Mississippi College

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Proceedings of the First Annual

Mississippi College STEM Research Symposium

November 21, 2019
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SCHOOL OF SCIENCE AND MATHEMATICS

Departments of Biology, Chemistry & Biochemistry, Engineering, Computer Science & Physics, Mathematics, and Physician Assistant Studies

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Proceedings of the
First Annual Mississippi College STEM Research Symposium
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About the
First Annual 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.

People's Choice Awards

Symposium attendees cast votes for their favorite poster presenters. Votes are tallied and the poster presenters receiving the three highest number of votes are determined. People's Choice Awards are presented to the poster presenters at the end of the symposium. Only current student presenters are eligible for People's Choice Awards.

Symposium Sponsors & Acknowledgments

The First Annual 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.

Easels for posters were provided by the Department of Chemistry.

Event photographs were provided by Dr. David Magers and Carlie Claudio.

Symposium Schedule and Poster Guide
First Annual Mississippi College STEM Research Symposium

Date …… November 21, 2019

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

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People's Choice Voting ……..……...…… 10:00 AM – 1:00 PM

Poster Presentations ……... 11:00 AM – 1:00 PM

People's Choice Awards ……..…… 3:00 PM – 3:30 PM

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8	**Mary K. McLeod**	**The Effects of the Environmental Pesticide Imidacloprid (IMID) and Trans-nonachlor (TRANS) on Macrophage Foam Cell Formation In vitro**
9	**Vipanpreet Kaur**	**Flavonoids Affect the Expression of Cytokines TNF-alpha, IL-6, and TGF-beta in Colorectal Cancer Cells Treated with Hydrogen Peroxide**
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Research Abstracts
First Annual Mississippi College STEM Research Symposium

Poster #1

Introduction of Free-Radical Scavenging Flavonoids to C2BBe1 Colorectal Cancer Cells In vitro Increases Expression of Pro-chemotaxic, Pro-metastatic β-chemokines

Jeanlouis, CJ, Balamurugan, K, Bear, M, Belton, A, Jago, C, Lewis, C, McCallister, A, McKenzie, N, Meregini, S, Moore, B, Peoples, T, Robinson, A, Snow, A, Stoll, K, Wang, N, Duncan, D, Prem, S, and Whittom Reiken, AA

Certain cancer cell lines exhibit a significant increase in pro-metastatic gene expression in the presence of oxidative stress. The colon cancer C2BBe1 cell line exhibits these properties, as these cells are known to thrive in oxidatively stressful environments. Flavonoid compounds are known to possess free-radical scavenging activities which theoretically would decrease oxidative stress and could be explored as a possible therapy for colorectal cancer. We hypothesized that the free-radical scavenging properties of flavonoid compounds would decrease oxidative stress on C2BBe1 colorectal cancer cells having anti-metastatic implications with regard to chemotaxic gene expression. C2BBe1 cells were treated in vitro for 24 hours under four different experimental conditions: flavonoid extract in DMSO and DMSO only control, both with and without hydrogen peroxide. Hydrogen peroxide simulated oxidative stress to induce free radical production. Antibody arrays were utilized to compare changes in gene expression between treatments. 4 pro-metastatic β-chemokines were analyzed. As expected, oxidative stress increased the expression of most examined pro-metastatic β-chemokines. Surprisingly, the expression of several increased significantly in the presence of flavonoids. Though these results were not expected, they are supported by previous studies suggesting that flavonoids have a variable threshold with regard to free-radical scavenging abilities in the presence of oxidative stress, and extremely high concentrations of free radicals, can cause flavonoids to release additional free radicals, causing an overall increase in oxidative stress. These results suggest that though flavonoids have been shown to have free-radical scavenging abilities, they may have adverse effects in certain cell types and physiological environments.

Presenting Author: Christopher J. Jeanlouis

MC Department: Department of Biological Sciences

Research Mentor: Angela A. Whittom Reiken, PhD

Research Sponsor: MC Department of Biological Sciences

Poster #2

Variations in Expression of Cancer Genes in Colorectal Cancer Cells treated with Capecitabine (Xeloda), Oxaliplatin (Eloxatin), or both Capecitabine and Oxaliplatin (CAPOX or XELOX)

Crooks, MD, Babu, JJ, Jeane, TJ, Bharany, S, Brown, KC, Butler, D, Hendry, ME, Holbrook, JB, Ingram, RG, Jeanlouis, CJ, Kaur, V, Singh, G, and Whittom Reiken, AA

Capecitabine (CAP) and Oxaliplatin (OX) are typically used in conjunction to combat colorectal cancer. This combination, also known as "CAPOX", is especially effective in the treatment of advanced stage colorectal cancer due to each drug's effect on the cellular reproductive cycle. In addition to the added benefit given by each on the "combative process" the combination of both drugs has an offsetive effect on some of the undesired "side-effects" experienced when only one is given. For this study, the C2 Human Cancer Array was used to test the effects of both Capecitabine and Oxaliplatin individually, as well as in combination, on genes specifically associated with cancer pathology. Once the testing protocol was completed, the results were organized and charted as to compare each set. The data was then used to determine the effects of each drug on the cancer genes expressed in a colorectal cancer cell line. Increase or decrease of expression for the different genes varied. Several genes decreased significantly with combination CAPOX treatment relative to individual Capecitabine or Oxaliplatin treatment.

Presenting Authors: Matthew D. Crooks, Jobin J. Babu, and Taylor J. Jeane

MC Department: Department of Biological Sciences

Research Mentor: Angela A. Whittom Reiken, PhD

Research Sponsor: MC Department of Biological Sciences

Poster #3

Relative Stabilities of Derivatives of 9-Methylanthracene and 9-Methylene-9,10-Dihydroanthracene and Derivatives of 6-Methylpentacene and 6-Methylene-6,13-Dihydropentacene

Plunkett, AW and 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, and if certain derivatives of these pentacene systems stabilize the methyl derivative relative to the methylene. Specifically, nitro and trifluoromethyl derivatives of anthracene are considered, and 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 the M06-2X high nonlocality hybrid functional from Thular and Zhao and the ωB97XD 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.

Presenting Author: Aaron W. Plunkett

MC Department: Department of Chemistry & Biochemistry

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

Research Sponsor: Mississippi College Catalysts

Poster #4

Enthalpies of Formation of Chloro and Cyano Derivatives of Heterocyclic Aromatics by Homodesmotic Reactions

Damon, DA, Shumaker, CL, and Magers, DH

Furan, pyrrole, oxazole, isoxazole, and imidazole are all examples of heterocyclic aromatic compounds. They and their derivatives have a variety of uses. 2,5-dimethyl-furan has been proposed as a possible biofuel; pyrrole is a component of both heme and chlorophyll; ibotenic acid, a derivative of isoxazole, is a powerful neurotoxin; and histidine is a derivative of imidazole. In the current study, we focus on the computation of the standard enthalpy of formation of chloro and cyano derivatives of these aromatic heterocycles 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, second-order perturbation theory, and density functional theory. The DFT functionals employed are Becke's three-parameter hybrid functional using the LYP correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ωB97XD 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.

Presenting Author: Dean A. Damon

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, PhD

Research Sponsor: Mississippi College Catalysts

Poster #5

Do Stable Hydrogen Bridge Bonds Form Between Boron and Silicon?

Overstreet, HM and Magers, DH

Hydrogen bridge bonds (μ-hydrido bonds) are examples of 3-center, 2-electron bonding. Such bonds are known to form easily between boron atoms. Diborane, B2H6, is perhaps the prototypical example. While hydrogen bridge bonds are not as common between silicon atoms, the ground state of Si2H2 is the butterfly structure of C2V symmetry with two hydrogen bridge bonds. In the current study, we investigate whether small molecules with one boron atom and one silicon atom might have stable configurations with hydrogen bridge bonds. Specifically, we investigate BSiH4, BSiH5, BSiH6, BSiH6 cation and BSiH7, and we compare the isomers with bridge bonds to the more common classical structures. The geometries, corresponding electronic energies, and the corresponding harmonic vibrational frequencies for all systems are computed using SCF theory, second-order perturbation theory, and density functional theory. The DFT functionals employed are

Becke's three-parameter hybrid functional using the LYP correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ωB97XD 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.

Presenting Author: Hannah M. Overstreet

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, PhD

Research Sponsor: Mississippi College Catalysts

Poster #6

Inhibition of Apoptosis Inhibiting Proteins in Colorectal Cancer Metastasis through Capecitabine, Oxaliplatin, and CAPOX Combination Treatment

Holbrook, JB, Babu, JJ, Bharany, S, Brown, KC, Butler, D, Crooks, MD, Hendry, ME, Ingram, RG, Jeane, TJ, Jeanlouis, CJ, Kaur, V, Singh, G, and Whittom Reiken, AA

Colorectal cell metastasis is accomplished through inhibition of apoptosis, normal cell death. Preservation of apoptosis is an important phase of preventing colorectal cancer formation. The aim of this study is to investigate the effects of chemotherapy drugs on the gene expression of proteins that inhibit apoptosis in colorectal cells. The C2BBe1 colorectal cell line was either untreated, treated with Capecitabine (Cap), treated with Oxaliplatin (Ox), or treated with a combination of Capecitabine and Oxaliplatin (CAPOX). The amount of gene expression for the protein, Growth/Differentiation factor 15 (GDF-15), was measured for each treatment group using an antibody array. Elevated GDF-15 levels have been associated with an adverse prognosis of colorectal cancer. Elevated GDF-15 levels leads to increased activation of the epithelial-mesenchymal transition (EMT) process which promotes an increased resistance to apoptosis. Successful chemotherapy treatment should lead to decreased gene expression of GDF-15. Gene expression for GDF-15 significantly decreased upon treatment with Ox and CAPOX. A significant change in gene expression upon treatment with Cap was not observed. As a result, our study indicates that treatment of colorectal cancer cells with Ox or CAPOX chemotherapy leads to a decrease in gene expression of GDF-15, decreasing the likelihood of colorectal cell metastasis.

Presenting Author: Jacob B. Holbrook

MC Department: Department of Biological Sciences

Research Mentor: Angela A. Whittom Reiken, PhD

Research Sponsor: MC Department of Biological Sciences

Poster #7

Capecitabine, Oxaliplatin, and CAPOX Combination Decrease Expression of Inhibitors of Apoptosis in Colorectal Cancer Cells

Hendry, ME, Babu, JJ, Bharany, S, Brown, KC, Butler, D, Crooks, MD, Holbrook, JB, Ingram, RG, Jeane, TJ, Jeanlouis, CJ, Kaur, V, Singh, G, and Whittom Reiken, AA

The inhibition of apoptosis, programmed cell death, is an important step in the formation and further metastasis of cancer cells. To prevent cancer formation, it is critical that the system for destroying damaged cells remains intact. In this study, we investigated the role of current pharmaceutical drugs on inhibitors of apoptosis in colorectal cancer cells. Caco-2 derivative cells, C2BBe-1, a colorectal cancer cell line resembling enterocytes of the small intestine, received either no treatment, treatment with Capecitabine (Cap), treatment with Oxaliplatin (Ox), or treatment with a combination of Capecitabine and Oxaliplatin (CAPOX). Using antibody arrays, the levels of expression for two pro-inflammatory proteins, Galectin-3 and Macrophage Migration Inhibitory Factor (MIF) were then determined for each treatment group. Galectin-3 and MIF are known to be capable of inhibiting apoptosis, allowing cancerous cells to survive indefinitely, as well as a variety of other functions that lead to the development of colorectal cancer. Overexpression of MIF and Galectin-3 is associated with poor prognosis in colorectal cancers, so gene expression for both proteins is expected to decrease with effective colorectal cancer treatments. Compared to the control groups, both MIF and Galectin-3 saw significant decreases in gene expression for all treatment groups. Our results, therefore, indicate that Cap, Ox, and CAPOX chemotherapy regiments decrease the expression of MIF and Galectin-3 in colorectal cancer cells, decreasing the formation, survival, and metastasis of colorectal cancers.

Presenting Author: Matthew E. Hendry

MC Department: Department of Biological Sciences

Research Mentor: Angela A. Whittom Reiken, PhD

Research Sponsor: MC Department of Biological Sciences

Poster #8

The Effects of the Environmental Pesticide Imidacloprid (IMID) and Trans-nonachlor (TRANS) on Macrophage Foam Cell Formation In vitro

Posada, DM, Moeller, C, McLeod, M, Howell, G, and Carmicle, S

Heart disease, the leading cause of death in the United States, is commonly caused by narrowing of the coronary arteries from plaque build-up, termed atherosclerosis. Recent studies have suggested a correlation between exposure to environmental insecticides and atherosclerosis. Imidacloprid is a neonicotinoid insecticide that disrupts nerves' ability to send signals. On the other hand, trans-Nonachlor, a component of the insecticide Chlordane, causes partial repolarization of a neuron and a state of uncontrolled excitation. Although Chlordane has been banned, its effects are still seen due to its accumulation in lipids/fats. In contrast, IMID, one of the main insecticides used in the U.S., has raised toxicity concerns. Elevated levels of LDL can damage an artery endothelium, increasing the risk for plaque formation. In this study, we examine and quantify the uptake of low-density lipoprotein (LDL) and oxidized-LDL in RAW 264.7 macrophages in vitro in the presence of two common environmental pesticides, Imidacloprid (IM) and trans-Nonachlor (TRANS). LDL and ox-LDL uptake was analyzed using Oil-Red-O staining, extraction and quantification. Significant increases in lipid absorbance are seen in macrophages when stimulated with TRANS but not IMID.

Presenting Author: Mary K. McLeod

MC Department: Department of Biological Sciences

Research Mentor: Stephanie Carmicle, PhD

Research Sponsors: MC Department of Biological Sciences, Mississippi State University Department of Basic Sciences, and Mississippi State University College of Veterinary Medicine

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Poster #9

Flavonoids Affect the Expression of Cytokines TNF-alpha, IL-6, and TGF-beta in Colorectal Cancer Cells Treated with Hydrogen Peroxide

Kaur, V, Balamurugan, K, Bear, M, Belton, A, Jago, C, Lewis, C, McCallister, A, McKenzie, N, Meregini, S, Moore, B, Peoples, T, Robinson, A, Snow, A, Stoll, K, Wang, N, Duncan, D, Prem, S, and Whittom Reiken, AA

Worldwide, colorectal cancer (CRC) is a frequently occurring cancer, with 70-80% sporadic cases. Research shows that colorectal tumors such as adenomas and carcinomas exhibit an increased level of oxidative stress when compared to non-affected cells. Increased oxidative stress a heightened level of proliferation that is indicative of colorectal cancer cells. One factor that may lead to this increase in proliferation under high oxidative stress conditions is increased cytokine expression. Tumor Necrosis Factor-alpha (TNF-alpha) and Interleukin 6 (IL-6) are cytokines that have been linked to the increase in proliferation of tumors in CRC, while Transforming Growth Factor-Beta (TGF-beta) has been shown to inhibit the proliferation of CRC cells. *Pseudognaphalium obtusifolium* is a plant which produces flavonoids having significantly more radical scavenging activity Vitamin C. These flavonoids may reduce the amount of oxidative stress that the carcinoma cells experience by reducing the expression of cytokines linked to increased proliferation. Hydrogen peroxide treated C2BBe1 colorectal adenocarcinoma cells were treated with flavonoids in order to see if the phytochemicals may have any effects on colon cancer cells under oxidative stress. Following treatment, antibody arrays were used to determine changes in expression. The flavonoids from *P. obtusifolium* were able to cause an increase in the expression of TGF-alpha and a decrease in TNF-beta, and IL-6. These results indicate that the flavonoids from *P. obtusifolium* do have an effect on cytokine expression during to oxidative stress.

Presenting Author: Vipanpreet Kaur

MC Department: Department of Biological Sciences

Research Mentor: Angela A. Whittom Reiken, PhD

Research Sponsor: MC Department of Biological Sciences

Poster #10

Expression of Metalloproteinases and Related Proteins in C2BBE-1 Colon Adenocarcinoma Cells under Oxidative Stress

Bharany, S, Balamurugan, K, Bear, M, Belton, A, Jago, C, Lewis, C, McCallister, A, McKenzie, N, Meregini, S, Moore, B, Peoples, T, Robinson, A, Snow, A, Stoll, K, Wang, N, Duncan, D, Prem, S, and Whittom Reiken, AA

Human colorectal adenocarcinoma cells are known to exhibit great oxidative stress due to the heavy metabolic usage and rapid division of the intestinal epithelium. It has previously been shown that tumor cells normally generate a great number of reactive oxygen species (ROS), and colon cancer cells can tolerate extreme ROS levels. In fact, increased oxidative stress leads to increased proliferation and metastasis in colon cancer. Metalloproteinases play a role in metastasis by degrading the extracellular matrix. Our lab has previously concluded that *Pseudognaphalium obtusifolium*, a member of the Asteraceae family, produces flavonoid phytochemicals having significantly more radical scavenging activity than ascorbic acid (Vitamin C). Numerous studies have shown that flavonoids have both anti-carcinogenic and antioxidant behavior. To determine if these phytochemicals may have significant therapeutic effects, we stressed the cell line using hydrogen peroxide. Cytokine expression was determined using antibody arrays for cells treated with or without hydrogen peroxide in addition to treatment with or without flavonoids. Specifically, analysis was performed for IFN-Gamma, VEGF, TIMP-1, TIMP2, MIF, TNF-alpha, TGFb2, TGFb3 and IL6 metalloproteinases and related proteins. Expression was decreased for most proteins under oxidative stress except TIMP2 was greatly increased and IL6 was slightly increased. Tissue Inhibitor of Metalloproteinase 2 (TIMP2) is a natural matrix metalloproteinase inhibitor. Treatment with flavonoids under oxidative stress conditions had the opposite effect expected, decreasing the expression of TIMP2 and increasing expression of the other proteins. Future experiments will continue to explore the roles of these and other proteins in colon cancer metastasis.

Presenting Author: Sajal Bharany

MC Department: Department of Biological Sciences

Research Mentor: Angela A. Whittom Reiken, PhD

Research Sponsor: MC Department of Biological Sciences

Poster #11

Using Time-Lapse Photography to Determine the Importance to Wildlife of Logs Near Streams

Saleem, K, Stockstill, S, and Hensley, FR

We tested the hypothesis that logs are important habitats for wildlife using time-lapse photography. Cameras were set at five locations spread over an 85-meter section of creek. Two cameras were set in sites with logs, and three cameras were set in sites without logs. Photos were taken at intervals of 1 minute or less. The stream itself - located in Hinds County, Mississippi - was < 3 meters wide at its highest point and < 1 meter deep. After retrieving data, teams of undergraduate students reviewed and recorded vertebrate occurrence in > 1.8 million photos collected from January 2017 to December 2018. Over 5,000 animals were detected, representing more than 15 species in > 4,500 photos. We identified vertebrates as precisely as possible within the limits of camera resolution and detection. Ultimately, we discovered that 12 of the 15 animal species were seen more frequently in

association with sites with logs than in sites without logs. Thus, we recommend that log removal to address stream bank erosion be considered only in comparison to the habitat value of logs for wildlife species present in the area.

Presenting Authors: Skylar Stockstill and Khunsa Saleem

MC Department: Department of Biological Sciences

Research Mentor: Frank R. Hensley, PhD

Research Sponsor: MC Department of Biological Sciences

Poster #12

Conventional Strain Energies of Thiirane, Thietane, Borylthiirane, 2-Borylthietane, and 3-Borylthietane

Nash, SL, Mohamed, MM, Smith, SA, and Magers, DH

A previous study in our group revealed that thiirane is less strained than cyclopropane and that thietane is less strained than cyclobutane. A different study of ours revealed that cyclopropylborane is much less strained than cyclopropane. The current study investigates if these effects might be additive. Could a boryl group on thiirane and thietane reduce their strain even more? To answer this question, the conventional strain energies for borylthiirane, 2-borylthietane, and 3-borylthietane are determined within the isodesmic, homodesmotic, and hyperhomodesmotic models and compared to the conventional strain energies of thiirane and thietane. 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 (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.

Presenting Author: Summer L. Nash

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, PhD

Research Sponsor: Mississippi College Catalysts

Poster #13

Regioselectivity of Acid-Catalyzed Epoxide Ring-Opening Reactions

Broom, PL, Smith, SA, and Magers, DH

Epoxide opening reactions occur through two known mechanisms: base catalyzed, in which nucleophilic attack opens the ring, followed by a proton transfer to produce the substituted alcohol, and acid catalyzed, in which the oxirane oxygen is protonated via proton transfer, followed by nucleophilic attack to produce the substituted alcohol. There is little debate in the literature about base catalyzed reactions involving the least substituted carbon in the epoxide. However, two undergraduate textbook authors disagree about the regioselectivity involving acid catalyzed epoxide opening reaction when the carbons are primary and secondary. Joel

Karty asserts that the more substituted carbon is attacked in the acid catalyzed mechanism and offers bond length data to augment his argument. David Klein, on the other hand, suggests that the less substituted carbon is attacked when the competing electrophiles are primary versus secondary due to "the steric effect predominating over the electronic effect." To investigate these dissenting opinions, the optimized equilibrium geometries of a series of asymmetric derivatives of oxirane are computed using SCF theory, second-order perturbation theory, and density functional theory. The DFT functionals employed are Becke's three-parameter hybrid functional using the LYP correlation functional, the M06-2X high nonlocality hybrid functional from Thular and Zhao, and the ωB97XD functional from Head-Gordan and coworkers which includes empirical dispersion. The basis sets employed are Dunning and coworkers' correlation consistent basis sets. Bond lengths should be indicative of bond strengths; thus, the different C-O bonds are compared in each optimized structure and in the corresponding protonated structures.

Presenting Author: Perry L. Broom

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, PhD

Research Sponsor: Mississippi College Catalysts

Poster #14

The Conventional Strain Energies of Cyclopropylborane, Borirane, Boretane, Borolane, and the Diboretanes

Logan, KS, Hartman, KL, and Magers, DH

In 2012, Rubina and Rubin reported the first generation and spectroscopic identification of boretane through a strain-release-driven ring expansion of cyclopropylborane. Prior to this discovery, all four-membered boracycles which had been reported were unsaturated. In the current study, we build upon this discovery by calculating the conventional strain energies of cyclopropylborane, borirane, boretane, 1,2-diboretane, 1,3-diboretane, and borolane 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 using the LYP correlation functional and the M06-2X high nonlocality hybrid functional from Thular and Zhao. Three correlation-consistent basis sets are employed: cc-pVDZ, cc-pVTZ, and cc-pVQZ. Results are compared to the conventional strain energies of cyclic hydrocarbons.

Presenting Author: Kelbe S. Logan

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, PhD

Research Sponsor: Mississippi College Catalysts

Poster #15

How Can Steric Hindrance Be Alleviated in the Formation of Dendrimer Precursors to Conserve π-Conjugation?

Brooks, RJ, Smith, SA, and Magers, DH

The Mississippi College Organic Research Group has an ongoing mission to design and prepare flat, two-dimensional dendrimers. In order for dendrimers to attain light-harvesting properties, conjugation of the π-bonding system must be conserved. It has been found that when twisting occurs about the single bonds of the dendrons, there is a decrease in energy transfer and therefore loss of conjugation and reduced light harvesting properties. In previous work, synthesized dendrimer precursors have shown this twisting, and therefore loss of π-conjugation, due to the hydrogens in the ortho positions of the phenyl rings. In the current project we investigate computationally if structures which incorporate diynes, as opposed to the ethynyl units previously used, will position the hydrogens far enough from one another that their steric interactions will be reduced and twisting of the structure will not occur and conjugation will be retained. Another goal of this research is to determine if twisting can be eradicated by changing the types of atoms and the length of the bridges that connect the phenyl rings. Nucleus-independent chemical shift calculations are also conducted to determine the aromaticity of the structures and prove whether conjugation is truly conserved. To investigate these questions, optimum structures are computed at the SCF and DFT levels of theory. The functionals employed are B3LYP, M06-2X, and ωB97XD. All calculations use correlation consistent basis sets.

Presenting Author: Ruth J. Brooks

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, PhD

Research Sponsor: Mississippi College Catalysts

Poster #16

Conventional Strain Energies of Thiaziridine and the Thiazetidines

Gramm, JD and 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 thiirane and thietane.

Presenting Author: Joshua D. Gramm

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Research Sponsor: Mississippi College Catalysts

Poster #17

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

Zetterholm, DL and 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 d33 coefficient. In seeking to extend research done by Arun Gagrai and co-workers which discovered a possible relationship between first-order polarizability of a molecule and its piezoelectric response (d33), 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 previous results and model them in the Hartree Fock level 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.

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Research Sponsor: Mississippi College Catalysts

Poster #18

The Combined and Individual Therapeutic Effect of Capecitabine (CAP) and Oxaliplatin (OX) on the MIF and ICAM-1 genes in Human Colorectal Cancer

Singh, G, Babu, JJ, Bharany, S, Brown, KC, Butler, D, Crooks, MD, Hendry, ME, Holbrook, JB, Ingram, RG, Jeane, TJ, Jeanlouis, CJ, Kaur, V, and Whittom Reiken, AA

Colorectal cancer is known to occur in the inner lining of the colon or rectum called the polyp. The cells can either become malignant or turn benign in the tissue. Colorectal cancer can be either inherited or the more common sporadic type caused accumulated DNA mutations acquired throughout a person's life. There are certain important genes that get disrupted in colorectal cancer including intercellular adhesion molecule - 1 (ICAM-1) and macrophage migration inhibitory factor (MIF). ICAM-1 is a ligand for leukocytes' LFA-1 surface receptor, which helps them move from the blood vessels to the site of infection through the process called diapedesis. Cells such as macrophages, monocytes, and granulocytes found in the

immune system will use ICAM-1 to go to the area of inflammation and fight abnormal cells. MIF act's as a regulator to those cells coming in to inflamed tissue site. In order to resolve the potentially serious effects of the mutated gene, the effects of both CAP and OX therapy was tested in a combined and individual fashion using a colorectal cancer cell line. Antibody arrays were used to determine gene expression. The results showed that either CAP and OX used alone decreased the expression of both the ICAM-1 and MIF genes. It also showed that the utilization of CAPOX in a combined form raised the expression of ICAM-1 and decreased the expression of MIF.

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Research Sponsor: MC Department of Biological Sciences

Poster #19

Lactate Production in Glucose-deprived Cells

Sarigul, AE, Bell, HL, Kirkland, BC and Reagan, JW

Many types of cancer cells are characterized by rapid and constitutive cell growth which is often associated with conversion of pyruvate to lactate even under normoxic conditions. This phenomenon, first described by Otto Warburg in the early part of the 20th century and commonly referred to as the Warburg Effect, was overlooked for decades. However, the need for a carbon source (e.g. lactate) to support unregulated cell growth has led to a renewed interest in the Warburg Effect. To determine whether incubation conditions that induce rapid cell growth increase lactate production, Chinese hamster ovary (CHO) cells were incubated at various temperatures and glucose concentrations. Media with a glucose concentration of 15 mM supports rapid cell growth and lactate secretion when incubation occurs at physiological temperatures (37oC). It is possible that suboptimal incubation conditions (31oC and low glucose concentration) that fail to support maximal cell growth activate the unfolded protein response (UPR). To test this hypothesis, our laboratory is in the process of developing robust assays for the detection of UPR activation including quantification of CHOP and Bip expression by Western blotting. This will allow our lab to determine whether stress-inducers that lead to quiescence activate the UPR and simultaneously decrease lactate production. Such a connection would suggest that the Warburg Effect occurs when cells exist under conditions that maximize growth potential and increase demand for membrane synthesis.

Presenting Author: AE Sarigul

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Poster #20

Effect of Dietary Carbohydrate on Growth and Lipid Accumulation in *Drosophila melanogaster* Larvae

Townsend, WR, Sumrall, DM, Haynes, AC, Norris, AC, Bryant, G and Reagan, JW

The mass of *Drosophila melanogaster* larvae increases about 200-fold between hatching and pupation. This makes them a tractable model system for the study of cell division and growth. Our laboratory is developing this model system to study the effect of dietary proteins and carbohydrates on metabolic pathways that impact growth rate. To this end, the rate of growth and accumulation of lipids is determined in larvae reared on chemically-defined diets with various protein to carbohydrate ratios. In this study, analysis of growth rate on a 1:1 diet was determined by measuring larval mass and length every 8 hours until the onset of pupation which occurred 168 hours after egg laying (AEL). After an initial lag phase of 72 hours AEL, growth accelerated to a rate of 0.02 mg/hr. The larvae achieved maximum size at 150 AEL with a weight of 1.6 mg/larvae. The effect of dietary carbohydrate on larval growth rate may be a function cytosolic triglyceride content. Due to their voracious feeding behavior, D. melanogaster larvae have well-developed salivary glands which can serve as a surrogate for overall cell function. Therefore, salivary glands were removed and analyzed for neutral lipid content by oil-red-O staining. The accumulation of energy-rich lipids such as triglycerides may affect the rate at which larvae achieve the ideal mass for pupation and development into adult flies. Continuation of these studies will shed light on the role of carbohydrates and lipids in the regulation of metabolic parameters that affect cell division and growth.

Presenting Author: WR Townsend

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Research Sponsor: MC Department of Biological Sciences

Poster #21

Antioxidant Effects of *Pseudognaphalium obtusifolium* on the Expression of Cytokines IL-6, IL-8, VEGF, and IGF-1 in Colorectal Cancer

Ingram, RG, Balamurugan, K, Bear, M, Belton, A, Jago, C, Lewis, C, McCallister, A, McKenzie, N, Meregini, S, Moore, B, Peoples, T, Robinson, A, Snow, A, Stoll, K, Wang, N, Duncan, D, Prem, S, and Whittom Reiken, AA

Colorectal cancer is one of the most prevalent cancers worldwide. Research has shown that human colorectal adenocarcinoma cells exhibit aggressive proliferation under abnormal levels of oxidative stress. Cells exhibiting increased oxidative stress have also been shown to have a marked increase in cytokines such as Interleukin-6 (IL-6), Interleukin-8 (IL-8), Insulin-like growth factor (IGF-1) and Vascular Endothelial Growth Factor (VEGF). These cytokines have been linked with tumor angiogenesis and metastasis. Some scientists believe keeping these cytokines in check would dramatically reduce metastasis. *Pseudognaphalium obtusifolium* produces flavonoids having potent antioxidative properties. To determine if these flavonoids have significant effects on colon cancer cells under oxidative stress, C2BBe1 colorectal

adenocarcinoma cells were treated with hydrogen peroxide to induce oxidative stress, both with and without the addition of flavonoid extracts from the plant. The expressions of IL-6, IL-8, IGF-1, and VEGF were analyzed for both groups using antibody arrays. Flavonoids caused decreased expression of IL-6 and IGF-1, while there was a marked increase in IL-8 and VEGF. However, increased VEGF should not promote angiogenesis due to the decrease in IGF-1. As such, one may conclude that while radical scavenging activity of *Pseudognaphalium obtusifolium* flavonoids may increase the expression of some cytokines, it also plays a role in decreasing the expression of others. The negative effects of increased cytokines, such as 1L-8 and VEGF, may be counteracted by a decreased expression of other factors involved in metastasis such as IGF-1.

Presenting Author: Richard G. Ingram

MC Department: Department of Biological Sciences

Research Mentor: Angela A. Whittom Reiken, PhD

Research Sponsor: MC Department of Biological Sciences

People's Choice Awards
First Annual Mississippi College STEM Research Symposium

The following presenters received the most votes from their peers and mentors and were awarded the People's Choice Award. People's Choice Award recipients received a gift card, sponsored by the Mississippi College Office of Research. Congratulations to these scholars!

Pictured: Ruth Brooks and Dr. Stan Baldwin, Dean, School of Mathematics and Science

Ruth J. Brooks

How Can Steric Hindrance Be Alleviated in the Formation of Dendrimer Precursors to Conserve π-Conjugation?

MC Department: Department of Chemistry & Biochemistry

Research Mentor: David H. Magers, PhD

Research Sponsor: Mississippi College Catalysts

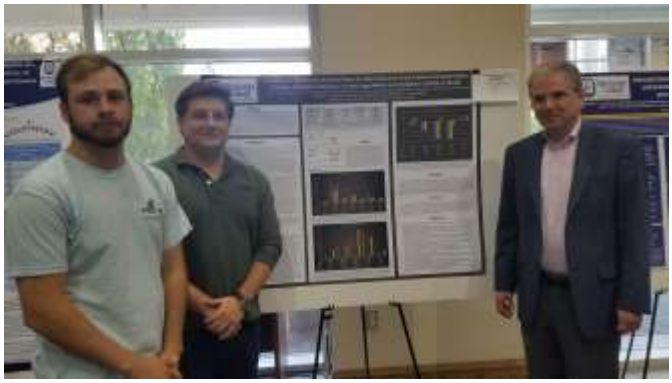
Matthew D. Crooks, Jobin J. Babu, and Taylor J. Jeane

Variations in Expression of Cancer Genes in Colorectal Cancer Cells Treated with Capecitabine (Xeloda), Oxaliplatin (Eloxatin), or Both Capecitabine and Oxaliplatin (CAPOX or XELOX)

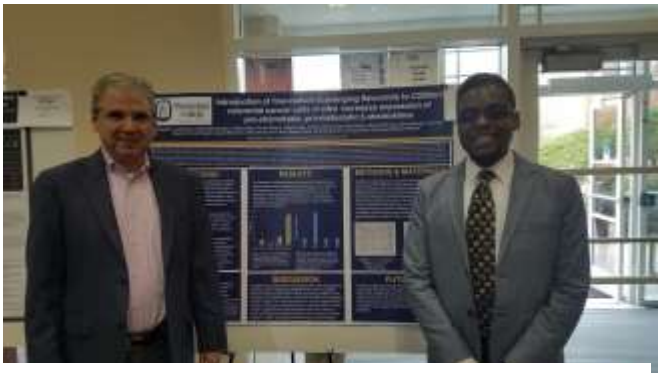
MC Department: Department of Biological Sciences

Research Mentor: Angela A. Whittom Reiken, PhD

Research Sponsor: Mississippi College Department of Biological Sciences



Pictured: Matthew Crooks, Taylor Jeane, and Dr. Stan Baldwin, Dean, School of Mathematics and Science



Pictured: Christopher Jeanlouis and Dr. Stan Baldwin, Dean, School of Mathematics and Science

Christopher J. Jeanlouis

Introduction of Free-radical Scavenging Flavonoids to C2BBe1 Colorectal Cancer Cells In vitro Increases Expression of Pro-chemotaxic, Pro-metastatic β-chemokines

MC Department: Department of Biological Sciences

Research Mentor: Angela A. Whittom Reiken, PhD

Research Sponsor: Mississippi College Department of Biological Sciences

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