



Mississippi
College

A CHRISTIAN UNIVERSITY

Proceedings of the
Fall 2022
Mississippi College STEM
Research Symposium

November 19, 2022
Math, Chemistry, Computer Science (MCC) Lobby
Mississippi College
Clinton, MS

SCHOOL OF SCIENCE AND MATHEMATICS
Departments of Biology, Chemistry & Biochemistry,
Engineering, Computer Science & Physics, Mathematics,
and Physician Assistant Studies

Proceedings of the
Fall 2022 Mississippi College STEM Research Symposium

Volume 3

Number 1

November 2022



Mississippi College Office of Research Director
David H. Magers, Ph.D.

Mississippi College School of Science and Mathematics Dean
Stan A. Baldwin, Ph.D.

Symposium Coordinators and Proceedings Editors
Angela Whittom Reiken, Ph.D.
Joseph Kazery, Ph.D.

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About the
Fall 2022 Mississippi College STEM Research Symposium

Student Poster Presentations

Undergraduate and graduate students from the Mississippi College School of Science and Mathematics are invited to submit an abstract and present a poster. Each student presenter should be a current student of the Department of Biology, Chemistry & Biochemistry, Engineering, Computer Science & Physics, Mathematics, or Physician Assistant Studies. New researchers with one semester of data and seasoned researchers with a complete project are all welcome to present.

Guest Poster Presentations

Faculty and alumni posters are welcome as guest presenters as space permits.

Symposium Sponsors & Acknowledgments

The Fall 2022 Mississippi College STEM Research Symposium is sponsored by the Mississippi College School of Science and Mathematics and the Mississippi College Office of Research.

Refreshments and gift cards for recipients of People's Choice Awards are provided by the Mississippi College Office of Research.

The MC Medical Dental Alumni Association provides two overall awards for best research projects judged by qualified faculty.

Members of the Mississippi College Chapter of Tri-Beta provide their assistance with voting and coordination of the event.

Easels for posters are provided by the Department of Chemistry.

Special thanks to event host Abdallah Zaitar and event photography provided by various students and faculty.

Symposium Schedule and Poster Guide

Fall 2022 Mississippi College STEM Research Symposium

Date November 19, 2022

Location College Math, Chemistry, Computer Science (MCC) Lobby

Poster Presentations and Refreshments 1:30 PM – 4:00 PM

People's Choice Voting 1:30 PM – 3:30 PM

People's Choice Awards 3:30 PM – 4:00 PM

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19	Whitney E. Schuler	Relative Stabilities of Amino, Nitro, and Methoxy Derivatives 6-methylpentacene and 6-methylene-6,13-dihydropentacene
20	Gabrielle D. Winters	Conventional Strain Energy and Hyperconjugation in Cyclopropylborane and Chloro Derivatives
21	Hanna K. Bynum	Stabilization Factors in Fluoro and Chloro Derivatives of Cyclopropyl Carbinyl Cation
22	David L. Zetterholm	Ab Initio Analysis of Polarizability in Molecular Piezoelectric Response for Organic Dimer Systems

Abstracts

Fall 2022 Mississippi College STEM Research Symposium

Poster #1

Analysis of Local Crayfish in Lotic Ecosystems

Ervin, J., Garteiser, J., Cockrell, C., Doubert, A., Hearst, S., Kazery, J.

Crayfish are common organisms in freshwater ecosystems & are of great ecological importance that can even impact public health. Crayfish are responsible for promoting nutrient cycling through decomposition, providing habitats to other organisms, & are prey to many organisms. Knowing the importance of crayfish to the environment as well as the public charges us with & understanding of what type of crayfish are found locally and baseline data for their health. This study provides baseline information of the local genera as well as the biometrics of crayfish found in flowing waters within Clinton, MS as well as to determine if there is variation in crayfish by local regions. Samples of crayfish were collected between May and October 2022 from lotic systems: streams, creeks, & springs. Specimens were keyed to genus, sexed, and biometric data (total length & mass) was collected and analyzed. The main genus of crayfish was *Procambarus* making up 93% of the samples & 7% *Lacunicambarus*. In total, the crayfish demonstrated a healthy distribution with a total mean length 6.5 cm. The mean length of crayfish varied significantly only between the industrial (7.2 cm) and suburban regions (6.0 cm). the mass of the crayfish, the suburban region (4.930 g) was demonstrated to be significantly lower than the other industrial (7.989 g), urban (8.714 g), & rural (6.615 g) regions. This data provides a baseline data for future studies or management. This study can be furthered by monitoring existing populations or comparing other specimens from the surrounding areas.

Presenting Author: Javian Ervin

Department: Biological Sciences

Research Mentor: Joseph Kazery, Ph.D.

Research Sponsor: This research was supported by the Department of Biological Sciences & in part from a grant from the Mississippi College Office of Research Department of Student Research at Mississippi College.

Poster #2

Crayfish as Sentinel Species to Monitor Trace Elements in Freshwater Ecosystems

Cockrell, C., Garteiser, J., Doubert, A., Ervin, J., Hearst, S., Kazery, J.

Crayfish are common in freshwater ecosystems being the largest invertebrate making up the largest amount of invertebrate biomass & are of great ecological importance that can even impact public health. Crayfish can be used as a sentinel species to monitor the health of environments. This provides information of substances that are in or have been passing through freshwater ecosystems and has accumulated in crayfish. Crayfish were sampled from 13 locations within Clinton, MS & each location was categorized into regions: industrial, rural, suburban, & urban. Abdominal muscles & exoskeletons were digested using HNO₃, HCl, & H₂O₂ as described in EPA Method 200.7, then analyzed by ICP-OES to determine the concentration of selected trace elements. The uptake of Al, Cu, Hg, Mn, Sr, & Zn was observed in crayfish and varied significantly in concentrations and by location. Our results indicated that most trace elements (Al, Cu, Mn, Sr) were concentrated in the exoskeleton, whereas Zn was concentrated in the abdominal muscle. Based on regions, results indicated there were significantly higher concentrations of Al, Cu, Mn, & Sr in the suburban & rural regions than industrial or urban. There was significantly more Zn in the industrial region, & significantly more Hg in the urban region. Crayfish are an integral part of freshwater habitats; therefore, potential ecological or public implications may occur due to toxic levels of trace elements. This may cause a decline in population or affect the public being a food source or being passed through the food chain to desirable fish.

Presenting Author: Carlee Cockrell & Jacob Garteiser

Department: Biological Sciences

Research Mentor: Joseph Kazery, Ph.D.

Research Sponsor: This research was supported by the Department of Biological Sciences & in part from a grant from the Mississippi College Office of Research Department of Student Research at Mississippi

Poster #3

Testing for Quicker Outcomes: HIV ELISA Rapid Testing Method

Bryant, J., Moore, C., Nguyen, C., Pierre, R., and Whitton Reiken, A

Human Immunodeficiency Virus is an RNA retrovirus that infects T helper cells of the immune system. HIV interrupts a normal part of a gene by putting self there instead of the natural gene. It may interrupt a less important gene at first causing less noticeable symptoms yet may eventually interrupt a serious gene and cause great physical defects and a weakened immune system. This RNA retrovirus was first documented and described in 1981 leading to the HIV/AIDS epidemic.

While initially considered a death sentence, advancement in research has produced a multitude of effective treatments reclassifying the condition as a chronic treatable infection. Accurate and early diagnosis is paramount due to the latent nature of the virus. Enzyme-linked Immunosorbent Assay (ELISA) utilizes antibody binding specificity to test for the presence of HIV specific antigens in patient samples. The assay protocol consists of a multi well microplate with capture antibodies bound to the bottom of each well. These antibodies specifically bind to HIV antigens and hold them in place. A detection antibody is then added to the microplates where it will also bind to the antigen. Conjugate, enzyme-linked detection antibodies, are then added where they will bind to the detection antibodies. In the presence of chromagen, the reagent which reacts with the enzyme, a reaction occurs which produces a color change indicating a positive or negative result. This specific assay produces a red color if the test is positive and a yellow one if it is negative. This project demonstrates the effectiveness of ELISA in detecting HIV antigens, which is the first step in diagnosing the infection.

Presenting Author: Joi Bryant

Department: Biological Sciences

Research Mentor: Angela Whittom Reiken, Ph.D.

Research Sponsor: This research was supported by the Department of Biological Sciences & in part from a grant from the Mississippi College Office of Research Department of Student Research at Mississippi

Poster #4

Alpha- and Gamma-linolenic Acid's Effect in Preventing Oxidative Stress in Chinese Hamster Ovary Cells

Wan, J, Lane, JA, Price, JC, Redhead, JT, Wheeler, DJ, and Whittom Reiken, AA

Common uses of Alpha and Gamma-Linolenic acid in medicine today include heart and blood disease such as hardening of the arteries and high blood pressure. Both fatty acids target cyclooxygenases-1 which trigger inflammatory response by oxygenates arachidonate (AA, C20:4(n-6)) to the hydroperoxy endoperoxide prostaglandin G2 (PGG2), with Alpha-Linolenic acid showing a higher probability than Gamma-Linolenic acid. Knowing these functions, our in vitro model is designed to address the ability of Alpha and Gamma-Linolenic acid in preventing cytotoxicity induced by oxidative stress. The model incorporates a Chinese Hamster Ovary cell line to mimic the mammalian cells. These were plated on to a twenty-four well plate for a 24-hour treatment with hydrogen peroxide, Alpha and Gamma-Linolenic acids as separate treatments. The potential changes in cell proliferation and cytotoxicity effect caused by hydrogen peroxide with Alpha and Gamma-Linolenic acids were measured through MTT and LDH assay. The first finding was that Gamma-Linolenic acid seems to induce higher cellular cytotoxicity and lower cellular proliferation in CHO cells, while Alpha-Linolenic acid downregulates both cellular proliferation and cytotoxicity. The second finding was both Alpha and Gamma-Linolenic

acid are shown to effective in preventing oxidative stress damage induced by hydrogen peroxide, with Alpha doing a better job than Gamma. The mechanism of the prevention remain unclear, but could be related to the fatty acids effect in reducing inflammation associated with the synthesis of prostaglandin E2. Future study could be done on its effect in a 48 hour treatment and also treating the cells with reactive oxygen species to measure the values of the oxidative stress induced in the cells.

Presenting Author: Jingxuan Wan

Department: Biological Sciences

Research Mentor: Angela Whittom Reiken, Ph.D.

Research Sponsor: This research was supported by the Department of Biological Sciences & in part from a grant from the Mississippi College Office of Research Department of Student Research at Mississippi

Poster #5

Evaluating the Individual Effects of Caffeine, Aspirin, and Acetaminophen on Chinese Hamster Ovary Cells to Evaluate Clinical Significance

Redhead, JT, Wheeler, DJ, Wan, J, Price, J C, Lane, JA, Ely, MG, Webb, KA, and Whittom Reiken, AA

Caffeine, aspirin, and acetaminophen are common drugs that are taken separately as well as in combinations, such as Excedrin or Goody's Powder, across the human population daily. To test the individual effects of each component on a cellular level, we used concentrations of each treatment from prior research in cell media to form a solution to treat Chinese Hamster Ovary cells. After treatments with media containing one of the three drugs or control media were executed, the cells were exposed for 24-hour incubation intervals under these conditions within a Thermo Scientific incubator. After incubation periods had concluded, cells were then analyzed for viability as a result of treatments using a MTT assay. Furthermore, the cytotoxicity as a result of the three drugs relative to the control was evaluated utilizing a LDH assay, revealing the rate of necrosis. Following these findings, we then stained cells with hematoxylin to investigate the transformation and morphology of cells treated with each of these substances relative to cells untreated. Next, we determined potential protein targets of the various treatments through bioinformatics to aid in the explanation of the results we received as well as the potential clinical consequences due to the use of these drugs. Our results revealed that treatment with these drugs causes potential damage to cells, which reduces their viability and, in some cases, does so by necrosis. Using bioinformatics, we determined potential protein targets of these drugs along with their pathways to aid in explanation of our findings.

Presenting Author: Dalton Wheeler & Tal Redhead

Department: Biological Sciences

Research Mentor: Angela Whittom Reiken, Ph.D.

Research Sponsor: This research was supported by the Department of Biological Sciences & in part from a grant from the Mississippi College Office of Research Department of Student Research at Mississippi

Poster #6

Analysis of the Effects of Letrozole on Chinese Hamster Ovary Cells

Lane, JA, Price, JC, Redhead, JT, Wheeler, DJ, Wan, J, and Whittom Reiken, AA

Letrozole, sold under the brand name Femara, is a drug that is FDA approved to treat metastatic breast cancer that is hormone receptor (HR) positive or has an unknown receptor status in post-menopausal women. To test the effects of different concentrations of Letrozole on a cellular model, we used concentrations of each treatment from prior research in cell media that was then used to treat Chinese Hamster Ovary (CHO) cells. Following treatment with media containing one of the two concentrations or control media, the cells were exposed for 24-hour incubation intervals in a Thermo-Scientific incubator. After the incubation periods were complete, cell viability was determined via the MTT cellular viability assay. Additionally, the cause of death of the CHO cells as a result of the two concentrations relative to the control was determined using the LDH assay, which provides the rate of cell necrosis. The cells were then stained with hematoxylin and eosin (H&E) in order to visualize morphology changes that the drug treatments induced. Finally, we determined potential protein targets of Letrozole through bioinformatics to elucidate some of the results we received and reveal potential clinical consequences due to the use of Letrozole. Our results showed that treatment with Letrozole causes potential damage to cells, reducing their viability and potentially leading to necrosis. Using bioinformatics, we determined potential protein targets of these drugs along with their pathways to aid in explanation of our findings.

Presenting Author: Austin Lane & Joseph Price

Department: Biological Sciences

Research Mentor: Angela Whittom Reiken, Ph.D.

Research Sponsor: This research was supported by the Department of Biological Sciences & in part from a grant from the Mississippi College Office of Research Department of Student Research at Mississippi

Poster #7

Effect of Dietary Cholesterol on Growth and Linear Mobility of *Drosophila melanogaster* Larvae

Tullos, EL, Robbins, CE, Dickerson, AL, Graddy, SR, Barkley, EK, Cook, AN, Frisbie, AE, Sullivan CS and Reagan, JW

Unlike vertebrate animals, which are able to synthesize cholesterol, insects are cholesterol auxotrophs. Consequently, an exogenous source of sterol is required for successful progression through the larval stage of development. To determine whether dietary cholesterol is also required for larval mobility (linear movement), synchronously collected eggs from wild-type (Oregon R strain) *D. melanogaster* were placed on one of two diets: a cholesterol-enriched (CR) diet containing 0.05% cholesterol or a cholesterol-free diet (CF). After hatching, the larvae fed on their respective diets for 6 days. A third group (CF-CR) fed on the cholesterol-free (CF) diet for 6 days before transfer to the cholesterol-enriched diet (CR). At the end of the 6th or 12th day (CF-CR) the larvae were placed in the center of a 100 mm petri dish containing the CR diet to a depth of ~0.3 cm. To document movement, photos of the larvae were captured every 15 seconds for an hour. Larval mass and length were quantified in identically treated larvae to document the effect of cholesterol starvation on growth and development. These data demonstrate that cholesterol starvation-induced decrease in growth and development of *D. melanogaster* larvae is accompanied by a reversible decline in linear mobility. Whether these two outcomes are linked by a common molecular pathway or mechanism is the subject of ongoing and future experiments.

Presenting Author: Ethan L. Tullos & Callie E. Robbins

Department: Biological Sciences

Research Mentor: Jerry W. Reagan, Ph.D.

Research Sponsor: This research was supported by the Department of Biological Sciences & in part from a grant from the Mississippi College Office of Research Department of Student Research at Mississippi

Poster #8

Ab Initio Analysis of Polarizability in Molecular Piezoelectric Response for Organic Dimer Systems

Pathology and Early Detection of Parasitic *Bolbophorus* Trematodes in Commercial Catfish Ponds

Charles Moore, Haleigh Hassinger, Emily Rodrigue, Matthew Sinclair, Lillian Sisson, Ridge Futral, Bethanie Prine, Breana Chastang, Daisia Rixter, Jingxuan Wan, Tyler Welch, and Scoty Hearst

Digenetic trematodes are a major problem for the commercial catfish industry. Trematodes from the genus *Bolbophorus* cause significant economic loss to the Mississippi commercial catfish industry each year. These parasites use the gut of the American white pelican (*Pelecanus erythrorhynchos*) and the gut of the ram's horn snail (*Planorbella trivolvis*) as intermediate hosts,

where these hosts can be infected with *B. damnificus* and *Bolbophorus* type II trematodes simultaneously. *Bolbophorus* infections causes visible skin lesions and mortality in commercial catfish, where infected catfish refuse to eat and eventual waste away. Since, *Bolbophorus* infect the gut of their hosts, we hypothesized that *Bolbophorus* may also infect the gut of commercial catfish resulting in mortality. In this study, we collected Mississippi commercial catfish and snails from Control ponds, where there were no visible signs of *Bolbophorus* infections and from ponds where there were visible signs of infection. We tested catfish skin and gut samples as well as snail gut samples for *B. damnificus* and *Bolbophorus* type II trematodes using the widely used 18S PCR diagnostic assay. We found *B. damnificus* and *Bolbophorus* type II positivity in catfish skin and gut samples from both the Control ponds and Infected ponds. We also found *B. damnificus* and *Bolbophorus* type II positivity in snail samples from Control ponds and Infected ponds. Our data suggests that the Control ponds were in the early stage of infection, though there were no visible lesions, infections were detected in catfish and snail samples. Furthermore, the fact that *Bolbophorus* infections were detected in the gut of catfish with no sign of infection and with visible infections suggest that *Bolbophorus* infections of the gut could be a major cause of the digestive issues linked to mortality in this disease pathology.

Presenting Author: Charles Moore

Department: Chemistry & Biochemistry

Research Mentor: Scoty Hearst, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #9

Environmental Analysis of Trace Elements in Fish Species Inhabiting a former Mississippi Gravel Quarry

Jose Alfonso Xavier, Takaye Farmer, Lillian Sisson, Caleb Dean, Joseph Kazery, Trent Selby, and Scoty Hearst

Gravel quarries are open mines where the natural vegetation, topsoil, and subsoil layers are removed creating pits or quarries for the extraction of gravel. These gravel pits naturally fill with water to form ponds or lakes. Potential environmental concerns for gravel mining include habitat fragmentation, dust, runoff pollution, and water contamination. There are no reports of the lack or presence of these toxic elements in gravel pits or their aquatic wildlife. In this study, we are the first to survey fish species, sediments, and water for trace elements from a former gravel pit lake located in Yazoo County, Mississippi. We collected White Perch (*Morone americana*), Largemouth Bass (*Micropterus salmoides*), and Bluegill (*Lepomis macrochirus*) from a gravel pit and analyzed samples of muscle, liver, and skin tissue for trace elements using an ICP-OES. Here, we compare trace elements and toxic metals in the various species of fish inhabiting a former Mississippi gravel pits and compare these levels with the maximum permissible levels established

by World Health Organization, USDA, and Food and Agriculture Organization of the United Nations.

Presenting Author: Jose Alfonso Xavier

Department: Chemistry & Biochemistry

Research Mentor: Scoty Hearst, Ph. D

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #10

A New Surveillance Strategy Using Kidney Tissue Reveals SARS-CoV-2 Positivity Trends in Mississippi White-tailed Deer

William Yarbrough, Scoty Hearst, Ryan Ivey, Caleb Young, Edward Facundus, Kaitlin A. McNeely, George T. Bates, Pedro Palermo, Doug Watts, John T. Bates

Early detection and monitoring of SARS-CoV-2 infections in animal populations living within close proximity to humans is crucial to preventing reverse zoonosis of new viral strains. *Odocoileus virginianus* (White-tailed deer, WTD) are one few animal species susceptible to zoonotic SARS-CoV-2 spill-over. SARS-CoV-2 infections into WTD populations have been reported in states such as Michigan, Pennsylvania, Illinois, Iowa, New York, Ohio, and Texas. The major challenges for SARS-CoV-2 surveillance are sample collecting expertise and manpower. In this study, we developed a new SARS-CoV-2 surveillance strategy using WTD kidney tissue collected from hunter harvested deer to lessen these challenges. Using this method, we report the first exposure of SARS-CoV-2 in WTD from the southeastern region of the United States in the great state of Mississippi. During the 2021-2022 Mississippi deer hunting season, we tested for SARS-CoV-2 positivity in nasal swabs, blood serum, and kidney tissues collected from hunter harvested deer throughout the state. PCR analysis revealed a 25% positivity rate (n=12). Serologic analysis indicated 67% positivity (n=15) and tissue analysis revealed a 26% positivity rate in WTD (n=62). However, assessing WTD positivity rates over time revealed increasing positivity trends mirroring SARS-CoV-2 rates in Mississippians. Comparison of WTD and human positivity trends in Mississippi showed a strong correlation of 83.9%. Overall, this study demonstrates the efficacy of this new SARS-CoV-2 tissue surveillance strategy, which can help to limit the burdens of future surveillance studies and monitoring programs.

Presenting Author: William Yarbrough

Department: Chemistry & Biochemistry

Research Mentor: Scoty Hearst, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #11

Analysis of Trace Elements of Metal Artifacts from an American Civil War Campsite Located in Bentonia, Mississippi

Mohammad Ibrahim, Landon Ashley, Analee Mobley, Jeremy Evans, Claire Stokes, and Scoty Hearst

The American Civil War, from 1861 to 1865, was a civil war in the United States between the United States "the North" and the Confederate States of America "the South". The Confederate States of America includes the states of: South Carolina, Mississippi, Florida, Alabama, Georgia, Louisiana, Texas, Virginia, Arkansas, Tennessee, North Carolina, Kentucky and Missouri. In this study, we examine metal artifacts found in a suspected Civil War camp site located in Bentonia, Mississippi. Local legends in the area tell of this particular location as an old Civil War camp site that was once occupied by Confederate soldiers. The site is located 5 miles away from the Battle of Benton Road, where 700 to 800 Confederate soldiers lost their lives in defense of Yazoo City. Using metal detectors, we uncovered multiple potential Civil War artifacts including tent nails, a fire starter, a pickaxe, a war axe, and a knife handle. We also found slag and evidence of smelting. Using an ICP-OES, we analyzed the elemental composition of each artifact and compared them to modern metals and certified reference materials. We found unique metal impurities in the potential Civil War artifacts not found in the modern metal samples. To further validate these as Civil War artifacts, we conducted elemental analysis of Civil War artifacts with certified providence as a comparison. We obtained Confederate canister shot from The Battle of Appomattox Court House, Appomattox, VA, and an axe head from the Confederate camp in Smyrna, GA as our certified reference samples. The certified Civil War reference material was a good match to the artifacts uncovered at the study site and suggest these artifacts are genuine and date back to the Civil War period. This data also validates the Bentonia campsite as a real Civil War camp.

Presenting Author: Mohammad Ibrahim

Department: Chemistry & Biochemistry

Research Mentor: Scoty Hearst, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #12

Analysis of Trace Elements in Ceramic Pottery Samples Collected from the Holy Land

Takaye Farmer, Jose Alfonso Xavier, Barbara Parks, Dean Parks, and Scoty Hearst

Pottery, made out of clay and other ceramic materials hardened by heat, is one of man's oldest inventions. The earliest pottery dates back before the Neolithic period in 29,000 BC. Ceramic pottery served as mainly cooking and storage vessels as well as functional art. Pottery is divided into three major types: earthenware, stoneware and porcelain. Each requires its own specific clay material and varying firing temperatures. The studying of pottery provides archaeological insight into cultures of the past. Understanding the unique characteristics of pottery collected from a particular location reveals a great deal the area's culture such as: technology, sophistication, and trade. In this study, we use ICP-OES to determine the chemical composition of pottery collected from various time periods and locations across the Holy Land. Pottery samples were collected throughout Israel at En Gedi, Hazor, Herodium, Masada, Timnah, Jerusalem, and Jericho. Samples were also collected from the Crusader's Banias Fort and Corinth, Greece. Here, we present our results and chemical findings. We speculate that identifying the chemical composition of these archaeological samples will allow us to determine locations with similar or distinct pottery characteristics and provide evidence of shared culture or cultural exchange such as trade. This can provide better insight into the daily life, religion, and social relationships between these vast location and cultures across the Holy Land.

Presenting Author: Takaye Farmer

Department: Chemistry & Biochemistry

Research Mentor: Scoty Hearst, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #13

Preparation of Conjugated Polyphenylethynylarene Macrocycles

McRae, E, Steen, B, and Selby, TD

The preparation of π -conjugated macrocyclic organic molecules is a focus of our group. The syntheses of several macrocycles, with varying degrees of conjugation will be presented and can all be prepared from the same key intermediate structure, (3-ethynylphenoxy)(tert-butyl)dimethylsilane. This key intermediate was prepared from the commercially available 3-hydroxybenzaldehyde. Protection of the hydroxyl with tert-butyldimethylsilyl chloride in the presence of a weak base (imidazole), under microwave conditions gave the protected compound in 94% yield. The aldehyde functional group was converted into the terminal alkyne via Corey-Fuchs olefination reaction conditions in 87% yield. Sonogashira coupling (palladium/copper(I) iodide catalyst) of the terminal alkyne with aryl halides gave polyphenylethynylarenes in high yields. Cyclization of the polyphenylethynylarenes alcohols can be accomplished under dilute conditions via nucleophilic substitution or acylation addition/elimination reactions. Structures of

this type are expected to show directed energy and electron transfer and thus should be effective in the preparation of photoreactive materials such as electronic sensors or light harvesting materials.

Presenting Authors: Elizabeth McRae

Department: Chemistry & Biochemistry

Research Mentor: Trent D. Selby, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #14

Synthesis of Macrocyclic Diaminopolyphenylethynylarenes and Diaminopyridinylethynylarenes

Schwartz, SJ; Stewart, M, and Selby, TD

Molecules containing high degrees of π -conjugation are ideal materials for advanced electronic and photonic applications. Conjugation should be promoted by constructing flat 2-dimensional architectures. We report here, the synthesis of highly-conjugated 2-dimensional diaminopolyphenylethynylarenes and diaminopyridinylethynylarenes. The synthesis of diaminopolyphenylethynylarenes begins with Sonogashira coupling of 1-ethynyl-3-aminobenzene with 1,2-diiodobenzene in good yield. The synthesis of diaminopyridinylethynylarenes is accomplished by coupling of 6-bromo-2-pyridinamine with 1,2-diethynylbenzene under Sonogashira conditions. Cyclization was accomplished by reacting the amino groups with glyoxal or oxalyl chloride. Additionally, these nitrogen containing molecules can easily be oxidized to radical cations giving rise to some unique electronic properties.

Presenting Author: Samantha J. Schwartz

Department: Chemistry & Biochemistry

Research Mentor: Trent D. Selby, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #15

Relative Stabilities of Amino, Nitro, and Trifluoromethyl Derivatives of 9-methylantracene and 9-methylene-9,10-dihydroanthracene

Stokes, CE; Sullivan, EP; Magers, DH

In 1949, Clar and Wright reported that 6-methypentacene exists as 6-methylene-6,13-dihydropentacene at room temperature due to a [1,5]-sigmatropic hydrogen shift (Nature 1949, 163, 921). Thus, the aromaticity of the central ring and the planarity of the overall compound is destroyed by this shift. The same does not occur in anthracene. While the 9-methylene derivative of anthracene is a local minimum, the planar 9-methyl derivative is the more stable. In the current study we investigate if certain derivatives of these anthracene systems stabilize the methylene system relative to the methyl. Specifically, amino, nitro, and trifluoromethyl derivatives of anthracene are considered. Optimum equilibrium geometries, harmonic vibrational frequencies, and the corresponding zero-point vibrational energies are computed for each set of isomers using density functional theory. The DFT functionals employed are Becke's three-parameter hybrid functional with the Lee-Yang-Parr correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ω B97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are Dunning and coworkers' correlation consistent basis sets cc-pVDZ and cc-pVTZ. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Presenting Author: Claire E. Stokes

Department: Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #16

Calculation of Conventional Strain Energies of Small Heterocycles of Carbon and Silicon by Model Reactions

Franklin, EM; Magers, DH

The conventional strain energies for three- and four-membered heterocycles of carbon and silicon are computed within the isodesmic, homodesmotic, and hyperhomodesmotic models. Isodesmic reactions conserve number and types of bonds. Homodesmotic reactions are isodesmic reactions which also conserve the valence environment around each atom. Hyperhomodesmotic reactions are homodesmotic reactions which conserve the valence environment around each set of two bonded atoms. Computed results for cyclopropane and cyclobutane are compared with experimental values for these systems to demonstrate the reliability of the method. Optimum equilibrium geometries, harmonic vibrational frequencies, and corresponding electronic energies

are computed for all pertinent molecular systems using SCF theory, second-order perturbation theory (MP2), and density functional theory. The DFT functionals employed are Becke's three-parameter hybrid functional with the Lee-Yang-Parr correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ω B97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are Dunning and coworkers' correlation consistent basis sets, cc-pVDZ, cc-pVTZ, and cc-pVQZ. Results indicate that silicon substitution reduces the conventional strain energy of cyclobutane most likely due to a reduction of Baeyer strain (bond angle strain), but increases the conventional strain energy in cyclopropane by destroying the stabilizing factor of sigma delocalization. Natural Bond Order analysis is employed to help explain the results. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Presenting Authors: Eli M. Franklin

Department: Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #17

Conventional Strain Energies of Thiaziridine and the Thiazetidines

Gramm, JD; Magers, DH

The conventional strain energies for thiaziridine, 1,2-thiazetidine, and 1,3-thiazetidine are determined within the isodesmic, homodesmotic, and hyperhomodesmotic models to investigate the effect of third-row elements on the strain energies of three- and four-membered rings. Optimum equilibrium geometries, harmonic vibrational frequencies, and corresponding electronic energies are computed for all pertinent molecular systems using self-consistent field (SCF) theory, second-order perturbation theory (MP2), and density functional theory (DFT). The DFT functionals employed are Becke's three-parameter hybrid functional using the LYP correlation functional and the M06-2X high nonlocality hybrid functional from Thular and Zhao. The basis sets employed are Dunning and coworkers' correlation consistent basis sets: cc-pVDZ, cc-pVTZ, and cc-pVQZ. In addition, cc-pV(D+d)Z, cc-pV(T+d)Z, and cc-pV(Q+d)Z basis sets are also investigated to determine the effect of the extra d function for sulfur on the overall results. Results are compared to the conventional strain energies of small cyclic hydrocarbons and to other heterocyclic systems. Natural Bond Order analysis is employed to help explain the results. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Presenting Authors: Joshua D. Gramm

Department: Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #18

Enthalpies of Formation of Quinoline Derivatives by Homodesmotic Reactions

Borbash, RG; McCormick, CE; Magers, DH

Derivatives of quinoline and quinolone, specifically 5-nitro-8-hydroxyquinoline and 5-chloro-8-hydroxyquinoline, are useful as ligands in coordination compounds with Zn(II), Al(III), Cu(II), and Ru(II) and can be used as antimicrobial or antineoplastic (anticancer) agents. In the current study, we focus on the computation of the standard enthalpy of formation of these quinoline derivatives by homodesmotic reactions. In homodesmotic reactions the number and types of bonds and the bonding environment of each atom are conserved. The enthalpy of all of the reactants and products in each homodesmotic equation is computed using SCF theory and density functional theory (DFT). The DFT functionals employed are Becke's three-parameter hybrid functional with the Lee-Yang-Parr correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ω B97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are Dunning and coworkers' correlation consistent basis sets, cc-pVDZ, cc-pVTZ, and cc-pVQZ. From the resulting enthalpy of reaction, the desired enthalpy of formation is determined by use of reference values for all other systems in the reaction, and the computation of atomization energies is avoided. The results are so consistent that computed enthalpies of smaller compounds can be used as reference values for the computation of the enthalpies of larger compounds. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Presenting Author: Ryleigh G. Borbash

MC Department: Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #19

Relative Stabilities of Amino, Nitro, and Methoxy Derivatives 6-methylpentacene and 6-methylene-6,13-dihydropentacene

Schuler, WE; Plunkett, AW; Magers, DH

In 1949, Clar and Wright reported that 6-methylpentacene exists as 6-methylene-6,13-dihydropentacene at room temperature due to a [1,5]-sigmatropic hydrogen shift (Nature 1949, 163, 921). Thus, the aromaticity of the central ring and the planarity of the overall compound is destroyed by this shift. In the current study we investigate if certain derivatives of these pentacene systems stabilize the methyl derivative relative to the methylene. Specifically, nitro, amino, and methoxy derivatives of pentacene are examined. Optimum equilibrium geometries, harmonic vibrational frequencies, and the corresponding zero-point vibrational energies are computed for each set of isomers using density functional theory. The DFT functionals employed are Becke's three-parameter hybrid functional with the Lee-Yang-Parr correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ω B97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are Dunning and coworkers' correlation consistent basis sets cc-pVDZ and cc-pVTZ. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Presenting Author: Whitney E. Schuler

MC Department: Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsors: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #20

Conventional Strain Energy and Hyperconjugation in Cyclopropylborane and Chloro Derivatives

Winters, GD; Wiget, PA; Magers, DH

Many studies of strain energies have considered those of cyclopropane and cyclobutane. Not only are these systems the prototypical small, cyclic hydrocarbons, but they generate additional interest because their conventional strain energies are usually reported to lie within one to two kcal/mol of each other despite cyclopropane obviously having more Baeyer strain (bond angle strain). This similarity is usually explained by the stabilizing sigma delocalization in cyclopropane. However, another study in our group has shown that cyclopropylborane is even less strained than cyclopropane. This added stability may be due, at least in part, to hyperconjugation of the C-C

bonds in the ring with the empty p orbital on the borane. In the current study, we investigate this stabilization by calculating the conventional strain energies of chloro derivatives of cyclopropylborane. Specifically, the conventional strain energies of cyclopropyl-chloroborane and cyclopropyl-dichloroborane are computed within the isodesmic, homodesmotic, and hyperhomodesmotic models. Optimum equilibrium geometries, harmonic vibrational frequencies, and corresponding electronic energies are computed for all pertinent molecular systems using SCF theory, second-order perturbation theory, and density functional theory (DFT). The DFT functionals employed are Becke's three-parameter hybrid functional with the Lee-Yang-Parr correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ω B97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are Dunning and coworkers' correlation consistent basis sets cc-pVDZ, cc-pVTZ, and cc-pVQZ. Natural Bond Order analysis is employed to judge the degree of hyperconjugation in each system. We gratefully acknowledge support from the MC Catalysts.

Presenting Author: Gabrielle D. Winters

MC Department: Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #21

Stabilization Factors in Fluoro and Chloro Derivatives of Cyclopropyl Carbinyl Cation

Bynum, HK; Wiget, PA; Magers, DH

While cyclopropyl carbinyl cation ($C_4H_7^+$) is a local minimum on the potential energy hypersurface, the global minimum is the cyclobutonium cation (lower in energy by approximately 2 kcal/mol). The same is certainly not true if the hydrogens of the CH_2 moiety are replaced with fluorines. In the current study we investigate the factors which stabilize the cyclopropyl configuration in fluoro, chloro, and methyl derivatives of cyclopropyl carbinyl cation. Specifically, optimum equilibrium geometries, harmonic vibrational frequencies, and corresponding electronic energies are computed for $C_3H_5CFH^+$, $C_3H_5CF_2^+$, $C_3H_5CClH^+$, $C_3H_5CCl_2^+$, $C_3H_5CHCH_3^+$, and $C_3H_5C(CH_3)_2^+$ with SCF theory, second-order perturbation theory, and density functional theory (DFT). The DFT functionals employed are Becke's three-parameter hybrid functional with the Lee-Yang-Parr correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ω B97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are Dunning and coworkers' correlation consistent basis sets cc-pVDZ, cc-pVTZ, and cc-pVQZ. Natural Bond Order analysis is employed to help explain the factors contributing to the stabilization of each system. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Presenting Author: Hanna K. Bynum

MC Department: Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsors: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Poster #22

Ab Initio Analysis of Polarizability in Molecular Piezoelectric Response for Organic Dimer Systems

Zetterholm, DL; Magers, DH

In seeking to describe macroscale piezoelectric response, having a better understanding of piezoelectric response at the single-molecule level is a necessity. In the case of organic molecules, there are millions of possible candidates which possibly have the desired properties, revealed in the magnitude of the d_{33} coefficient. In seeking to extend research done by Daniel Lambrecht and co-workers which discovered a possible relationship between first-order polarizability of a molecule and its piezoelectric response (d_{33}), the current study seeks first to confirm this relationship with different levels of computational theory and to extend the previous work to application, where new molecules with even higher responses can be designed from principles discovered in the calculations. These results specifically take the calculations from Arun Gagrai and coworkers' previous results and model them in the Hartree Fock and MP2 levels of theory to see if the relationship is maintained, and then consider the extension of period 16 of the Periodic Chart to see if the relationship is maintained for heavier atoms, for which relativistic effects would need to be considered for in their computation, using tailored basis sets and effective core potentials. We gratefully acknowledge support from the Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry.

Presenting Author: David L. Zetterholm

Department: Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

People's Choice Awards – Physical Sciences

Fall 2022 Mississippi College STEM Research Symposium

During the symposium, attendees voted for their favorite poster presentations for the “People’s Choice Awards” sponsored by the Mississippi College Office of Research. 1st, 2nd, and 3rd place presenters were awarded \$50, \$30, and \$20, respectively with an award certificate. Congratulations scholars!

Elizabeth McRae

1st Place Physical Sciences

Preparation of Conjugated Polyphenylethynylarene Macrocycles

MC Department: Department of Chemistry & Biochemistry

Research Mentor: Trent D. Selby, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Claire E. Stokes

2nd Place Physical Sciences

Relative Stabilities of Amino, Nitro, and Trifluoromethyl Derivatives of 9-methylantracene and 9-methylene-9,10-dihydroanthracene

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry and Mississippi College School of Science & Mathematics Office of Research

Eli M. Franklin

3rd Place Physical Sciences

Calculation of Conventional Strain Energies of Small Heterocycles of Carbon and Silicon by Model Reactions

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Whitney E. Schuler

4th Place Physical Sciences

Relative Stabilities of Amino, Nitro, and Methoxy Derivatives 6-methylpentacene and 6-methylene-6,13-dihydropentacene

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

People's Choice Awards – Biological Sciences **Fall 2022 Mississippi College STEM Research Symposium**

During the symposium, attendees voted for their favorite poster presentations for the “People’s Choice Awards” sponsored by the Mississippi College Office of Research. 1st, 2nd, and 3rd place presenters were awarded \$50, \$30, and \$20, respectively with an award certificate. Congratulations scholars!

Ethan L. Tullos & Callie E. Robbins

1st Place Biological Sciences

*Effect of Dietary Cholesterol on Growth and Linear Mobility of Drosophila
Melanogaster Larvae*

MC Department: Department of Biological Sciences

Research Mentor: Jerry W. Reagan, Ph.D.

Research Sponsor: Mississippi College Department of Biological Sciences

Carlee Cockrell & Jacob Garteiser

2nd Place Biological Sciences

*Crayfish as Sentinel Species to Monitor Trace Elements in Freshwater
Ecosystems*

MC Department: Department of Biological Sciences

Research Mentor: Jerry W. Reagan, Ph.D.

Research Sponsor: Mississippi College Department of Biological Sciences

Charles Moore

3rd Place Biological Sciences

Pathology and Early Detection of Parasitic Bolbophorus Trematodes in Commercial Catfish Ponds

MC Department: Department of Biological Sciences

Research Mentor: Scoty Hearst, Ph.D.

Research Sponsor: Mississippi College Department of Biological Sciences

Jose Alfonso Xavier

4th Place Biological Sciences

Environmental Analysis of Trace Elements in Fish Species Inhabiting a Former Mississippi Gravel Quarry

MC Department: Department of Biological Sciences

Research Mentor: Scoty Hearst, Ph.D.

Research Sponsor: Mississippi College Department of Biological Sciences

MDAA Research Awards
Fall 2022 Mississippi College STEM Research Symposium

The Medical Dental Alumni Association (MDAA) sponsored two overall research project awards and the research teams associated with each project was presented with \$250 and a plaque during the MDAA meeting in 2022.
Congratulations scholars!

Tullos, EL, Robbins, CE, Dickerson, AL, Graddy, SR, Barkley, EK, Cook, AN, Frisbie, AE, Sullivan CS, and Reagan, JW

Presented by Ethan L. Tullos and Callie E. Robbins

Effect of Dietary Cholesterol on Growth and Linear Mobility of Drosophila Melanogaster Larvae

MC Department: Department of Biological Sciences

Research Mentor: Jerry W. Reagan, Ph.D.

McRae, E, Steen, B, and Selby, TD

Presented by Elizabeth McRae

Preparation of Conjugated Polyphenylethynylarene Macrocycles

MC Department: Department of Chemistry & Biochemistry

Research Mentor: Trent Selby, Ph.D.

Research Sponsor: Mississippi College Catalysts, the alumni support group of the Department of Chemistry & Biochemistry

Event Photos

Fall 2022 Mississippi College STEM Research Symposium



















