jose Alfonso Xavier Fernandez, Caroline Armstrong, Christian Leach, Trent Selby, and Scoty Hearst
Mississippi College Chemistry and Biochemistry Dept, Clinton, MS

P2-BM6 **Surveillance for Zoonotic Parasites in Mississippi River Fish**

Fritz Valerio, Christian Leach, Javian Ervin, Stephen Mills, William Janous, Chinaza Nwaiwu, Wilson Hooker, Jose Alfonso Xavier Fernandez, Caroline Armstrong, Javian Ervin, Joseph Kazery, Trent Selby, and Scoty Hearst
Mississippi College, Chemistry and Biochemistry Dept, Biology Dept, Clinton, MS

P2-BM7 **Binding Chromium(III) to Form Mixed Cr(III),Fe(III) Serum Transferrins**

Dylan R. Graham, Eilidh Drummond, Marlena Barrido, and John B. Vincent
Department of Chemistry and Biochemistry, The University of Alabama, Tuscaloosa, AL 35487-0336

P2-BM8 **An inexpensive, 3D-printed biofilm reactor for testing nanoparticle treatments under flow conditions**

Elizabeth R. McCaffrey, Dhanush L. Amarasekara, Tanveer K. Shaikh, Nicholas C. Fitzkee
Department of Chemistry, Mississippi State University, Mississippi State, MS 39762 USA

P2-IM4 **Synthesis & Characterization of Alpha-Zirconium Phosphate Nanoplatelets**

Chandni Bhat[1], Ataur Rahman[2], Avinash Srivastava[2], and Jonathan D. Burns[2]
1. Department of Chemistry and Biochemistry, University of Alabama, Tuscaloosa,AL
2. Department of Chemistry, University of Alabama at Birmingham, Birmingham, AL

P2-IM5 **Synthesis of bipyridine-containing bio-inspired ligands to support manganese and iron for oxidative catalysis**

Jennifer R. Greer, Fernanda Garcia, Sidney E. Creutz
Department of Chemistry, Mississippi State University, Starkville, MS

P2-OP7 **N-methylpyridinium as a novel charged acidifying group for squaramide organocatalysts**

Aiden Leise, Julie A. Pigza
School of Mathematics and Natural Sciences, University of Southern Mississippi, Hattiesburg, MS

P2-OP8 **Development of activated palladium-acyl complexes as precatalysts for cross-coupling catalysis**

Blake Yuenger, Kevin Shaughnessy, Makynna Koper
Department of Chemistry and Biochemistry, The University of Alabama, Tuscaloosa, AL

P2-OP9 **Evaluation of the use of Zinc oxide for an Undergraduate Friedel – Crafts Acylation Experiment**

Ketron Charles K., Baron Verna B.
Department of Chemistry and Physics, The University of Tennessee at Martin, Martin, TN

P2-OP10 **Synthesis of Pyridine-based HIV Integrase Inhibitors**

Brenna R. Macaluso[1], Christopher T. Bruni[1], Sharon E. Suffern[1], R. Victor Mishoe[1], Gavisha Mugon[1], Sarah J. Hayek[1], Jacques J. Kessl[2], Julie A. Pigza[2], Matt G. Donahue[2], Wolfgang H. Kramer[1]*
[1]Department of Chemistry and Biochemistry, Millsaps College, Jackson, MS
[2]Department of Chemistry and Biochemistry, The University of Southern Mississippi, Hattiesburg, MS

P2-OP11 **An Environmentally Conscious Approach to the Synthesis of Nitrosodiphenylamine**

Chloe B. Amos, Misa S. Meadows, Karlee McKinney, S. Ariel Kelley
Department of Chemistry, Belhaven University, Jackson, MS

P2-OP12 **Preparation of conjugated polyphenylethynylarene macrocycles**

Alana Latorre, Elizabeth McRae, Trent Selby
Department of Chemistry & Biochemistry, Mississippi College, Clinton, MS

P2-PC10 **DFT + F12 QFFs for Cost-Effective Rovibrational Spectral Data Predictions of Ground and Excited Electronic States**

Noah Garrett, Megan Davis, Ryan Fortenberry
Department of Chemistry and Biochemistry, University of Mississippi, University MS
Theoretical Division Division, T-1 and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos NM

P2-PC11 **Conventional Strain Energies of Thiasilirane and the Thiasiletanes**

Avery C. Foret, Mia K. Hyme, Kayla E. Ryan, and David H. Magers
Computational Chemistry Group, Department of Chemistry & Biochemistry, Mississippi College, Clinton, MS

P2-PC12 **Conventional Strain Energy and Hyperconjugation in Cyclopropylborane and Fluoro and Chloro Derivatives**

Gabrielle D. Winters and David H. Magers
Computational Chemistry Group, Department of Chemistry & Biochemistry, Mississippi College, Clinton, MS

P2-PC13 **Enthalpies of Formation of Chloro, Cyano, and Methyl Derivatives of Heterocyclic Aromatics by Homodesmotic Reactions**

Gracie Bassett, Dean Damon, Carmen Shumaker, and David H. Magers
Computational Chemistry Group, Department of Chemistry & Biochemistry, Mississippi College

P2-PC14 **Conventional Strain Energies of Small Heterocycles of Carbon and Silicon and their Amino and Nitro Derivatives by Model Reactions**

Eli M. Franklin and David H. Magers
Computational Chemistry Group, Department of Chemistry & Biochemistry, Mississippi College

P2-PC15 **Theoretical Anharmonic Vibrational Analysis of Nitrosamines**

Kerany Un, Ashley Davidson, S. Ariel Kelley, and D. Brandon Magers
Department of Chemistry, Belhaven University, Jackson, MS

P2-PC16 **Reaction Pathways for the Formation of Magnesium Oxide from Water and Metal Hydrides**

Kailey M. Bell, Rebecca A. Girth, and Ryan C. Fortenberry
Department of Chemistry, University of Mississippi, Oxford MS

P2-PC17 **Systematic analysis of various models, theories, and basis sets on the energy of solvation of small cations with Python data science tools**

Justin Humphrey, Desmond Simms, David Emenike, Ryan C. Fortenberry, and D. Brandon Magers

Department of Chemistry & Physics, Belhaven University, Jackson, MS

Oral Presentation Abstracts

Oral Session 1

9:00 a.m. in President's Dining Room B

O1-1 **In Silico Strategy for Modelling of SARS-CoV-2 Immune Escape.**

Allyson McGowan, Jordhan D. Booth, Karina Kapusta
Department of Chemistry and Physics, Tougaloo College, Tougaloo, MS

Over nearly four years, SARS-CoV-2 has undergone numerous mutations. Some of these mutations have been associated with increased mortality rates, enhanced transmission, repeated infections, evasion of immune responses, and more effective replication of the virus. Meanwhile, the consequences of other mutations remain either unclear or insignificant. Despite the extensive data available on such effects, inconsistencies and gaps in information continue to exist. Advanced computational chemistry methods may help bridge these knowledge gaps and enhance our understanding. This project aimed to develop a strategy for predicting immune response evasion based on mutations occurring in the SARS-CoV-2 spike glycoprotein. Known and available crystallographic structures of the wild type, as well as alpha, beta, gamma, delta, epsilon, kappa, and the original omicron (BA.1) variants, were utilized. Additionally, a constructed 3D homology model of the newest omicron (JN.1) subvariant was used to scan against the murine antibody 2B04. Receptor-binding domain (RBD) complexes with antibodies were subjected to Molecular Dynamics simulation to evaluate the strength of their interactions and the stability of the complexes. The results from these simulations were validated against existing research and used to deepen our understanding of viral mutations. They also provide a method for quickly predicting the immune escape of newly emerging variants of SARS-CoV-2, based on limited data such as the sequence of a protein.

This work was supported by the Mississippi INBRE, funded by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103476.

O1-2 **Better safe than sorry: Preventing the next pandemic by studying newly emerging coronaviruses**

Misa Meadows, Uttara Jayashankar, Sydney Beechboard, Emma Lendy, Arun K. Ghosh, Andrew D. Mesecar

Department of Chemistry, Belhaven University, Jackson, MS
Department of Biological Sciences, Purdue University, West Lafayette, IN
Department of Biochemistry, Purdue University, West Lafayette, IN
Department of Chemistry, Purdue University, West Lafayette, IN

The effects of the Covid-19 global pandemic caused by the *betacoronavirus*, SARS-CoV-2, has emphasized the importance of studying newly emerging coronaviruses that could potentially cause further pandemics. The recent emergence of CCoV-HuPn-2018 (CCoV), a human-infecting canine coronavirus, was detected in patients with pneumonia in Malaysia, identifying CCoV as a zoonotic virus. Upon sequencing, the novel CCoV was classified as an *alphacoronavirus*, similar to other animal-infecting coronaviruses such as the feline infectious peritonitis virus (FIPV), which infects cats. Coronaviruses are single-stranded positive RNA viruses that translate their genome into two large polypeptides, pp1a and pp1ab. The 3-Chymotrypsin-like protease (3CLpro) is responsible for cleaving these polypeptides at eleven sites to form smaller, non-structural proteins that are essential for viral replication. The importance of the 3CLpro and its conservation amongst various coronaviral genera make it an attractive drug target. The objective of our study is to repurpose small molecule inhibitors designed against SARS-CoV-2 in efforts to establish broad-spectrum inhibition against *alphacoronaviruses* CCoV and FIPV. In this study, we use a fluorescent-based peptidomimetic substrate to characterize and compare the 3CLpro enzymatic properties. We further performed Structure Activity Relationship (SAR) studies to identify characteristics of the inhibitors contributing to broad-spectrum efficacy. To understand how the identified inhibitors affect the stability of the protein, the melting temperatures of the 3CLpros bound to these inhibitors were quantified using Differential Scanning Fluorimetry (DSF). Together, this study provides valuable information for the future development of broad spectrum inhibitors against various coronaviral genera.

O1-3 **Natural Chemical Compounds as Potential Inhibitors Of an Omicron SARS-CoV-2 Mutants' Spike Glycoprotein. Computational Approach**

Jordhan D. Booth, Karina Kapusta
Department of Chemistry and Physics, Tougaloo College, Tougaloo, MS

COVID-19, a respiratory illness caused by the coronavirus SARS-CoV-2, has claimed numerous lives since it first appeared in 2019. This virus is distinguished by its rapid genetic mutations, which allow it to adapt swiftly to new environments, impacting key factors like transmissibility and resistance to immune responses. Consequently, there is a growing interest in inhibitors that can effectively target various viral strains simultaneously. Our prior research identified potent natural compounds, such as hesperidin in citrus fruits, that hinder the binding of the SARS-CoV-2 spike glycoprotein to the ACE2 receptor in human cells. These findings have been corroborated by in-vitro studies conducted by other scientific teams. However, hesperidin showed little to know affinity towards the novel omicron variant of a virus. Inspired by these results, we are now exploring the efficacy of other compounds present in the essential oils of citrus fruits against various new subvariants of an omicron. In this study, we focused on the Spike Glycoprotein's Receptor Binding Domains (RBD) of recent SARS-CoV-2 subvariants. We constructed 10 homology models and utilized 7 reference RBD structures for comparative analysis. Our research employed the Schrodinger Software Package for all computational tasks. Techniques such as molecular docking, molecular mechanics, and molecular dynamics were used to assess the potential inhibitors' effectiveness. This research demonstrates the value of homology modeling in predicting the RBD's secondary structure, paving the way for innovations in drug discovery. These advancements could lead to the development of new, non-toxic, natural treatments that are effective against multiple coronavirus variants at the same time.

This work was supported by the Mississippi INBRE, funded by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103476.

O1-4 **CRISPR-mediated genome editing tool development for targeting and addressing USH2A mutation for patients with Usher syndrome type II**

Katerina Anamisis, Piyush K. Jain, and Noah Rakestraw
Department of Molecular Genetics and Microbiology, University of Florida
Department of Chemical Engineering, University of Florida

Usher syndrome is a rare genetic disease that affects both hearing and vision. This inherited autosomal recessive condition affects 4 to 17 per 100,000 people and accounts for about 50 percent of all hereditary deaf-blindness cases.

There are three distinct types of Usher syndrome, of which type II is the most common. Usher syndrome type II is caused by mutations of the *USH2A* gene, a 15.7 kb gene that encodes for the protein usherin which localizes to photoreceptor cilium and cochlear hair cells. This triggers progressive deterioration of photoreceptor function, commencing with the more susceptible rod cells. This subtype of Usher syndrome includes moderate to severe sensorineural hearing loss from birth and progressive loss of vision, prompting retinitis pigmentosa (RP). In RP, the photoreceptors progressively lose function, causing loss of peripheral vision that can lead to blindness by midlife and decreased night vision by adolescence.

The large size of the *USH2A* gene makes gene therapy challenging as a potential treatment. However, precision genome editing in the eye could enable precise gene correction and potentially treat a wide range of inherited diseases, including genetic disorders of vision.

The objective of my project is to develop a CRISPR-mediated prime editor tool to target and correct the *USH2A* mutation for deletion of exon 66, c.14483del (p.Pro4828Hisfs*56). This project can be broken down into three major parts, which include inducing the mutation in HEK293T cells and producing a cell line that exhibits this mutation, testing a variety of prime editing tools and techniques to target and address this mutation, and testing the prime editing tool on organoids and mouse models. My overall goal is to apply a CRISPR-mediated prime editor tool to correct *USH2A* gene mutations that can be used in clinical trials.

Oral Session 2

9:00 a.m. in Meeting Room B

O2-1 Synthesis of Densely Functionalized Pyrroles from Alpha-Aminoketones and Alkynes

Andrew J. Rowell, Matthew G. Donahue

Department of Chemistry, University of Southern Mississippi

The pyrrole ring is a five-membered aromatic heterocycle containing four carbon atoms and one nitrogen atom. The pyrrole ring is found in small molecule prescription drugs including atorvastatin, ketolorac, sunitinib and tolmetic. The various substitution patterns in these molecules showcases the nature of the synthetic challenges in construction of the pyrrole nucleus. In this talk, a strategy for the de novo synthesis of densely functionalized pyrroles will be discussed. Starting from commercially available alpha-amino ketones, the nitrogen is sulfonylated with para-toluenesulfonyl chloride to the secondary sulfonamide. This increases the acidity of the N—H bond allowing for a subsequent Michael addition to an alkyne under mild conditions with cesium carbonate. Upon addition of the sulfonamide nitrogen to the alkyne, the resultant allenoate anion undergoes a 5-exo-trig ring closure upon the pendant ketone. The isolable product of this sequence is a five membered ring nitrogen heterocycle with a tertiary alcohol that is primed for elimination to the pyrrole. Upon treatment with BF3•OEt, this alcohol is readily ionized resulting in aromatization of the ring. Thus far, this research has been carried out with alpha-amino ketones that have a non-ionizable substituent including phenyl and tert-butyl ketone. The alkynes must have an electron-withdrawing group such as an ester or ketone. New compounds produced from this work have been characterized by spectroscopic methods including IR and 1H and 13C NMR.

O2-2 **Synthesis of Terminal Methylidyne Ligands by a Novel "C-H" Transfer Reagent**

Chandler Woo, Rajesh Mukkera, Sidney Creutz
Department of Chemistry, Mississippi State University, Starkville, MS

The electronic structure and reactivity of earth-abundant terminal metal-carbon multiple bonds remain poorly explored despite their importance in facilitating catalytic reactivity involving unsubstituted hydrocarbons. Investigations of these species are currently impeded by the lack of direct synthesis of these complexes. Hence, we have developed a new "C-H" transfer reagent to readily access methylidyne ligands for fundamental studies. This reagent features anthracene elimination, which has been previously employed to synthesize other terminal metal-ligand multiply-bonded species. Methylidyne-containing complexes, such as [N3N]Mo≡CH, were synthesized with the transfer reagent to probe the reactivity and give insight on the kinetics and mechanism of the reagent. Furthermore, complexes featuring a pseudo-tetrahedral environment have also been tested due to the high-lying π*-bonding orbitals in the d-manifold, which have been proven to assist in metal-ligand multiple bonding. The development of this reagent serves to greatly facilitate investigations into the reactivity of these species, as earth-abundant metal-carbon multiple bonds play an important role in catalytic cycles such as Fischer-Tropsch catalysis and a multitude of coupling reactions.

O2-3 **Photochemical Key Steps in the Synthesis of Isoindolone Piperidines As Kinase Inhibitors: Asymmetric Photochemical Cyclization**

Zoe O. Elder[1], Tynai J. Bridges[1], Caroline A. McKinney[1], Mariam R. Bhatti[1], Hayley T. Allen[2], Matthew G. Donahue[2], Wolfgang H. Kramer*[1]

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Cancer cells are the result of disruption of tightly regulated metabolic pathways. This leads to uncontrolled proliferation of cells as seen in invasive tumors. Inhibition of certain metabolic enzymes thus might provide a tool to minimize the harmful effects of excessive cell growth. Two key phosphorylating enzymes, glycogen synthase kinase-3 (GSK3) and cyclin-dependent kinases (CDKs) are the target of researchers to interfere with cancer metabolism. Valmerins are isoindolone piperidines that have been shown to inhibit GSK3/CDK enzymes during cell proliferation. In this project, we are using the photodecarboxylative cyclization as a key step in the synthesis of GSK3/CDK inhibitors. The syntheses are initiated from affordable building blocks and culminate in the stereo-controlled synthesis of the target molecules. Variations in the chromophore lead to the formation of regioisomers, the control of which is important. Electron-donating and electron-withdrawing effects of the substituents might direct the cyclization to one side of the imide.

Acknowledgement: This work was supported by the Mississippi INBRE, funded by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103476.

Oral Session 3

1:00 p.m. in President's Dining Room B

O3-1 **Performance of a hybrid explicitly correlated coupled cluster method for the use in anharmonic vibrational frequency computations**

Alexandria Watrous, Brent Westbrook, and Ryan Fortenberry
Department of Chemistry and Biochemistry, University of Mississippi, University, MS

A hybrid quartic force field approach that produces the same accuracies as non-hybrid methods but for less than one quarter of the computational time is introduced as an alternative to calculate highly accurate theoretical rovibrational spectral data for application to observations from both ground-based radio telescopes and space-based missions like JWST. This method utilizes explicitly correlated coupled cluster theory at the singles and doubles level inclusive of perturbative triples (CCSD(T)-F12b) in conjunction with a triple- basis set, core electron correlation, and scalar relativity for the harmonic terms and CCSD(T)-F12b with a valence double- basis set for the cubic and quartic terms. There is no sacrifice in the prediction of fundamental anharmonic vibrational frequencies or vibrationally-averaged rotational constants as compared to experiment, but the time saved is notable. As such, this work reports a hybrid approach (F12-TcCR+DZ) in the computation of rovibrational spectral data which can be applied to the observation of novel molecules in the gas phase in the laboratory and potentially even in astrophysical environments.

O3-2 **Single Molecule Spectroscopy and Super-resolution Microscopy Imaging**

James Ethan Batey, Geun Wan Kim, Meek Yang, Darby Heffer, Elric Pott, Hannah Giang, and Bin Dong*

Department of Chemistry and Biochemistry, University of Arkansas

Single-molecule localization microscopy (SMLM) has become a strong technique in the toolbox of chemists, biologists, physicists, and engineers in recent years for its unique ability to resolve characteristic features quickly and accurately in complex environments at the nanoscopic level. Super-resolution multicolor imaging has seen the greatest advancement among SMLM techniques, drastically improving the differentiation ability of nanostructures beyond the diffraction limit and increasing the precision with which previously unresolvable structures are studied. However, traditional multicolor SMLM methodologies present low spatial resolution, pseudo-spectral resolution, and require complex optical systems. Here, we overcome these drawbacks by constructing an ultrahigh-throughput SMLM methodology that allows for fast and accurate multicolor imaging of complex environments at the nanoscopic level by a multichannel ratiometric analysis. This method overcomes traditional SMLM issues by separating signals used for spectral and localization analysis, permitting ultrahigh-throughput with high spatial and spectral resolution and true color analysis from a simple optical system. Our methodology can readily distinguish between close emitting fluorophores and achieves sub-10 nm localization precision with single molecule emission wavelengths at sub-5nm variance

O3-3 **Predicting F-SAPT Interaction Energies from MM/GBSA Analysis for the Chorismate Mutase Enzyme**

Nathan DeYonker, Jose Bachega, Khawlah Almurisi
Department of Chemistry, University of Memphis, Memphis, TN

Our group uses molecular modeling and quantum chemistry to quantitatively understand the interactions between amino acid residues and enzyme substrates. A unique and powerful enzyme catalyst, chorismate mutase is an established model for probing enzyme mechanisms and has been a frequent case study both in the community and in our group. We have been investigating Functional Group Symmetry Adapted Perturbation Theory (F-SAPT), a new technique that can accurately calculate amino acid-substrate interaction energies. However, F-SAPT is very time-consuming, requiring days of computational effort. MM/GBSA (molecular mechanics/Generalized Born Surface Area) is a versatile and extremely inexpensive method used to calculate protein-substrate free energies. Combined with molecular dynamics simulation, we compute protein-substrate interaction energies of the chorismate mutase enzyme at one-picosecond intervals with MM/GBSA. The long-term aim is to train a function that can predict F-SAPT interaction.

Oral Session 4

1:00 p.m. in Meeting Room B

O4-1 The Synthesis of Piperidines via the Intramolecular Prins Cyclization of N-Sulfonyl Alpha-Aminoacetals

Damien D. Cooper, Matthew G. Donahue

Department of Chemistry, University of Southern Mississippi

The saturated nitrogen heterocycle known as piperidine has five carbon atoms and one nitrogen atom. Piperidines are common heterocyclic cores of natural products and small molecules that have biological activity. The synthesis of piperidine presents many unique challenges in consideration of the configurational and conformational disposition of the substituents along the carbon backbone. Inspired by natural products such as (-)-lasubine I, which has been synthesized in the Donahue lab, this talk discusses current investigations toward the use of the Prins reaction to access 3,5-disubstituted piperidines. Starting from a commercially available alpha-aminoacetal, in three chemical steps, these structures have been prepared in high yield with excellent control of the 3,5-configuration. The sequence involves sulfonylation of the alpha-aminoacetal to create a secondary sulfonamide that is readily alkylated with allyl bromide under mild SN2 conditions. This cyclization precursor has been subjected to both Bronsted and Lewis acids that have resulted in the formation of cis-3,5-disubstituted piperidine core. We imagine the reaction proceeds through the formation of an oxonium ion that is trapped by the pendant alkene. This results in the formation of a secondary carbocation that is trapped by the conjugate base of the acid. We further hypothesize that due to the chair-like transition state, both the 3 and 5 substituents end up cis and ultimately in an equatorial disposition. Work toward post-cyclization functionalization will also be discussed as a demonstration of the value of these heterocycles.

O4-2 **Pyridine-based HIV Integrase Inhibitors: Side-Chain Development**

Tyler D. Twedt[1], Brenna R. Macaluso[1], A. Margaret Miller[1], Hannah J. N. Mattke[1], Christopher T. Bruni[1], Sharon E. Suffern[1], R. Victor Mishoe[1], Gavisha Mugon[1], Sarah J. Hayek[1], Jacques J. Kessl[2], Julie A. Pigza[2], Matthew G. Donahue[2], Wolfgang H. Kramer[1*]

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Retroviruses employ three unique enzymes, reverse transcriptase, integrase and protease, that are essential for their life cycle. Antiviral therapy targets those enzymes preferably, as less side effects are expected. Human immunodeficiency virus (HIV), which causes acquired immunodeficiency syndrome (AIDS), is generally combated with triple therapy, consisting of usually two reverse transcriptase inhibitors and one integrase or protease inhibitor. As the high mutation rate of the virus causes resistance, HIV drugs are constantly optimized. HIV integrase incorporates the viral DNA into the host cell genome. HIV Integrase inhibitors are mostly based on aromatic heterocycles such as pyridine and quinoline. This project aims to synthesize new inhibitors based on the pyridine core. The heterocycle is generated by reaction of substituted malonic esters with an aminocrotonate ester. The development of the side chain in the 3-position which consists of a methine carbon carrying a tert-butoxy group and a carboxylic acid, is essential. Several methods have been attempted and are discussed. Further incorporation of substituents on the pyridine core will determine the efficiency of the inhibitors.

Acknowledgement: This work was supported by the Mississippi INBRE, funded by an Institutional Development Award (IDeA) from the National Institute of General Medical Sciences of the National Institutes of Health under grant number P20GM103476.

O4-3 Synthetic Efforts Toward Halofuginone as a Therapeutic for Tick-Borne Diseases

Oussama Errida, Matthew G. Donahue
Department of Chemistry, University of Southern Mississippi

According to the US Centers for Disease Control and Prevention, ticks are responsible for the transmission of over 15 different diseases with symptoms ranging from mild to chronic. In Mississippi, the Gulf Coast tick (*Amblyomma maculatum*), is responsible for the transmission of *R. parkeri* to human through direct bites resulting in fever, headaches, rash, and muscle aches. It has been shown that the febrifugine, bioactive constituent of *Dichroa febrigua* Lour. of the Saxifragaceae family, has validated antimalarial activity. A halogenated analog of febrifugine, called halofuginone, is used globally as a feed-additive to prevent diseases in poultry farms. Recently, both febrifugine and halofuginone have been tested in the treatment of tickborne diseases, however it is prohibitively expensive to purchase either febrifugine ($35/millgram) or halofuginone ($51/milligram) from commercial suppliers to synthesize derivatives for testing. Assays for testing require hundreds of milligrams so the only viable method for obtaining them is through chemical synthesis from commercially available starting materials. In this talk, current efforts underway toward the total synthesis of halofuginone are discussed. The route follows an existing literature precedent from Organic Process Research and Development 2019, 23(5), 990 "A Scalable Total Synthesis of Halofuginone." In a survey of the literature, this route was determined to be the most robust with use of the least expensive chemicals. To date, the first three steps have been reproduced with the fourth currently under investigation. The goal of this work is to create novel derivative of halofuginone once synthetically useful quantities have been prepared.