

STEM Posters at the Capitol



February 6, 2013

“It is essential, if we want to continue to reap the benefits of science, to commit as a nation to preparing more young people for extraordinary careers in science.”

—Carol W. Greider, 2009 Nobel laureate in physiology & medicine

Highlights

- Over 90 students
- From 14 Arkansas colleges and universities
- Presenting 62 different posters of original work
- Encompassing all aspects of natural science and math



UNIVERSITY OF
Arkansas at Pine Bluff

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Catalytic production of hydrogen: clean energy for a sustainable economy

Robert Bowman and Charles Mebi*

Department of Physical Sciences, Arkansas Tech University,
Russellville, AR

Our society is currently dependent on carbon-based non-renewable fossil fuels (coal, oil and natural gas) to meet our fast growing global energy demand. This dependence is unsustainable and contributes to large amounts of carbon dioxide released into the atmosphere with potential environmental and health consequences. Hydrogen is a clean alternative to fossil fuels and can be produced from water which is abundant and readily available. Hence, there is great interest in the development of hydrogen fuel-cell technology and basic research on the production and storage of hydrogen. Current method of hydrogen production from water requires expensive platinum-based catalysts. The goal of this project is to develop new catalysts based on cheap metal (Iron) as a substitute for platinum. Our catalysts are iron-carbonyl clusters coupled to polyaromatic thiolate ligands. They are designed to mimic the structure and function of the active site of the efficient hydrogen producing enzyme, [Fe-Fe] hydrogenase. We have studied a series of these compounds and the results show that they are effective hydrogen generation catalysts. The preparation and evaluation of these catalysts will be discussed.

Hydrogen generation through the electrolysis of water

Esgar Jimenez and M. Jeffrey Taylor*

School of Mathematical and Natural Sciences, University of Arkansas at Monticello, AR

We are currently generating hydrogen and oxygen through the electrolysis of water avoiding any exotic or expensive equipment or materials. This involves the splitting of water molecules into hydrogen gas and oxygen gas by applying an externally direct current potential. Water is oxidized (loss of electrons) at the anode to form oxygen gas. Hydrogen ions are reduced (gain of electrons) at the cathode to form hydrogen gas. Currently, we use a 120 V AC house current and an AC/DC converter as an energy source for the voltameter or electrolyzer. The anode and the cathode are placed in separate enclosed tubes connected by a bridge, immersed in an electrolyte solution. The DC current is supplied with a voltage exceeding ~ 1.5 V. The cathode produces twice as much of hydrogen as oxygen gas is produced at the anode. We have employed different electrodes and different electrolyte solutions to generate the hydrogen and oxygen.

We propose to scale up our current production methods by constructing a larger voltameter or electrolyzer to produce and capture the hydrogen gas. We intend to power the electrolyzer with a solar photovoltaic panel. A multitude of uses can be considered for inexpensive, clean burning hydrogen fuel.

Affordable small-scale vertical axis wind turbine for Arkansas

Henry Mitchell, Chris Soekenson, Ernesto Lopez Chan,
Ted Song*

Division of Engineering, John Brown University, Siloam Springs, AR

The objective of this project was to build a functional and efficient wind turbine with a budget of \$200.00. The key element was an easy to construct overall design using materials that could be resourced locally. The idea behind this is to give rural communities throughout the state of Arkansas and the world an affordable option in the use of renewable energy sources, such as wind, in their area. For the reasons noted above, a vertical axis wind turbine (VAWT) design was chosen. Since VAWT requires low wind speeds to generate electricity and is a simple design, the chosen design may be a good solution for harvesting the wind in the state of Arkansas. The materials used were 4" PVC pipes, 2 bicycle wheels, and a bicycle chain and gears for connecting the wind turbine to the generator, and metal angle iron for building a base for the turbine in conjunction with a low rpm dc motor as a generator. Experimental results show that the proposed turbine may produce usable power in wind speeds found in many places in the state of Arkansas.

An efficient passenger size electric vehicle

Chris C. Arnold, Kevin T. Tran, Kevin R. Lewelling*

Department of Engineering, University of Arkansas at Fort Smith, AR

Acceptance of Battery Electric Vehicles (BEVs) has been slow due to limited driving range, lengthy recharging times, and vehicle size. An answer to address these limitations may involve combining cutting edge technologies with traditional automotive standards. A BEV is being developed at the University of Arkansas – Fort Smith which combines state of the art electronics and Lithium Ion (LI) batteries with a common 5-speed transmission. This new powertrain allows a relatively small 8 horse power electric motor to match driving demands and stay within the limits of the battery output. If this 5-speed powertrain is successful, plans will be developed to design and construct a Continuous Variable Transmission (CVT) which will further increase vehicle efficiency for passenger vehicles and light-weight delivery trucks. This project continues to build a bridge between local business and industry and the University of Arkansas –Fort Smith in motor development and specialized parts needed in this powertrain. As this technology matures, it is foreseeable that new businesses and industries could result.

Feasibility study of a grid-tied photovoltaic system in Arkansas

Gunnar Shaffer, Francis Morales, Ted Song*

Division of Engineering, John Brown University, Siloam Springs, AR

A feasibility study of a grid-tied photovoltaic (PV) system in the state of Arkansas is presented. Arkansas has good insolation measurements which may allow home owners to invest and install a grid-tied PV system. In order to promote grid-tied PV systems in the state of Arkansas and reduce carbon dioxide (CO₂) emissions, this study discusses the financial and environmental benefits of this type of PV system. Moreover, this research discusses some of the challenges of a grid-tied PV system and proposes possible solutions—such as tax incentives and installation adjustments for allowing maximum efficiency—that may help to overcome the obstacles. An example grid-tied PV system in the state of Arkansas is provided as an outcome of the research, which shows the feasibility of a PV system that can be both financially profitable and used to reduce CO₂ emissions. Analysis results have been presented to provide the future PV owners with possible payback times as well as exact system sizing and government requirements for consistent regulations.

CdTe/In₂S₃ solar cells by electrodeposition and evaporation

Joshua Vangilder^a, Maqsood Ali Mughal^a, Michael Jason Newell^a, John Hall^c, David McNew^c, Frederick Felizco^b, Shyam Thapa^a, Robert Engelken^{*c, a}, B. Ross Carroll^d, and J. Bruce Johnson^d

^aEnvironmental Sciences, ^bEngineering Management, ^cElectrical Engineering, ^dPhysics Arkansas State University, Jonesboro AR

We report exploratory research involving formation of p-CdTe/n-In₂S₃ heterojunctions by a combined electrodeposition and vacuum evaporation technique. These structures have potential to support photovoltaic conversion of light energy into electrical energy. The most successful approach involves deposition of thin In₂S₃ films by electron beam vacuum evaporation onto commercial indium tin oxide (ITO)-coated glass, followed by electrodeposition of the CdTe film and, finally, application of a front contact, usually silver, to the CdTe. The presentation will discuss both the deposition processes and characterization of the films and junctions, for example, by electron microscopy, energy dispersive X-ray analysis, optical spectroscopy, X-ray diffraction, and current-voltage-illumination curves. This work is being conducted under the auspices of the “Vertically Integrated Center for Transformative Energy Research” (VICTER) as part of the Arkansas ASSET II Initiative administered through the Arkansas Science and Technology Authority, and funded by the National Science Foundation EPSCoR Program (Grant EPS-1003970). The goal of VICTER is improvement of energy conversion systems all of the way from “materials to grid”, with a major focus on solar cell modules. It involves faculty from Arkansas State University, the University of Arkansas-Fayetteville, the University of Arkansas-Little Rock, and the University of Arkansas-Pine Bluff, with Dr. Alan Mantooth of UAF the center coordinator.

Near-thermal reactions of $\text{Au}^+(^1\text{S}, ^3\text{D})$ with CH_3X ($\text{X}=\text{F}, \text{Cl}$)

Kendall G. Fancher, Ashley J. Hicks, Cullen C. Matthews,
and Li Chen Chen, William S. Taylor*

Department of Chemistry, University of Central Arkansas-
Conway, AR

The focus of this work is to further our understanding of the mechanistic controls on reactions involving metal ions and small molecules. Such experimentally-accessible parameters might somehow be exploited in order to selectively form desired products. Gold nanoparticles have the demonstrated ability to induce chemical processes in hydrocarbon substrates utilizing a mechanism which could involve gold ions. Activation of the C–H bond in methane, the prototypical model for hydrocarbon activation, is the first step in the conversion of this abundant resource into molecules that are more useful as fuels and feedstocks; however activation of the C–H bond is energetically demanding. Here we react gold ions in two different electronic states with the methyl halides CH_3F and CH_3Cl , which offer the advantage of a weaker C–X bond ($\text{X}=\text{Cl}, \text{F}$). With both methyl halides, two parallel reactions are observed to arise from the ground state of Au^+ corresponding to simple clustering and elimination of HX . HF elimination is also observed to occur in the reaction of the excited state of Au^+ with CH_3F . Excited Au^+ also induces a second process with both methyl halides to yield CH_2X^+ . All observed products can be understood using thermochemical and quantum-mechanical arguments.

Molecular tweezers: controlling metals for diverse applications

T. Ryan Rogers, Jeremy Rodman, Patrick Desrochers*
Department of Chemistry, University of Central Arkansas,
Conway

Molecular tweezers can be made from small molecules capable of binding metals. These “tweezers” (referred to generally as chelates) are used to grasp various metals, establishing fine control over the metal’s activity. Metals are essential elements with roles as diverse as life-sustaining biochemistry to the preparation of bulk industrial commodities. In either case, the metal must be closely supervised to ensure effective results. For example, a vehicle’s catalytic converter, molecules that transport oxygen in blood, and industrial medicine synthesis all required metals to function. If the metals in each of these processes were not controlled, undesirable outcomes would result: expensive auto-parts, rust in the blood, and toxic metals in otherwise life-saving medicines. Our lab has demonstrated the use of microwaves to produce chelate “tweezers” capable of forming chemically active and useful complexes with several metals. Our chelates render metals more easily recyclable and their utility more sustainable. Our synthesis method allows these chelates to be made much cheaper and over 250 times faster than conventional methods. Ongoing research focuses on improving the chelate to control a wider variety of metals and allow more diverse applications from protein sensors to catalysts for the polymerization of plastics for the electronics industry

Expert-like physics problem-solving framework: utility for the classroom and teacher training

Mishal Benson, Andrew Mason*

Department of Physics and Astronomy, University of Central Arkansas, Conway, AR

STEM education reform is currently underway in Arkansas. Physics education research (PER) has recently begun at the University of Central Arkansas that could address this reform. Computer modules in development for introductory calculus-based physics courses, as part of collaboration with the University of Minnesota, are a toolset for possible use to this end. The modules are intended to explicitly introduce and “coach” an expert-like problem-solving framework to novice students. Several coaching modules have already been adapted to algebra-based physics. These coaches could be used in high school physics classrooms and training for pre- and in-service teachers in teaching the framework. The first step is collaborating with Arkansas high school physics teacher volunteers in evaluating these coaches for use in the classroom. Then we would adapt as necessary for trial among volunteers in high school physics courses. Eventually, these coaches will be available online. Other avenues of interest include creating modules with life-science oriented physics problems and developing applications for mobile devices and tablets.

Simulation of powder X-ray diffraction using polystyrene microspheres

J.S. Pennington and R.J. Tackett*

Department of Physical Sciences, Arkansas Tech University,
Russellville, AR

Powder x-ray diffraction is a common technique for determining the microstructure of crystalline material. As diffraction is a phenomenon that occurs when a wave encounters an obstacle that has the same characteristic size as the wavelength of the diffracted wave, by scaling up the size of the scattering obstacles, it is possible to simulate x-ray diffraction using electromagnetic radiation in the visible spectrum. In this experiment, a film of polystyrene microspheres (radius = $5\mu\text{m}$) was deposited onto a transparent medium, and a He-Ne laserbeam (633nm) was then diffracted by the microspheres; the resulting pattern was projected onto a thin piece of paper, captured by a camera, and the pattern was analyzed using free ImageJ software. The purpose of this experiment is to introduce the theory and practice of powder x-ray diffraction without the considerable equipment and operating costs that are required to run a diffractometer.

Regeneration of resin beads for commercial use in biofuel cleaning

Beatty, J. and A. Williams*

School of Mathematical and Natural Sciences, University of Arkansas at Monticello, AR

Commercial preparation of biofuels can involve various techniques, of which a non-aqueous technique is used at nearby production facilities. In the preparation, purification of the biofuels is first seen to by running the fuel mixture through a series of resin columns. As the resin is used its purification ability decreases and it must be replaced. In an effort to decrease the cost of buying additional resin we are looking at methods of regenerating the resin for continued use. To this end used samples of resin have been regenerated, and were tested by analyzing their ability to clean biofuel compared to that of unused resin.

Method Development for the Characterization of Fatty Acid Content in Freshwater Eustigmatophyceae

T. Snider, M. Jager, A. Williams*

School of Mathematical and Natural Sciences University of
Arkansas at Monticello, AR

Characterization of algae for their fatty acid content is one of a variety of tests done to determine the applicability of the algae. Applications include use as nutrients for aquaculture, in human consumption, or potential ability as biofuels. A number of freshwater eustigmatophyceae have been collected by Nathan Probst and Dr. Karen Fawley at UAM. These samples will be tested to determine if there are any differences in fatty acid concentration between species. Modification of previous methods of sample preparation has been required, and will be described. Results of fatty acid content will be determined through GC-MS analysis. Current results show that methodology needs significant work, as the techniques did not result in clean GC-MS spectra of the individual fatty acids, though they are distinctly different. However, fragmentation patterns appeared to match with that of diglyceride fatty acids.

References:

1. Krienitz, L; Wirth, M. *Limnologica* **2006**, 36. 204-210.
2. Prior, S; Fawley, M; Fawley, K. *J. Ark. Acad. Sci.* **2010**, in press.
Mass Spectroscopy work performed by the High Performance Structural Mass Spectrometry Laboratory, located in Chemistry and Biochemistry, University of Arkansas, Fayetteville

Monte Carlo Studies of the Hall C Compton Polarimeter

Erik G. Urban,^a David Gaskell^b

^aPhysics Department, Hendrix College, Conway, AR

^bThomas Jefferson National Accelerator Facility, Newport News, VA

Nuclear physics experiments at Thomas Jefferson National Accelerator Facility help us to understand the fundamental underpinnings of our universe. Many of these experiments require extremely precise measurements in order to measure very small quantities. One device used in experimental Hall C of Jefferson Laboratory is known as the Compton polarimeter and is used to obtain a precision measurement of the electron spin polarization of the lab's electron beam. After designing various Monte Carlo simulation packages for the electron detector within this apparatus, tests were performed to better understand the processes that influence the polarization measurement, assess the validity of the current analysis methods, and gauge the size of various systematic sensitivities. Many processes influencing the measurement are now understood more clearly, leading to better analysis methods. Additionally, several basic systematic sensitivities have been quantified, the largest to date estimated at $\pm 0.55\%$ polarization. Once all the uncertainties associated with the Compton polarimeter have been determined, an overall systematic error can be assigned to the beam polarization measurement.

Mars Rover Project (MRP)

Theva N. Chanthaseny and Kevin R. Lewelling*

Department of Engineering, University of Arkansas at Fort Smith, AR

A joint research project to design and construct a Mars rover between the University of Arkansas – Fort Smith (UAFS) and Harding University started summer 2012 after receiving funding from the NASA Collaborative Research Program grant and both universities, respectively. This research project is unique due to the rover's capabilities of scanning large areas of the Martian terrain. A group of undergraduate students at Harding University has designed a suite of optical instruments to sense and measure extraterrestrial atmospheric compositions, including biomarker gas presence on solid-surface solar system bodies such as Mars and Enceladus. We are in the final stages of designing and constructing the on-board power supply system based on 12 V Lithium Ion (LI) battery pack and microcontroller hardware. The task also includes programming used to guide the rover autonomously. The rover's capabilities to quickly scan large areas are made possible by deploying a retroreflector and then driving the rover at distances up to 100 meters away. Technologies employed in this project could be used in rovers designed for varied applications from dangerous police work to nuclear power plant operations.

Acoustic Properties of Various Flight-Approved Materials

Justin Mann, Matthew Sisson, William Slaton*

Department of Physics and Astronomy, University of Central Arkansas, Conway, AR.

How do sound waves interact and move through different materials? This is a question that concerns NASA's Johnson Space Center when trying to minimize the excess noise in manned spacecrafts. Numerous potentially flight-approved materials and some of the necessary laboratory equipment were sent to UCA in order to help answer this question. A technique requiring a cylindrical tube and two microphones was implemented to essentially determine how much sound gets absorbed into a certain material at various frequencies. This can be used to decide which material is optimal to diminish noise at a certain frequency. In addition, density considerations were taken into account to possibly minimize the cost of sending these into space. Further, this research would be very useful in determining the choice of materials used in auditoriums, concert halls, classrooms, etc. For example, an instructor would not want a classroom in which it is difficult to hear because of reverberations of their voice. Though the original motivation for this research applies to spacecrafts, it can be easily directed to situations and environments that are closer to home.

Protecting humanity, one flying space rock at a time

Jeremy Ward and Jeff Robertson*

Department of Physical Sciences, Arkansas Tech University,
Russellville, AR

We provide astrometry observations of minor planets designated Near-Earth-Object Potentially Hazardous Asteroids (NEO-PHA). Follow up observations of these objects, both newly discovered and those with poor orbital parameters, are obtained analyzed and processed to yield astrometric positions. Our asteroid astrometry results in improved accuracy of their orbits and lessens the chance of losing track of them resulting from lack of timely follow-up observations after initial discovery. The astrometry is also used to accurately determine their long-term trajectories and Earth impact hazard probabilities. These observations support NASA in fulfilling its congressional mandate to identify potentially hazardous space objects and can also help in solar system mission planning. But really, we do it for humanity.

Investigating the mechanical properties of medicinal microbubbles

Kristin Kovach^a, Gregory J. Salamo^a, Michael J. Borrelli^b

^aUniversity of Arkansas, Department of Physics, Fayetteville, AR; ^bUAMS, Department of Radiology, Little Rock, AR

Microbubbles are being investigated as a novel technique for breaking apart blood clots, for selective drug delivery, and to increase permeability in the body. When ultrasound is applied to the bubbles inside the bloodstream at a location of interest, the subsequent vibration of the bubbles could allow for blood clots to be physically broken apart or for the drug permeability to increase in that location. The goal of this project is to determine how these bubbles behave when force is applied to them. In order to do this, an atomic force microscope (AFM) is used to press upon individual bubbles. Data collected by the AFM records how much the bubble resists deformation when a probe presses on the bubble. This deformation can be used to determine how much force has been applied to the bubble, and therefore the Young's Modulus of the bubble. This information is useful for the determination of the limits of motion of the bubbles when they are being manipulated within the body.

Tuning magnetoconvective flow for redox-magnetohydrodynamic analytical devices

Preston G. Scrape and Ingrid Fritsch*

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

Miniaturization is a holy grail of modern analytical chemistry because miniaturized analysis entails a favorable decrease in the amount of resources, power, and time required by the analytical procedure. Small-scale devices such as drug tests and blood analyzers require a microfluidic pumping method compatible with the analysis to be performed. Redox-magnetohydrodynamics (MHD), a relatively new pumping method, is a promising addition to the microfluidics repertoire. Our work expands the applicability of redox-magnetohydrodynamic pumping to microfluidic systems by “tuning” the fluid flow produced in a redox-MHD system; in particular we are interested in mixing and catalytic applications.

Our experimental results indicate the power of redox-MHD to transport fluids to anywhere in a microfluidic device, based on the geometry and polarity of electrodes and magnets in the device. In previous work, redox-MHD was used to transport a biological sample from an injection port to an electrochemical analysis site. Subsequent developments allow such a procedure to be performed on a wider selection of samples. The ability to “tune” redox-MHD fluid flow also invites advances in other sample handling procedures: for instance, redox-MHD can combine fluids for catalytic applications, as well as introduce turbulence into the fluid for mixing.

A comparison of the self-organizing map and growing neural gas network performance in the context of handwriting recognition

Kaleigh Clary and Gabe Ferrer*

Mathematics & Computer Science Department,
Hendrix College, Conway, AR

The self-organizing map (SOM) is capable of great performance in handwriting recognition. As such, it has become a benchmark in machine learning—particularly in handwriting recognition. In spite of its popularity, it does have some significant shortcomings. The growing neural gas network (GNG) is an alteration of the SOM that was developed to address these shortcomings. Both networks correctly identified 100% of drawings with a small number of letters (2-3). As the number of letters increased, however, the GNG outperformed the SOM. At eight letters, the SOM correctly identified 76% of drawings. The GNG network correctly identified 90%. The GNG also completed training much faster than the SOM. With a small (2-3 letters) data set, the SOM and GNG are both quick to train at about 2 seconds. With a larger data set (eight letters), the SOM takes 15-30 seconds to train, depending on the size of the map, while each GNG network takes 3 seconds to train. The results clearly indicate that the growing neural gas algorithm is the superior method for classifying letter drawings. It outperforms the SOM in both speed and accuracy.

Quality dimensions of e-science platforms: content analysis approach

Dimond Hawkins and Samar Swaid*

Department of Applied Mathematics and Computer Science
Philander Smith College, Little Rock, AR

This work focuses on identifying the quality of e-science platforms through content analysis to the Extreme Science and Engineering Discovery Environment (XSEDE) and the National Center for Biotechnology Information (NCBI) projects. Based on literature review and content analysis of the features and services offered by XSEDE and NCBI, we find that e-service quality can be measured on the dimensions of: accessibility, communication, competence, courtesy, credibility, reliability, responsiveness, security, usability, and learnability. This is the first phase in a multi-layered project that aims to understand quality dimension of e-science projects to meet the needs of the scientific and the academic communities. The study provides a number of implications for theory and practice of software engineering and human-computer interaction field *This study was supported, in part, by a grant from NSF/HBCU-UP award no. 238895; 0625410J.*

Proposing a new TEXT-based CAPTCHA

CeDale Smith, Terecia Jones, Samar Swaid*

Department of Applied Mathematics and Computer Science,
Philander Smith College, Little Rock, AR

CAPTCHA stands for Completely Automated Public Turing Test to Tell Computer and Human Apart. It is the test that human can pass easily but computer cannot. For example, humans can read distorted text, but current computer programs cannot. As more services are offered free via websites such as Google, Yahoo and Facebook, more people register to different service providers. However, intelligent CAPTCHAs are needed to prevent hackers from registering to these websites via bots. CAPTCHAs have proven very useful for many reputable, Web-based email and application service providers, including social networking sites and online auction sites, for the purpose of deterring automated registration. CAPTCHA methods varied in their methods and approaches (e.g., text, image, audio ... etc). This project attempts to provide a new text-based CAPTCHA based on drawing lines as the main distortion method. The Proposed CAPTCHA is compared to other existing text-based CAPTCHAs. We provide implications and areas for future research.

Usability of text-based CAPTCHA

Terecia Jones, CeDale Smith and Samar Swaid*

Department of Applied Mathematics and Computer Science
Philander Smith College, Little Rock, AR

The adoption of Completely Automated Public Turning Tests to Tell Computers and Humans Apart (CAPTCHA) to differentiate between humans and computers is an increasingly adopted practice by websites. One of the most familiar of these CAPTCHAs is to ask users to type in some sequence of distorted but common characters, what we term here text-based CAPTCHA. However, these text-based CAPTCHAs are found to be unusable and difficult to interpret, even for humans with near perfect vision. This study aims to investigate usability issues in the widely adopted text-based CAPTCHAs. We develop a scale to measure the usability on dimensions of: (i) distortion; (ii) content; (iii) presentation; and (iv) convenience. Survey instrument and screen capture software are used to collect data from 85 users. An exploratory factor analysis and equation modeling are applied to test the dimensions proposed to measure CAPTCHA's usability. The study offers its implication for research and practice and provides its guidelines in designing usable text-based CAPTCHAs. *[This study was supported, in part, by a grant from NSF/HBCU-UP award no. 238895; 0625410]*

Acute Effects of Exercise on Cognitive Functions in Older Adults

Rachel Pennington, Shellie Hanna,* and S. Kirkconnell*

Biological Sciences Department, Arkansas Tech University,
Russellville, AR

The primary focus of this study is to test the effects of acute aerobic exercise on cognitive functioning of adults over the age of 60. A second purpose is to emphasize that the positive neurological effects of exercise can start taking place immediately and that strenuous 6-month programs aren't the only way to get positive results. This is important because it encourages older adults to maintain active lifestyles in order to prolong high-quality life. We hypothesize that memory retention, mental processing speed, and selective attention acutely improves after exercise.

Participants completed a timed Stroop test to evaluate cognitive performances both before and after exercise. Results before and after exercise were compared, and all participants completed the post-exercise test with improved scores ($p=0.000$). Cognitive performance was significantly enhanced post exercise. Our results show that exercise acts immediately to promote mental health and wellbeing.

Effect of chickpea and white bean puree as a fat replacer in cheesecake

Holly Imes and Lisa Ritchie*

Department of Family and Consumer Sciences, Harding University, Searcy, AR

The purpose of this experiment was to determine the effects on color, texture, flavor, density, weight, height, viscosity, and overall consumer acceptance of cheesecake when replacing the fat with 50% white bean puree and with 50% chickpea puree with xanthan gum. Obesity is a growing problem in the United States, and a diet high in fat is a leading contributor. By replacing half of the cream cheese in cheesecake with a legume puree, the caloric and fat content decreased substantially. The products were evaluated by a test group using a score card that focused on texture, flavor, color, density, and appearance. Then the researcher conducted objective tests as well. Overall, the control proved to be the most desirable product in all categories. Next, Variation 1 (White Bean Puree) came in second; every category received over 50% in rating 1 or 2. Variation 2 (Chickpea Puree) was unacceptable to 98% of the test group. Considering the data, substituting up to 50% of the cream cheese with white bean puree would be an acceptable way to decrease the fat content in cheesecake.

Chia: a little seed with big benefits

Danielle Morton and Lisa Ritchie*

Department of Family and Consumer Sciences, Harding University, Searcy, AR

Cardiovascular disease is now the leading cause of death in the United States (Remig, et. al, 2010). The Centers for Disease Control and Prevention recorded that 599,413 died from heart disease in 2009. Cardiovascular disease is most commonly a consequence of obesity due to a high fat diet. These overwhelming statistics of those dying due to this fat-enriched lifestyle makes fat one of the most researched topics in food science. The problem with reduced fat products is that consumers are not willing to sacrifice the pleasing characteristics that accompany products high in fat (Sharp, 2001).

The purpose of this study is to investigate the physical, textural, and sensory properties of spice muffins when replacing margarine with chia seeds at two different levels. Chia seeds were used to replace 25% and 75% of the margarine in muffins. A group of panelists rated the muffins using a scorecard. Objective tests compared the volume, weight, height, and batter viscosity of the three products. Substituting chia seeds with margarine decreased the fat content as well as adding important nutrients such as omega-3 fatty acids. Replacing margarine with chia seeds is an acceptable method to decrease fat content and increase the nutritional value in baked goods.

Can you smell that fruit?

Trevor Drury, Ed Wilson*

Department of Chemistry, Harding University, Searcy, AR

Because the economy of northeast Arkansas relies heavily on agriculture, any advancement which speeds up the harvesting process would be a benefit to farmers. Detecting when fruit is ripe for market would be an economic advantage for producers and consumers. The purpose of this research was to see if there was a way that technology could be used in this process.

As fruit begins to ripen, it releases a gas called ethylene. The riper the fruit the more ethylene it produces. By using a gas sensor, the amount of ethylene given off by the fruit could be measured. Therefore, the focus of the experiment centered around whether or not a computer controlled gas sensor could be developed to measure ethylene and thereby determine if the fruit was ready for harvest.

The development of this ethylene sensor would help farmers detect the optimal harvesting time and for the canning industry to determine when fruit is no longer viable.

Fermi resonance effects in fourier transform infrared (FT-IR) spectroscopy for carbonyl compounds

Brandon Merriweather, Terry Anderson, Kayla Kimbrough, Frank Hahn*

Department of Chemistry, Division of Natural and Physical Sciences, Philander Smith College, Little Rock, AR

The radiation in the infrared (IR) region of the electromagnetic spectrum has been used to gain insights of molecular-level vibrational energy transitions and to understand better and elucidate the molecular structures. If an inherent bond vibration couples with an overtone or combination band in a molecule during the IR absorption process, accidental energy degeneracy in their wave functions occurs, which is called Fermi resonance. This Fermi resonance in IR spectroscopy results in coupled vibration frequencies and frequency shifts. The typical case of the Fermi resonance has been observed in carbonyl stretching vibration, C=O, in a molecule. At the atomic level, this coupling interaction is due to an overlapping of the p orbitals. The carbonyl stretching vibration, C=O, in a molecule has been also known to be affected by solute and solvent interaction. In this study, selected carbonyl compounds (e.g. benzoic acid, sodium benzoate, benzophenone, 2-pentanone, n-heptaldehyde, etc) have been radiated by FT-IR and Attenuated Total Reflectance (ATR) Fourier Transform Infrared (FT-IR) spectrometers to investigate quantum chemical Fermi Resonance variations in absorption frequencies of the analytes with obtaining detailed structural information. With a conventional FT-IR spectrometer, Fermi resonance was observed for ketones, a salt form of carboxylic acid, and aldehyde. However, the compound having a carboxylic acid group didn't show the Fermi resonance. These spectra by the conventional FT-IR will be compared to the ones by ATR-FT-IR to further investigate the instrument selectivity for this Fermi resonance effect.

Searching for beetles (Coleoptera: Scarabaeidae and Histeridae) associated with the dung of native Arkansas mammals

Bo Kelley^a, John L. Hunt^a, and Matthew B. Connior^b

^aUniveristy of Arkansas at Monticello, AR

^bSouth Arkansas Community College, El Dorado, AR

Beetles are important ecological components of natural ecosystems. One primary function is the fragmentation and recycling of animal dung. Two of the families of beetles associated with dung are Scarabaeidae and Histeridae. Scarab beetles fragment and bury excrement, while Histerid beetles prey on organisms living within these habitats (*i.e.*, dung). Little is known about the ecological impact of beetles associated with the dung of mammals native to Arkansas. Thus, we surveyed the dung of native mammals within Arkansas to determine the species and distributional patterns associated with dung. We opportunistically searched and collected beetles *in situ* from the dung or nests of native mammalian species within Arkansas. We also set simple pitfall traps using dung of various Arkansas mammals as bait. Preliminary results of our survey are presented.

Low susceptibility of invasive Indo-Pacific red lionfish (*Pterois volitans*) to a common Caribbean ectoparasite

Starlene M. Loerch,^a Amber McCammon,^{b*}
Paul C. Sikkell^a

^aDepartment of Biological Sciences, Arkansas State University, Jonesboro, AR

^bUniversity of the Virgin Islands, St. Thomas, VI

The enemy release hypothesis proposes that introduced species can become invasive by leaving behind natural enemies (predators, competitors and parasites) when they are introduced to a non-native habitat. Indo-Pacific red lionfish, *Pterois volitans*, are one of the most devastating species invasions to occur in the tropical Atlantic Ocean (Albins & Hixon 2011). The goal of this project was to test the susceptibility of red lionfish to a common Caribbean parasite, the monogenean capsid, *Neobenedenia melleni*. Fish were placed in the overflow of an oceanarium containing large numbers of *N. melleni* larvae. Despite exposure to high concentrations of the parasite, only a single parasite was found on one lionfish. Our findings thus far suggest that *Pterois volitans* is highly resistant to infection by *N. melleni*.

Mimicry in scarlet snakes

Christopher K. Akcali and George R. Harper*

Hendrix College, Biology Department, Conway AR

Batesian mimicry occurs when a palatable species mimics the color pattern of a dangerous species and thereby benefits from a predator's instinctual avoidance of the mimicked color pattern. The non-venomous scarlet snake is presumed to be a Batesian mimic based on the fact that its red, white, and black body bands closely resemble the red, yellow, and black body bands of the eastern coral snake and the Texas coral snake with which it co-occurs. Batesian mimicry theory predicts that geographical variation in the resemblance between mimics and models should reflect geographical variation in the relative abundance of mimics and models. To determine whether scarlet snakes vary in their resemblance to eastern and Texas coral snakes throughout their geographical range, photographs of preserved scarlet snakes (917), Texas coral snakes (328), and eastern coral snakes (344) collected throughout the geographical range of each species were taken and the amount of color on each snake was measured. The results suggest the possibility that the presumed scarlet snake mimic may not actually be benefiting from mimicry, especially in regions such as Arkansas where coral snakes are known to be absent.

Comparative analysis of venom from venomous snakes native to Arkansas

Sloane Zimmerman, Jessica Hook, and Randall Kopper*

Chemistry Department, Hendrix College, Conway, AR

Venom toxicity results from the combination of effects caused by protein and small peptide components selectively expressed in the venom glands, which have specific activities that contribute to subdue, kill, and/or digest the prey. Little is known about variations in venom protein components from snakes of the same species.

Most published investigations of snake venom components combined venom from multiple individuals. That provides larger samples for analysis, but often masks individual differences. Therefore, variations between individuals and between subsequent samples from the same snake have rarely been observed.

This study involves the analysis and comparison of venom from individual snakes in order to detect these differences. The volume, total protein concentration, electrophoretic profile, and specific enzyme activity of venom samples were analyzed from coralsnakes of similar size and ecological habitat.

These results suggest that protein concentrations and enzyme activities obtained from pooled samples represent only an average of highly variable individual components. This underscores the importance of understanding the variation among individuals in order to understand the significance of any differences found as the result of environmental or ecological factors. Knowledge of variation at the individual level will become increasingly important for understanding the ecology and evolution of snake venoms.

Status and dispersal of the exotic eurasian collared-dove (*Streptopelia decaocto*) in Arkansas

Jessie N. Cunningham and Ragupathy Kannan*

Department of Biology, University of Arkansas at Fort Smith, AR

The exotic Eurasian Collared-Dove (ECD) was first sighted in Arkansas at Harrison on 25 June 1989. Since this initial sighting the species has grown in numbers and is now present in 42 of 75 counties throughout the state. Using the national Christmas Bird Count (CBC) online database, I tracked the numbers and dispersal of this species from 1997-98 to 2011-12. ECD numbers showed a general upward trend with some fluctuations. The number of counties in the state reporting ECDs on CBCs has increased steadily since 1997-98. I plotted a state map for each of these years and showed presence-absence information for all CBCs in the state which recorded the species. In a 5-year time span, the species dispersed from the southeast corner of the state to the northwest corner, a distance of approximately 500 kms. With a dispersal rate of 100 kms/year, this exceeds the previously demonstrated dispersal rate of 45 kms/year for the species in Europe. I therefore predict that the species will soon cover most of North America at a faster pace than it colonized Europe.

Histochemical organization of the dorsal thalamus in the nine-banded armadillo (*Dasypus novemcinctus*)

J. Fletcher, B. Moffitt, C. Sherwood, N. Scroggins, J. Padberg*
Department of Biology, University of Central Arkansas, Conway, AR

Most comparative neurobiological studies of mammals have focused on species within five of the six mammalian superorders. However, there remain gaps in our understanding of the organization of mammalian sensory systems, which will only be filled by examining representative species from all six superorders. Notably, the neural organization of members of Xenarthra remains largely unexamined. The nine-banded armadillo, a member of Xenarthra, constitutes an excellent model for studies of evolutionary neurobiology. We are currently examining the functional organization of sensory areas in the armadillo with recording techniques in order to generate a map of sensory cortices. We are also examining the neuroanatomical organization of the armadillo thalamus using classical (Nissl) and modern (cytochrome oxidase) staining methods. In cytochrome oxidase series, the medial ventroposterior nucleus shows moderate to dense staining and is relatively homogenous, while the lateral ventroposterior nucleus is densely stained and interrupted by small fiber bundles. The ventrolateral nucleus is lighter and very homogenous. While generally in support of the earlier parcellation, these divisions are very clear in CO stained tissue. Through these ongoing studies, we will gain insight into the evolution of mammalian brains and how morphological differences between Xenarthran and Epitherian species translate into distinct neural organization.

Are the Sky Island pines unique?

Adam Bigott and Ann Willyard*

Biology Department, Hendrix College, Conway, AR

There are about 17 species in subsection *Ponderosae* (Pinaceae), mostly from the mountains of Mexico. Many botanists suspect that there are additional unrecognized species within the broadly described *Pinus ponderosa* in the United States. The Sky Islands are a collection of isolated mountains arising from the desert of the American southwest and potentially home to one of these hidden species. Some distinguishing features suggest that the Sky Island ponderosa are distinct from the ponderosa pines in the Rocky Mountains and from the large pine forests of the southwest. Chloroplast DNA was isolated from 339 individuals representing 12 populations from the Sky Islands and their potential relatives, including geographically overlapping *P. arizonica*. Using variable and genetically informative repetitive DNA sequences and clustering algorithms, we created a visual representation of the genetic variation. We also used Ecological Niche Modeling based on 19 biologically meaningful climate variables to test if the geographic distribution forms a distinct habitat. We discuss the usefulness of considering both molecular and ecological criteria to support species delimitation questions: *i*) are the Sky Island pines a unique species; or *ii*) are the Sky Island pines, as well as the ponderosa pines of the American southwest, a single species?

Molecular genetic survey of extremophile microbes from Blanchard Springs caverns, Arkansas

Mark Castleberry^a, Shannon Fiser^a, Jonathan Shields^a, Lauren Story^a, Charlotte Wetzlar^a, Claudia Gonzalez^b, James Engman^{a,*}

^aDepartment of Biology, Henderson State University, Arkadelphia, AR ^bNicholas School of the Environment, Duke University, Durham, NC

Microbes are increasingly considered important members of cave communities, facilitators of cave formation, and agents of disease, including white nose fungus, responsible for the death of millions of bats across North America. This project is using molecular genetic techniques to survey the bacterial flora of Blanchard Springs Caverns, Arkansas. Although considered the most biologically diverse cave in the Ozark Plateau, no previous survey of its microbes has been published. Samples from undeveloped reaches of the caverns were plated on selective media, with resulting cultures stored at -80°C. A conserved region of ribosomal DNA (18S subunit) from these colonies was amplified by polymerase chain reaction (PCR) and sequenced using universal bacterial primers. Sequences were compared with those in the GenBank database using the BLASTN program, allowing identification to genus and species level. This survey has resulted in identification of 12 taxa, including rare and unusual species. *Aminobacter lissarensis* and *Oerskovia enterophila* are previously unknown from North America. *Rhodococcus erythropolis* and *Pseudomonas putida* are documented degraders of numerous hydrocarbons. Some species of *Bacillus* and *Pseudomonas* isolated are not consistent with any published sequences, and work is proceeding to determine if these are new to science.

The effect of riparian zone alterations on the levels of macroinvertebrate “shredders” and “grazers” in Sager Creek, a first order stream

Neil Miller, London Smith, Timothy Wakefield*

Division of Natural and Health Sciences, John Brown University, Siloam Springs, AR

The upper reaches of Sager Creek in Siloam Springs, AR should be classified as a first order stream according to the River Continuum concept. According to this concept, the benthic macroinvertebrate assemblage should be reflective of the proportionally high levels of allochthonous detritus contributed by a substantial riparian vegetation. Specifically, invertebrates classified into the “shredders” group should be proportionally higher than those classified as “grazers”. However, the biota of Sager creek could be skewed due to heavy land development in the riparian zone of the stream, allowing more sunlight into the creek than would be seen in a typical first order stream, thus increasing the amount of photosynthetic activity in the stream. Using samples of macroinvertebrates collected over a three year period, the biota of the headwaters of Sager Creek were analyzed to see how closely it mirrors a typical first order stream as predicted in the River Continuum Concept.

Analysis of water samples for the presence of mercury at historical mining operations in Clark County Arkansas

Zabrina Ruggles, Austin McKown, T. David Bateman*

Department of Chemistry, Henderson State University, Arkadelphia, AR

Mercury content was analyzed in various sites throughout Clark County Arkansas implementing the EPA approved Manual Cold Vapor Technique. Locations include but were not limited to different sites along the Ouachita, Caddo, and Antoine rivers, as well as the historical logging town of Graysonia. Historical data pertaining to mining locations and dates was considered when collecting data, as well as current weather patterns, which may influence current Mercury concentrations. A Buck Model Buck 410 Mercury Analyzer was used for sample analysis. Sampling location sites were recorded and topographically mapped through the use of a Garmin eTrex HC series personal navigator. Obtaining current and accurate data pertaining to the mercury content of Clark County water sources is important to the safety of the residents and ecosystems.

Role of PDR13 ATP-binding cassette transporters in arsenic sequestration

Nalita Holt,^a Anissa Buckner,^a Sathish Kumar Ponniah,^b and Muthusamy Manoharan^b

^aDepartment of Biology, ^bDepartment of Agriculture, University of Arkansas at Pine Bluff, AR

Among heavy metals, arsenic (As) is an extremely toxic metal which adversely affect plants, animals, and human beings. In Arkansas, the rice field has cotton growing history, and there are higher residual As in the soil due to usage of pesticides. Rice grain from arsenic contaminated field has been found to contain elevated levels of arsenic. Therefore it is very important to reduce arsenic uptake in rice. Arabidopsis contain approximately 130 ATP-binding cassette transport proteins (ABC); which includes PDR (Pleiotropic Drug Resistance) and MRP (Multi-drug Resistance Protein) gene subfamilies. The ABC proteins are known to sequester toxic materials from the plant; therefore we are interested to know the role of ABC protein genes in arsenic sequestration in Arabidopsis. The mutants were screened for the presence or absence of the gene. Full length *AtPDR13* gene was cloned and over-expressed in Arabidopsis to test arsenic sequestration. The selected mutant lines along with wild type, *AtPDR13* over-expressed, *AtPDR13* RNAi were cultured on the half strength MS medium with sodium arsenate. The fresh and dry weights of both shoots and roots from wild type, mutants, *AtPDR13* over-expressed and *AtPDR13* RNAi lines will be recorded to understand the effects of arsenic on Arabidopsis.

Determination of bioactivity in *Ilex decidua*

Cynthia Holland and Martin J. Campbell*

Department of Chemistry, Henderson State University,
Arkadelphia, AR

Plants have been used for medicinal purposes for thousands of years and many people still use primitive medicines today. Most plants, however, remain unexplored. One such example is *Ilex decidua* (Aquifoliaceae), or the deciduous holly, which grows wild in the Southeast United States, including much of Arkansas. Recently literature reports indicate other hollies in the genus *Ilex* (Aquifoliaceae), for example, *Ilex vomitoria*, or the yaupon holly, have shown cytotoxic, anti-inflammatory, or chemopreventative activity. Also, ursolic acid, a known cancer cell growth-inhibitor, was found in the berries of *Ilex verticillata*. In view of evidence of anti-cancer bioactivity in other *Ilex* species, the deciduous holly was chosen for investigation. Samples of twigs, leaves, and berries were collected in southwest Arkansas. We report our initial sample preparation and compound isolation findings.

Towards the synthesis of Antascomicin B: a beneficial natural product

Kaneshia D. Day, Matthias C. McIntosh, Dharma T.
Nannapaneni, Brian L. Walker

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

As our population continues to age, Alzheimer's Disease and other neurodegenerative diseases become more prevalent. With no cure and few medications to treat these diseases, the demand for research to provide a cure or a more effective treatment is great. A natural product, a chemical compound produced by living organisms, called Antascomicin B has been considered for treatment of neurodegenerative diseases such as Alzheimer's when bound with a protein called FKBP12 which can aid in the regeneration of neurons. By devising an effective synthesis of Antascomicin B, it can be produced on a large scale to further test its effectiveness in treating neurodegenerative diseases, and can then be formulated into a useful medication. Not only will this allow a natural product to be created over a synthetic one, but the process also utilizes "green" chemistry which is better for the environment. In finding an effective total synthesis for this natural product, this can possibly provide insight for other syntheses of natural products that can be effective in treating other diseases.

Allylic diazene rearrangement approach to C-C bond formation in natural product synthesis

Katarina Bejarano, Savannah Stevens, T. David Bateman*

Department of Chemistry, Henderson State University,
Arkadelphia, AR

The synthesis of aromatic bicyclic compounds via an allylic diazene rearrangement (ADR) is described. Commercially available aromatic aldehydes are introduced to toluenesulfonylhydrazide and acetic acid catalyst to yield the corresponding hydrazones. The hydrazones are reduced to hydrazines by catecholborane at low temperature. The resulting compounds are treated with pyridine to eliminate the sulfinic acid and yield the allylic diazene intermediate. Upon rearrangement, the aromaticity of the substrate is disrupted producing a reactive isoaromatic species which will react with olefins via 2+2 addition. This methodology provides a facile route to C-C bond formation, and will be used in natural product total synthesis.

Synthesis of amino acid radical precursors

Claire Desrochers, W. Ryan Parker, Jordan Wilkerson,
K. Nolan Carter*

University of Central Arkansas Department of Chemistry,
Conway, AR

Free radicals are important intermediates in the damage of biological molecules such as proteins. There is evidence that protein radicals can transfer damage to DNA, a process which could cause mutations and possibly cancer. Mutated DNA can also lead to cell death, which can ironically be beneficial to a cancer patient by targeting his or her tumor cells. In our research, we are synthesizing amino acid derivatives that contain a carbon-selenium bond. This bond can be cleaved by ultra violet (UV) light to produce specific amino acid radicals. Because proteins are merely a combination of many amino acids, a single amino acid radical can serve as a model for the larger, damaged biomolecule. The synthesis for one such amino acid radical precursor is currently being optimized. Furthermore, work is currently underway toward the synthesis of other selenium-containing derivatives of the amino acids phenylalanine and valine. These compounds are being prepared from reductive amination of the corresponding α -oxoesters.

Oxidative stress and its relationship to Arkansas agriculture and human disease

Stephen Raines, Kristen Johnson, Nathan Reyna*

Department of Biology, Ouachita Baptist University,
Arkadelphia, Arkansas

At Ouachita Baptist University we have created genetically modified plants that serve as a model system for understanding the role oxidative stress plays in human disease development and prevention. Interestingly, our system was originally created to help Arkansas agriculture and is also used to study how crops respond to disease in the field. While one may think plants and animals are very different, a recent study found that almost 70% of the genes related to cancer and disease in humans were also found in plants. The similarities between plants and animals are especially strong in relation to how their cells respond to oxidative stress. As a result of these similarities, we have expanded our research to include aspects of human health. Through funding by the Arkansas Space Grant Consortium/NASA and AR-INBRE program, we have begun to identify new signaling pathways associated with relieving oxidative stress and the prevention of cell damage. Once identified, these pathways become targets for new drug discovery. In the context of understanding areas of importance to human health and agriculture, students at OBU are given the opportunities to participate in intensive training activities in molecular biology, physiology, and biotechnology.

Development of transgenic rice plants

Cameran Faucette,^a Anissa Buckner,^a Sathish Kumar Ponniah,^b and Muthusamy Manoharan^b

^aDepartment of Biology, ^bDepartment of Agriculture, University of Arkansas at Pine Bluff, AR

Isoflavones play an important role in human health as a dietary component. Consumption of Isoflavones is associated with health benefits such as decreased risk of heart disease, reduced risk of some hormone related cancers. Rice is one of the most important grains with regard to human nutrition but it does not naturally produce flavonoids. Synthesis of Isoflavones in rice may enhance its dietary value. Isoflavonoids are synthesized as a part of the phenylpropanoid pathway, and one of the key enzymes in the phenylpropanoid pathway is chalcone synthase (CHS), which catalyzes the formation of the central intermediate, naringenin chalcone. Therefore, our main objective was to transform soybean chalcone synthase gene (CHS) into the rice genome using *Agrobacterium*-mediated transformation. Sixteen transgenic lines were generated from the callus on hygromycin-containing medium. The results of the southern blot and PCR analyses showed that the CHS transgene was stably integrated into rice genome and also stably inherited to their progenies. RT-PCR analysis confirmed that CHS was expressed in T2 progenies of each transgenic line. Transgenic plants were normal and fertile.

Sequence analysis of conserved baculovirus genes in plodia interpunctella granulovirus

Josh Morgan, Victoria J. Bennett, Thomas J. Galliguez, Joel Funk*

Biology Department, John Brown University, Siloam Springs, AR

Baculoviruses are large double stranded DNA viruses that are divided into two groups: granuloviruses (GV) and nucleopolyhedroviruses (NPV). This group of viruses has been used for a number of applications, including insect control, gene therapy, and the production of recombinant vaccines. Three different highly conserved genes have been found in baculovirus genomes: late expression factor 9 (lef-9), late expression factor 8 (lef-8), and polyhedrin/granulin (pohl/gran) (Jehle et al. 2006). Because these genes are highly conserved, comparing nucleotide sequences for these genes in different baculoviruses is useful when constructing a phylogenetic tree. The purpose of this study was to detect and amplify three conserved baculovirus genes (lef-9, lef-8, and pohl/gran) in the *Plodia interpunctella* granulovirus (PiGV) and determine how they were related to the same genes in other baculoviruses. The DNA from PiGV was purified and amplified with polymerase chain reaction (PCR) using degenerate primers. After running the PCR product on an agarose gel, the PCR product on the gel was purified and sequenced. Bioinformatic software was then used to analyze the sequence and construct a phylogenetic tree. This phylogenetic tree allowed the relationship of PiGV to other baculoviruses to be determined.

Function of a dual gene in growth and tumors

Shana Chancellor and Mary Stewart*

School of Mathematical and Natural Sciences, University of Arkansas at Monticello, AR

Many human disease genes are conserved with *Drosophila melanogaster* (fruit fly) genes, including those that cause a set of human conditions called ribosomopathies. Ribosomopathies are characterized by pathologies such as anemia, skeletal defects and predisposition to some types of leukemia. Many types of ribosomopathies are caused by mutation of a ribosomal protein gene. In *Drosophila*, mutation of ribosomal protein genes causes abnormalities such as delayed development, small adult size, reduced fertility and in a few cases, tumorous growth. Because *Drosophila* is a valid model for understanding human disease and is easily manipulated, we are studying the *Drosophila* ribosomal protein S6 (*RpS6*) gene. The *Drosophila RpS6* gene is actually a “dual gene” in that it codes for a ribosomal protein as well as a small nucleolar RNA (snoRNA). In a strain of flies called *hen*², which have a mutation in the *RpS6* gene, a variety of abnormalities occur including delayed development, death and hematopoietic tumors. The goal of our research is to test the hypothesis that each component of the *RpS6* dual gene makes distinct contributions to the abnormalities seen in *hen*² flies. Using the simple model system of *Drosophila* to understand how reduced expression of a ribosomal protein or a snoRNA causes abnormalities could provide information that may be applicable to humans.

Promoter methylation and gene profile expression in systemic lupus erythematosus (SLE) patients

Jarren Oates,^a Beverly Word^b and Beverly Lyn-Cook^b

^aDepartment of Biology, University of Arkansas at Pine Bluff, AR

^bNational Center for Toxicological Research, Jefferson, AR

Systemic lupus erythematosus is a multifactorial autoimmune disease that affects women at a 9:1 ratio when compared to men. In addition, women of specific ethnic groups, such as African Americans, Hispanic/latinos, Asia and Native American, have a higher incidence when compared to European Americans. Pathogenesis of lupus remains unknown, however emerging data are beginning to show that aberrant epigenetic mechanisms may play a central role in its onset and progression. Our hypothesis is that specific genes involved in cytokine production will be expressed at higher levels in lupus patients compared to non-lupus patients. Furthermore, the expression profile will be regulated through epigenetic mechanisms. Using a cytokine production DNA methylation PCR array, this study demonstrated that Foxp3 promoter showed an increased methylation profile, while ELANE gene showed a decreased methylation profile in lupus patients compared to age-matched non-lupus patients. The gene profile expression array revealed three genes with a significant increase in expression, IL-18, TNFSF13B (BlyS) and FASLG. Increased methylation of the Foxp3 gene suggests inactivation of Foxp3. Decreased expression of Foxp3 gene has been noted in another autoimmune disease, rheumatoid arthritis. These studies further suggest that epigenetic mechanisms may play an important role in lupus onset and progression.

Progress towards synthesis of novel RNA phosphoramidite monomer protecting groups

Kenda Syler, Seth Jones, Rachael Kew, Wezley Griffin,
Vincent Dunlap*

Department of Chemistry, Henderson State University,
Arkadelphia, AR

With the explosion of new research in the field of RNA, a significant demand for synthesis of oligoribonucleotides has materialized thus allowing the phosphoramidite method to become a very valuable tool in biochemical research. As a result, the demand for synthesis of phosphoramidite monomers has increased. However, there is a lack of selectivity between the 2'- and 3'-hydroxyl groups in RNA for phosphite addition, resulting in a reduction in efficiency of synthesis. Silyl protecting groups have been developed to improve selectivity for the 2'-hydroxyl; but, in order to obtain the greatest utility, yields of the monomer still need to be improved. In order to improve these yields, we have developed structural analogs of the 5'-hydroxyl protecting group dimethoxytrityl (DMT) which contain linker arms aimed at improving selectivity for 3'-hydroxyl phosphitylation. Synthetic methods for assembly of the protecting groups as well as additional developments are presented.

Intratumoral chitosan/IL-12 neoadjuvant to tumor resection reduces breast cancer metastasis

Jimmy N. Vo, Lirong Yang, David A. Zaharoff*

Department of Biomedical Engineering, Laboratory of Vaccine and Immunotherapy Delivery, University of Arkansas, Fayetteville, AR

Interleukin-12 is a potent antitumor cytokine that exhibits significant clinical toxicities after systemic administration. We have previously shown that intratumoral injections of IL-12 co-formulated with a solution of chitosan can eliminate established primary tumors by maintaining high concentrations of IL-12 in the tumor microenvironment while minimizing systemic exposure.

Because of IL-12's ability to generate tumor-specific cell-mediated immunity, we are exploring the anti-metastatic potential of intratumoral chitosan/IL-12 immunotherapy in a highly metastatic model of breast cancer (4T1). Thus far, we have found that intratumoral chitosan/IL-12 neoadjuvant prior to tumor resection confers a long-term survival benefit. Specifically, mice bearing 4T1 tumors were treated intratumorally with saline, chitosan, IL-12 alone or chitosan/IL-12. Primary tumors were then resected. Mice treated with either saline or chitosan died within 33 days after resection. 20% of mice treated with IL-12 remain alive more than 100 days after resection. 63% of mice treated with chitosan/IL-12 remain alive more than 100 days after resection. In addition, 80% of previously cured mice were protected from tumor rechallenge. Furthermore, toxicological studies indicate that chitosan/IL-12 does not adversely affect leukocyte levels or hematocrit. Based on data obtained thus far, intratumoral chitosan/IL-12 shows promising potential as a neoadjuvant immunotherapy to reduce metastatic disease.

Characterization of Na⁺-dependent dicarboxylate transporter (NaDC) in bovine brain Microvessel endothelial cells (BBMEC)

Kameron Lee, Kelin Key, Trenton Ware, Antonie H. Rice*

Department of Chemistry and Physic, University of Arkansas at Pine Bluff, AR

The delivery of therapeutic drugs to the brain continues to be a challenge for the pharmaceutical industry. The blood-brain barrier (BBB) regulates the influx and efflux of a wide variety of substances, and remains the major obstacle in the delivery of drugs to the central nervous system (CNS). Various strategies have been devised to circumvent the BBB in order to increase drug delivery to CNS. The purpose of this work was to assess the potential mechanistic pathways present at the Blood-brain barrier in bovine microvessel endothelial cells (BBMECs) and to demonstrate that active transporters exist at the BBB that may provide alternative routes for delivering therapeutics to the brain that may exhibit poor brain/CNS bioavailability, and to also assess the potential mechanistic pathway of a newly synthesized taxane, TX-67, across the BBB. The following work demonstrates the presence and activity of Na⁺-dependent dicarboxylate transporter (NaDC) in BBMEC cell culture system. To characterize the functionality of the NaDC transporter, typical substrates were selected to perform uptake and transport experiments. The NaDC substrates selected were succinate, glutarate, fumarate, •-ketoglutarate, and maleate. The results demonstrate that the transporter is present and functional in BBMECs. The data also suggest that the enhanced permeation of Tx-67 may be explained by the utilization of the NaDC transporter at the BBB.

Amelioration of rhabdomyolysis-induced kidney failure in mice using metal complexes

Twymenia Liggins,^a Nicholas Braman,^a KeiSharra Eldridge,^a Richard B. Walker,^a Alexei G. Basnakian,^b Grant W. Wangila^a

^aDepartment of Chemistry and Physics, University of Arkansas at Pine Bluff, AR

^bDepartment of Pharmacology and Toxicology, University of Arkansas for Medical Sciences, Little Rock, AR

Rhabdomyolysis is a common clinical and biochemical syndrome that may result from a large variety of diseases, trauma, or toxic insults that damage the integrity of the sarcolemma of skeletal muscle, leading to the release of potentially toxic muscle cell components into the circulation. This may result in potential life-threatening complications of acute renal failure that needs urgent preventive measures to eliminate or reduce the condition. Since rhabdomyolysis is mediated by reactive oxygen species (ROS), the new antioxidant metal complexes of salicylate and aminothiols derivatives would be useful in scavenging the ROS. Two specific aims were accomplished in this study; synthesis of several metal-complexes and cytoprotective activity of the metal complexes in kidney injury in mice. The focus was on ligands, which have or contribute to cytoprotective activity. The ligands from the substituted salicylate and aminothiols were examined. Also the assessment of cytoprotective activity of metal chelates *in-vivo*. The stable water-soluble compounds with the highest antioxidant and cytoprotective activities were tested for cytoprotection against rhabdomyolysis-induced kidney injury in mice. Our data suggest that the cytoprotective properties of these compounds are due both to the ROS-scavenging properties of the ligands and the ability of the chelates to deliver complex to cells. ZnRibCys is more effective in reducing rhabdomyolysis injury as shown by the results of measurement of BUN and serum creatinine.

Characterization of a GTPase effector catalytic domain derivative protein of phosphodiesterase 4D

Hans Wang, Paul Adams*, Reena Chandrashekar

Department of Biochemistry, University of Arkansas,
Fayetteville, AR

The purpose of this study is to characterize the interface of two proteins which play a key role in controlling cell growth: Ras homology enriched in brain (Rheb) and Phosphodiesterase 4D (PDE4D). Rheb is a GTPase which cycles through an active GTP bound state (on) and an inactive GDP bound state (off). Rheb is a regulator protein of the mammalian Target of Rapamycin (mTOR) and regulates cell growth when bound to GTP and has no function when GDP bound. Rheb has been shown to form a complex with the PDE4D class of GTPase Affecting Proteins (GAP). Binding to PDE4D inactivates Rheb by hydrolysis of the GTP to the GDP state. In diseases such as asthma, inflammation occurs which leads to an increased concentration of cAMP, which activates relief enzymes and also disrupts the Rheb-PDE4D complex which leads to an increased amount of free Rheb. This could cause over activation of the mTOR pathway, which could have negative effects. Examination of the binding action and the Rheb-PDE4D complex could yield strategies to stop the disassociation seen in increased concentrations of cAMP. Initial studies will examine a catalytic fragment of PDE4D called the F2 site, and the F2-Rheb complex.

Site-specific incorporation of an extrinsic fluorescence reporter group to characterize protein interactions of the Ras protein Rheb

Padma Mana, Paul Adams*

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

Because structure-function relationships among proteins underlie the chemical and molecular basis of biological processes, a detailed understanding of protein interactions involved in biochemical regulation are important. Rheb (**R**as **h**omology **e**nriched in **b**rain) is a Ras GTPase that cycles between an active GTP form and an inactive GDP form. The biological activity of Rheb is controlled in part by a protein interaction with the **T**umor **S**uppressor **C**omplex protein **2** (TSC2) that stimulates cell growth, through the **m**ammalian **T**arget **O**f **R**apamycin (mTOR) pathway. We plan to characterize the usefulness of extrinsic reporter group fluorescence in monitoring Rheb protein interactions. Rheb will be over-expressed, purified, and then labeled with environmentally sensitive fluorophore succinimidyl 6-[(7-nitrobenz-2-oxa-1,3-diazol-4-yl)amino]hexanoate (sNDB), an extrinsic fluorophore that emits light at a wavelength well-shifted from the intrinsic fluorescence emission maximum of tryptophan in the protein. As sNDB is known to attach to the side chain of lysine, digestive enzyme assays will be performed on Rheb in order to establish if sNDB attaches to one lysine specifically, or if it attaches to other lysines as well. If the latter is the case, we will design site-specific mutations on Rheb to remove lysines where unwanted sNDB reactions occur. We will then begin important protein interactions involving Rheb, using the sensitive fluorescence character of the extrinsic sNDB fluorophore.

Expression of a G-protein coupled receptor in a cell free expression system

Rodney O. Ballard,^a Eric B. Gonzales^b

^aDepartment of Chemistry and Physics, University of Arkansas at Pine Bluff, AR

^bDepartment of Pharmacology & Neuroscience, University of North Texas Health Science Center, Fort Worth, TX

One hurdle in the determination of protein structures is the ability to produce large quantities of pure protein. This problem is compounded when the protein in question is an integral membrane protein. Integral membrane proteins require large volumes of culture (up to 24 liters) and yield lower quantities of properly folded protein. The purpose of our investigation is to determine if a cell-free expression system, one that will produce protein in a 'test-tube', is a feasible substitute to large cell culture. We used the MembraneMax Expression system, from Invitrogen, to generate a carboxyl terminally histidine tagged bacteriorhodopsin, a member of the G-protein coupled receptor family. If bacteriorhodopsin is produced and folded properly, the protein expression system will turn pink in the presence of trans-retinal. We isolated expressed bacteriorhodopsin using metal affinity chromatography and analyzed protein fractions using SDS-PAGE electrophoresis. To observe the protein fractions collected, we concentrated each fraction prior to SDS-PAGE electrophoresis or loaded a larger sample onto the gel. We determined that concentrating the collected fractions or loading larger volumes of the protein fractions to larger protein gels provided sufficient protein for visualization. Further optimization of growth conditions and analysis will be essential before applying this technology to other integral membrane proteins.

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Purification and characterization of novel affinity tag

Emily Crossfield, Srinivas Jayanthi, Suresh Kumar
Thallapuram*

Department of Chemistry & Biochemistry, University of
Arkansas, Fayetteville, AR

Fibroblast growth factors (FGFs) are messenger proteins which regulate key cellular processes such as cell production, cell differentiation, wound healing and tumor growth. Heparin, a highly sulfated polysaccharide, binds to fibroblast growth factors (FGF) and triggers the FGF signaling process. Heparin facilitates the dimerization and activation of the FGF receptor. Large number of proteins containing positively-charged arginine and lysine have high binding affinities to heparin. In the present study, we have developed a novel clone where the fusion protein HCW was overexpressed in *E. coli* with an N-terminus Heparin affinity tag and was subjected to one-step purification using heparin affinity chromatography. The purified Hep-tag, was characterized using various biophysical tools to understand structure and mode of interaction with heparin. Purification of proteins for drug manufacturing can be very expensive with certain methods. This affinity tag has the potential to provide a more cost-effective method for purification of recombinant proteins. Funding for this project was provided by University of Arkansas Honors College, Howard Hughes Medical Institute, and the SURF grant by the Arkansas Department of Higher Education.

Drug discovery through simple analog synthesis and toxicity determination in the undergraduate laboratory experience

Megan Huffstickler, Connor Rayburn, Hunter Wayland,
T. David Bateman*

Department of Chemistry, Henderson State University,
Arkadelphia, AR

Tramadol is an opioid prodrug that exhibits biological activity, along with its O-desmethyl metabolite. The drug has a dual mechanism of action, and varied prescribed and off-label uses. Its metabolite is a μ -opioid receptor agonist, and tramadol itself inhibits the reuptake of serotonin and norepinephrine. We are synthesizing a focused library of simplified analogs, based on tramadol by altering the amino, aryl, and hydroxyl positions. The simplicity of the synthetic procedure will allow us to develop the preparation for the undergraduate organic chemistry laboratory. We will test the toxicity of our analogs in a brine shrimp bioassay that can be carried out by undergraduate biochemistry students. The analogs that exhibit the least toxicity will be subjected to MTT assays, and those with promising activity will receive NCI 60 cancer screenings.

Discovering drug interactions using chemical computer simulations

Shelby C. Cobb,^a Timothy M. Horton,^a Hollyn M. McCarty,^{a,b}
Joseph W. Levy,^{a,b} Lori L. Hensley,^b Grover P. Miller,^c Martin D. Perry, Jr.^a

^aDepartment of Chemistry, ^bDepartment of Biology, Ouachita Baptist University, Arkadelphia, AR

^cDepartment of Biochemistry and Molecular Biology, University of Arkansas for Medical Sciences, Little Rock, AR

Molecular level interactions of drugs with proteins play a critical role in how the human body processes their products. For many drugs, including many currently on the market, a complete understanding of these interactions is unknown. Ajulemic acid (AJA), a synthetic analog of marijuana, is a promising new therapeutic agent for pain and inflammation. Isolated Ewing's sarcoma (ES) cells treated with this novel drug undergo cell death. Experimental data reveals AJA bound to only one protein, PPAR γ , which is not expressed in ES cells. To locate other proteins, a computational approach is taken comparing the geometric shape of PPAR γ to known proteins and determining interactions with AJA. Several proteins of interest include retinoic acid and vitamin D receptors. About 50% of drugs are mixtures of two different forms of the same molecule. Warfarin is a prime example with one structural form metabolizing 1000-fold more effectively. The motivation behind such selective metabolism is likely the arrangement of amino acids, or residues, within the protein. Certain residues steer metabolism based on the drug's 3D structure. Computational approaches help identify the residues responsible in multiple drugs. Several residues show more favorable interaction with one form of a drug. This evidence allows for tailoring of drugs to specific proteins or altering the protein to enhance the drug's effectiveness.

In vitro UGT-mediated metabolism of 5-fluorouracil

Landry K. Kamdem and Julia R. Davis

Department of Pharmaceutical Sciences, College of
Pharmacy, Harding University, Searcy, AR

The compound, 5-Fluorouracil (5-FU), is a widely used drug in the treatment of cancer. It has a narrow range of efficacy, and its metabolic pathways should be better understood to improve the efficacy. In this study, we showed that 5-FU does undergo glucuronidation as a mechanism of detoxification *in vitro* and that 5-FU-glucuronide (5-FU-G) formation is time-dependent.

Ajulemic acid: a potential therapeutic for Ewing's sarcoma

Elizabeth A. Blankenship,^a Ryan K. James,^a Caroline J. Gill,^a Sara E. Huneycutt,^a Amy G. Eubanks,^a Robert J. Griffin,^b and Lori L. Hensley^a

^aOuachita Baptist University Department of Biology, Arkadelphia, AR; ^bUniversity of Arkansas for Medical Sciences Department of Radiation Oncology, Little Rock, AR

Ewing's Sarcoma is a pediatric bone cancer that is highly aggressive, leading to a five-year survival rate of only 30%. Improved therapeutic options are desperately needed. Our research has focused on the use of ajulemic acid (AJA), a synthetic cannabinoid, as a potential therapeutic agent for this and other solid pediatric cancers. Our data demonstrate this compound can successfully kill Ewing's sarcoma cells in vitro and in a novel bioluminescent mouse model. Our data further suggest AJA can limit the migration of tumor cells and endothelial cells (required for new blood vessel formation to feed the tumors). Additionally, we demonstrate the drug's ability to inhibit angiogenesis, the process by which new blood vessels are formed. This should help limit tumor size and decrease metastases. Our current experiments focus on the mechanism by which AJA inhibits this process. Thrombospondin is a protein with known anti-angiogenic properties, whereas vascular endothelial growth factor (VEGF) is a protein known to promote angiogenesis. Using 3-dimensional spheroids, we investigated the ability of AJA to modulate the levels of these proteins in order to elucidate the mechanism by which it inhibits angiogenesis. It is our hope that our collective data provide the rationale for the development of improved therapies for children in Arkansas with Ewing's sarcoma.

Identification of a nucleosomal region required for the proper distribution of the transcription elongation factor Spt16 across transcribed genes in *Saccharomyces cerevisiae*

Hoai-Trang T. Nguyen, William Wharton II, Jennifer A. Harper, Jimmy Dornhoffer and Andrea A. Duina

Biology Department, Hendrix College, Conway, AR

In eukaryotic cells, DNA associates with several proteins to form a compacted structure referred to as chromatin. The basic unit of chromatin is the nucleosome, a particle consisting of a stretch of DNA wrapped around the histone octamer, itself composed of pairs of four core histone proteins: histones H2A, H2B, H3 and H4. In previous studies we described a mutant of histone H3 – H3-L61W – that causes abnormal accumulation of the transcription elongation factor Spt16 at the 3' ends of transcribed genes. We now report that a mutation in histone H4 – H4-R36A – causes a similar defect in Spt16 association with chromatin during transcription. Genetic evidence indicates that the H3-L61W and H4-R36A mutations affect Spt16 function through a common mechanism and an inspection of the crystal structure of the core nucleosome particle revealed that the H3-L61 and H4-R36 residues are located in close proximity to each other. These results suggest that a nucleosomal region defined by H3-L61 and H4-R36 plays a key role in ensuring proper Spt16 interactions with genes. We propose a model in which the region defined by these residues participates in a signal required for Spt16 to properly disengage from genes following the transcription process.

Shape memory alloy thin-films

Anthony Keener, Mete Ozturk, Abhijit Bhattacharyya*

Department of Systems Engineering, University of Arkansas
at Little Rock, AR

Micron-thick Nickel(Ni)-Titanium(Ti) SMA films are being fabricated using a magnetron sputter deposition machine in the Micro-Electromechanical Systems (MEMS) Laboratory in the Department of Systems Engineering. The objective was to fabricate SMA films with a stoichiometry of 50-50 atomic weight % of Ni (Nickel) and Ti (Titanium) respectively. Samples have been fabricated and characterized over a range of DC Power settings with similar parameters to obtain the 50/50 ratio. The parameter we have changed, which has had the most significant effect on the atomic percentage is the DC Power supply for the pure Ti target. The samples with a smaller Ti power setting have continued to be Ni rich. A few more samples will be fabricated to lock down the desired Ti target DC Power setting. It is important to know the deposition rate of the co-sputtering to control the thickness of the film. Experimental data shows a deposition rate of the co-sputtered NiTi to be 1 • m/hr. A desired thickness of 10 to 100 nanometers should be deposited for less than 1 minute to 6 minutes. A good starting point is 6 minutes to confirm a thickness of 100 nanometers and work down to thinner films.

Helping people to relate to information quality

Daniel Pullen, M. Eduard Tudoreanu*

Department of Information Science, University of Arkansas at Little Rock, AR

Big Data is at the core of a computer driven renaissance, growing at a huge rate, and impacting more and more aspects of economy, society, and culture. Data is also gaining complexity, which poses problems in determining and using the quality of this data. Information requires complex feature characterization, and even with data quality tools, end-users may not be able to extract the most value from this data. Our research is looking into various factors of information quality and is characterizing how users, such as analysts and businesses, respond to quality of data. We are using visualization as the interface to present objective and subjective measurements of data quality. One particular application of this concept is in the domain of aeronautics, where more and more data with differing quality is available in the cockpit, but pilots may not be able to take full advantage of this data. To improve the quality of this information we implemented a flight simulator in the CAVE, and are experimenting with visual ways of helping pilots extract more out of the displayed information.

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General information source

<http://campus.murraystate.edu/services/ursa/>
with tips on planning poster-at-capitol events

<http://faculty.uca.edu/wvslaton/ARposters/>

Luncheon Keynote Speaker

Dr. Richard Jacobs
Arkansas Children's Hospital
Research Institute

STEM POSTERS AT THE CAPITOL

Patrick Desrochers
Department of Chemistry
University of Central Arkansas
Conway, AR 72035

Phone: 501-450-5939
Fax: 501-450-3623
E-mail: patrickd@uca.edu