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WHITEFLY SENSITIVITY TO PLANT VOLATILES. F. Djibodé-Favi[1], W. Mallory[1] & C. Cantrell[2], [1]Agricultural Research Station, Virginia State University, Petersburg, VA 23806 & [2]Natural Products Utilization Research Unit USDA-ARS National Center for Natural Products Research, University Ave., University, MS 38677. Sweet potato whitefly, which costs 1.6 billion to U.S. agriculture, is a sap feeder that also transmits viruses to crops. The adult stage produces wax particles, which profusely dust any visited surface. Our objective was to show that wax particles were also induced by infected plant volatiles. Young adult whiteflies harvested in 25 ml vials were fumigated with volatiles from either lemon grass or produced by the leaves' peltate glands of *Vernonia galamensis* identified as the sesquiterpene lactone Prevercistifolide-8-o-isobutyrate with no fumigated control. The lemon grass grown in our greenhouse mainly produces Citral (70%). Wax produced was collected on no. 2 Whatman paper, visualized using a scanning electron microscope and analyzed with a gas chromatograph. They barely produced wax when fumigated with lemon grass volatiles because they died in 15 min. Wax produced by non-fumigated whiteflies was made of 49.9% of C_{32} Aldehyde, 22.9% of C_{32} Alcohol, 30% of C_{34} Aldehyde, 13% of C_{34} Alcohol and five types of wax esters that made up 22.77% of the particle composition. Fumigation with vernonia gland extract showed 13.4%, 14.3%, 2.9% and 13% respectively. By contrast, the later has eleven wax esters that made up 56.3% of the particle composition. We discovered that wax particles mop up peltate gland secretions to increase whitefly fitness on vernonia leaves.

PHENOLOGY AND NATURAL ENEMIES OF THE PINE BARK ADELGID, PINEUS STROBI, IN VIRGINIA FORESTS. Holly A. Wantuch, Scott M. Salom & Thomas P. Kuhar, Va. Polytechnic Inst. & State Univ., Blacksburg VA 24061. The pine bark adelgid, *Pineus strobi* (Hemiptera: Adelgidae), is a native herbivore of eastern white pine, *Pinus strobus*, in eastern North America. Like many other adelgid species, the pine bark adelgid is a phloem feeding insect with limited mobility. Spending the majority of its life anchored to a single location on a tree, it can be found either on the bark, stem, or needle base. The only known predator to specialize on pine bark adelgid is *Laricobius rubidus* (Coleoptera: Derodontidae), about which relatively little is known. *L. rubidus* is closely related to *Laricobius nigrinus*, a biological control agent introduced to the eastern U.S. to manage the hemlock woolly adelgid, *Adelges tsugae*. These species successfully hybridize and produce fertile offspring, but it is unknown if interaction with an introduced sibling species and its respective adelgid

prey species will have any implications for *L. rubidus* or the pine bark adelgid. Thus, it is important to characterize the phenological patterns of these insects, specifically in their southern ranges, where they have not been studied previously. This study was funded by the USDA Forest Service Grant 11-DG-11083150-010.

POLAR VORTICES: CAN THEY REALLY KILL THE STINK BUGS? Thomas P. Kuhar & John D. Aigner, Department of Entomology, Virginia Tech, Blacksburg, VA 24061-0319. The brown marmorated stink bug (BMSB), *Halyomorpha halys* (Stål), was accidentally introduced from Asia into Pennsylvania in the late 1990s, and is spreading across North America. As it moves to more northerly regions, we are uncertain about how severe winter climate might affect this species. The supercooling point (SCP), is the temperature at which crystallization of the body fluids occurs, and provides an estimate of the lethal low temperature limit of insects. From 2013 to 2014 we determined the SCPs of BMSB adults collected each month. Supercooling points changed with season, all fall and winter SCPs, which averaged about -13 to -14°C, were significantly colder than SCPs taken from insects in summer. During early January 2014, much of North America experienced a "polar vortex", of uncommonly cold arctic air from the North Pole, which enabled us to measure field mortality of BMSB under extreme conditions (temperatures < SCP). Virtually 99% mortality occurred to BMSB adults held in insulated containers outside, compared to very low mortality of bugs held indoors. Wild BMSBs often overwinter in aggregations beneath loose bark on dead trees and in rock crevices. BMSBs that exhibit this behavior probably suffered high mortality in the extreme low temperatures of the 2014 polar vortex. However, because many BMSBs also seek winter refuge in human-built structures, recent polar vortices have not noticeably impacted BMSB populations as a whole. Thus, uncertainty remains about the impact of severe winter temperatures on BMSB populations.

CHANGES IN PHYSICAL, CHEMICAL AND ANTI-NUTRITIONAL PROPERTIES DURING DEVELOPMENT OF VEGETABLE SOYBEAN (EDAMAME). Arrieyana Cartier, Yixiang Xu, Daniel Kibet, Krystal Jordan, Ivy Elena, Stephanie Davis, Edward Sismour, Maru Kering & Laban Rutto, Agricultural Research Station, Virginia State University, Petersburg, VA 23806. Changes in physical, chemical and anti-nutritional characteristics of two vegetable soybean varieties ('Asmara' and 'Mooncake') during seed development were investigated. Pods were sampled weekly for six weeks starting from developmental stage 5 (R5) to 8 (R8). Changes over time in measured attributes were similar but the rate of change differed among the two varieties. In both varieties, seed moisture content and intensity of green color decreased as seed developed with the most significant decline observed in the last two weeks of sampling. Seed weight peaked at R6 then gradually decreased thereafter, while seed hardness increased throughout the sampling period with 'Asmara' recording significantly higher seed hardness at R8. For both varieties, protein accumulation occurred mostly in the later stages, while significant lipid accumulation was observed in the early stages of development. Among the sugars, fructose content decreased with seed development,

sucrose content increased to R6 before decreasing, and there was rapid accumulation of raffinose and stachyose in the last two weeks of sampling. Total phenolic content decreased between R5 and R6, but increased with further seed development and maturation. Tannin and phytate content in seed increased throughout the sampling period. Changes in trypsin inhibitory activity varied with variety reaching a maximum at R6 for 'Asmara, and closer to maturation for "Mooncake." Our data provide the physical, chemical and anti-nutritional basis for harvesting vegetable soybean at R6 namely: peak seed weight and sucrose content, lower values of oligosaccharide and anti-nutrients, and intense green color.

ELUCIDATING THE ANOREXIGENIC MECHANISM OF NEUROPEPTIDE AF. M. S. Delp[1], B. A. Newmyer[2], M. A. Cline[1] & E. R. Gilbert[1], [1]Department of Animal and Poultry Sciences, Virginia Tech, Blacksburg, VA 24060 & [2]Department of Neuroscience, University of Virginia, Charlottesville, VA 22904. Neuropeptide AF (NPAF), a member of the RFamide family, is encoded by the same gene as neuropeptide FF (NPFF), which causes short-term anorexia. However, reports on the role of NPAF on appetite-related process are lacking. Thus, central injections of 4.0, 8.0 and 16.0 nmol NPAF were administered to chicks to observe its effect on food and water intake. Chicks treated with 8.0 and 16.0 nmol central NPAF decreased both their food and water intake. In a second experiment, chicks that received central NPAF had an increased number of c-Fos immunoreactive cells in the dorsomedial (DMN), paraventricular (PVN) and ventromedial (VMH) nuclei. The arcuate nucleus and lateral hypothalamic area were not affected. In the third experiment, there were no differences in mRNA abundance of appetite-associated factors in NPAF-injected chicks in whole hypothalamus. In the fourth experiment, the DMN, PVN and VMH were isolated and the abundance of melanocortin receptor 4 (MC4R) mRNA and neuropeptide Y receptor 5 (NPY5R) mRNA increased in the VMH of NPAF-injected chicks. In a fifth experiment, NPAF-treated chicks exhibited fewer feeding pecks and spent less time perching, whereas they spent an increased time in deep rest. We conclude that NPAF causes anorectic effects that are associated with the hypothalamus.

BLUEBERRY EXTRACTS PROTECT AGAINST ALCOHOL-INDUCED BODY DEFECTS IN FETAL MICE. Zach S. Gish, Sharang Penumesta, Diana J. Valle & Roman J. Miller, Department of Biology, Eastern Mennonite University, Harrisonburg, VA 22802. Nutrient dense blueberries have been shown to combat aging, osteoporosis, cancer, and insulin resistance, while enhancing vision, hepatic, renal, cardiovascular, and brain functions. In contrast, alcohol is a powerful teratogen, systematically affecting prenatal development as well as postnatal functioning. Our study explored the effects of anthocyanins derived from blueberries in protecting/mitigating ethanol-induced prenatal developmental deficiencies in a murine model. Swiss mice were administered alcohol (25% v/v of absolute ethanol in normal saline at 0.03 ml/g per maternal body weight) or normal saline, through IP injections on days 5 and 7 following impregnation. Anthocyanin injections (30 mg/kg per maternal body weight) were administered through subcutaneous neck injections on days 0, 5, 7 and 12.

Statistical analysis showed that the anthocyanin group was protected from gross developmental deficiencies over the binge alcohol group in regards to average body weight, crown-rump length, telencephalon size and liver size ($p<0.05$). While not delineating the mechanism, these preliminary results are the earliest support of the hypothesis that the antioxidant properties of blueberry anthocyanins mitigate the gross teratology effects of prenatal binge alcohol exposure. (Research supported in part by the Daniel B. Suter Endowment in Biology, Eastern Mennonite University.)

Posters

DEVELOPING TOOLS FOR TRAP CROPS: ELUCIDATING THE BIOSYNTHETIC PATHWAY OF THE AGGREGATION PHEROMONE MURGANTIOL IN THE HARLEQUIN BUG STINK BUG (*MURGANTIA HISTRIONICA*). Jason Lancaster[1], Dawn Gundersen-Rindal[2], Donald C. Weber[2] & Dorothea Tholl[1], [1]Biological Sciences, Virginia Tech, Blacksburg, VA 24061 & [2]USDA-ARS, Beltsville, MD. Harlequin bug (*Murgantia histrionica*) is a stink bug pest in the southeastern United States that feeds on crucifer crops and can cause considerable economic loss. Adult male harlequin bugs release the sesquiterpenoid aggregation pheromone murgantiol, which attracts other conspecifics to the host plant to feed and mate. Terpenoid aggregation or sex pheromones are produced by a variety of insect taxa, but their biosynthesis is largely unexplored. This project aims to identify the biosynthetic pathway as well as the tissue-specific site of biosynthesis of murgantiol in harlequin bug. We hypothesize that murgantiol is synthesized in a two-step pathway with a dual function prenyldiphosphate synthase/terpene synthase enzyme catalyzing its first step. RNAseq analysis identified a candidate gene, *MhFPPS1*, which is highly expressed in mature males but not in females, and may encode the proposed dual function synthase in murgantiol biosynthesis. We are in the process of functionally characterizing recombinant MhFPPS1. Moreover, we are currently using tissue dissection and transmission electron microscopy to examine the presence of murgantiol pheromone glands and *MhFPPS1* expression in these tissues.

Astronomy, Mathematics, and Physics with Material Science

TAPE-INFLUENCED INFRARED AND THERMAL POWER GENERATION. Graham P. Gearhart, Brian C. Utter, & Giovanna Scarel, Department of Physics & Astronomy, James Madison University, Harrisonburg VA 22807. Infrared (IR) radiation can be harvested and turned into an alternative source of energy through the use of a power generator (PG) device. A glowbar source generates IR radiation which is then directed onto the PG device for an extended period of time, and a voltage is generated. Our data suggests voltage and temperature are influenced by both the color and presence of tape in IR power generation, and that it does not behave as thermoelectric power generation.

DESIGN OF A NOBLE GAS CERENKOV FOR THE SUPER HIGH MOMENTUM SPECTROMETER FOR 12 GEV AT JEFFERSON LAB. Donal Day & Mikhail Yurov, Department of Physics, University of Virginia, Charlottesville, VA 22904. The 12 GeV upgrade of the accelerator and the associated experimental facilities at Jefferson Lab will provide innumerable new opportunities for nuclear science. In Hall C the new Super High Momentum Spectrometer (SHMS) will provide excellent angular and momentum resolution up to a maximum central momentum of 11 GeV/c and a diverse set of directed studies, from the spin structure of the neutron to multi-nucleon correlations in nuclei, are planned. These and other approved experiments demand robust particle identification. As part of the electron identification and pion rejection package, a 2 meter long, 4-mirror noble gas Cerenkov counter is being built. The design principles, expected performance and status of the project will be presented.

DETERMINING A MATHEMTICAL MODEL FOR A VOLTAGE INDUCED, EXCLUSIVELY TEMPORAL SOLITON. Aidan L. Gordon, Brian C. Utter, & Giovanna Scarel, Department of Physics & Astronomy, James Madison University, Harrisonburg VA 22807. Infrared radiation (IR) can be converted into a usable alternate source of energy. Here we study the voltage produced by a power generator device irradiated by IR radiation over a long period of time. We find features that suggest the existence of solitons and here we present some results of our study of their dynamics.

TWO-PHOTON EXCHANGE CONTRIBUTION TO ELASTIC ELECTRON-PROTON SCATTERING. Mikhail Yurov, Department of Physics, University of Virginia, Charlottesville, VA 22904. Two experimental techniques, Rosenbluth separation and recoil polarization transfer, used to extract proton's electromagnetic form factors ratio G_E/G_M yield markedly different results. Modern theoretical calculations suggest that two-photon exchange might be responsible for the observed discrepancy and that it is epsilon dependent. Jefferson Lab Experiment E05-017 was designed to measure the two-photon exchange contribution over a wide range of ε and Q^2. In contrast with the conventional Rosenbluth method, E05-017 detected the elastically scattered proton rather than the electron. This approach returns a much more precise extraction of the form factor ratios. After a brief description of the experimental goals and techniques, the current status of the analysis will be presented.

A PRECISION MEASUREMENT OF ISOSPIN DEPENDENCE IN THE 2N AND 3N SHORT RANGE CORRELATION REGION. Dien Nguyen & Donal Day, Department of Physics, University of Virginia, Charlottesville, VA 22904. Short Range Correlations (SRCs) have been recognized as responsible for the high momentum tail of the nucleon momentum distribution. Several experiments at Jefferson Lab have exploited inclusive scattering to study these SRCs. In an upcoming tritium experiment (E12-11-112) at Jefferson Lab, we will perform a precision test of the isospin dependence of two- nucleon short range correlations using mirror nuclei: ^{3}He and ^{3}H. The data taken at x>2 will also be used to study three-nucleon short-range

correlations. In this talk we will briefly present the motivation for this experiment as well as some of the experimental details and the expected results. In addition, we will discuss a method to check the absolute target thickness of both targets through elastic scattering.

OPEN EDUCATIONAL RESOURCES IN COLLEGE MATHEMATICS. Thomas C. Mosca III, Rappahannock Community College, Department of Mathematics, Warsaw, VA 22572. An open source teaching resource was examined and applicability to teaching undergraduate mathematics was discussed. The resource, MyOpenMath, is available free and without restrictions. The resource consists of PDF textbooks, and software having testing capability, self-grading homework, and tutorial videos, many of which are linked to particular homework problems. While not as well polished as textbooks and testing/ homework software available from established publishers, it was found to be adequate to the needs. Further refinements in grade keeping, homework and the ability to add and edit test problems are needed. Textbooks are lacking in scope, requiring the use of two texts by different authors to cover course material, leading to clumsiness in the transition from one to the other.

COMPUTATIONAL METHODS AND TOOLS FOR MODELING AND SIMULATING THE ELECTRONIC STRUCTURE AND TRANSPORT PROPERTIES OF MATERIALS USING THE PYTHON PROGRAMING LANGUAGE. Anthony A. Teate, Dept. of Integrated Science & Technology, James Madison University, 701 Carrier Drive, Harrisonburg, VA 22807. The Python Programming language has proven to be quite a robust tool for scientists and engineers. Several widely used packages, from computational physics to molecular modeling, have been developed primarily in the Python language or provide an interface to their API via Python. The extensibility of the language with open source add-on packages such as NumPy and SciPy as well as plotting packages such as Matplotlib can serve as the foundation for a complete exploratory research environment in numerical modeling and simulation. Here we use Kwant, another open source Python package, to perform numerical calculations on tight-binding models. We compute the electronic band structure and quantum transport properties of simple two-dimensional nanoscale (mesoscopic) systems. We show how sparse tight-binding Hamiltonians for graphene are easily solved by Kwant, and are used to calculate energy band structure as well as the quantum conductance even in the presence of localized defects in the system lattice. We also demonstrate how the combination of the tight-binding model approach and the Kwant package can be used in an undergraduate class on computational modeling and simulation of nanoscale materials using the Python programming language.

IONIC SELF-ASSEMBLED MONOLAYERS THIN FILMS FOR OPTICAL pH SENSORS. D. M. Topasna, M. Liu, & CH. Tseng, Department of Physics & Astronomy, Virginia Military Institute, Lexington, VA 24450. Ionic self-assembled monolayers thin films made from polymer and organic dye molecule were studied for optical pH sensing coatings. A number of films were fabricated in order to determine

the optimized parameters of the polymer and of the organic dye solutions. Optical pH responses of these films were also studied. The transparent films were immersed in solutions at various temperature and pH values. We found that the films are stable when immersed in solutions with pH values below 9.0 and temperatures below 90°C and they are still functional after longer immersion times. We will use the results of this project as a basis for future work with ionic self-assembled monolayers to build various sensors and exploit more sensing platforms.

ANALSIS OF THE POLARIZATION TECHNIQUES USED WITH THE VMI OPTICAL POLARIMETER. G. A. Topasna, Dept. of Physics & Astronomy, Virginia Military Institute, Lexington, VA 24450. An analysis of the precision of the aperture photometry technique used to determine the linear polarization of stellar radiation with the VMI optical polarimeter is presented. It is shown that variations in the ON aperture radius and OFF annulus radii contribute no greater than 0.01% to the uncertainty in the degree of polarization and that the polarization position angle has an uncertainty on the order of 0.1° for high S/N ratio measurements. Using these results we show that three polarization standards, HD 198478, HD 183143, and HD 187929 exhibit variation in polarization with a maximum difference of 0.2%, 0.3%, and 0.1% over the time period spanning 3 September 2013 to 21 November 2014.

HISTORICAL NOTES ON TWO COLD WAR SURVEILLANCE PROJECTS. James D. Lehman, Retired, Physics Department, James Madison University, Harrisonburg, VA 22807. Post WWII saw a concerted effort by the military and private agencies to collect information on the Soviet Union and Allies as to military capabilities. The National Security Agency was formed in 1948 from separate Intelligence Services of the Army, Air Force and Navy. A National Forest site in a mountain valley of Pendleton County, West Virginia was available for the first of two major projects. The Washington Naval Research Laboratory, NRL, advocated using the Moon as a passive reflector of Earth's electronic communication. After two preliminary testing projects, the 600 foot diameter Big Dish Radio Telescope was under construction in 1956 and was scheduled to be completed in five years. "Cover" of the highly secret installation was provided by staff astronomers and the close proximity of NRAO, Green Bank, WV. From the beginning there were cost over runs and little sequential movement from planning to design to actual construction. The Dept. of Defense killed the project in 1962. Site preparation began immediately for the second of the major projects. Double 900 ft. diameter Wullenweber antennas were constructed on site. An inland Naval Base accessed use of the receiving facilities, and served as "cover" for this highly secret interceptor project. The Wullenweber era served well in surveillance for three decades of the Cold War. Fifty or more of these sites worldwide were dismantled by the mid-1990's.

Posters

ARCTIC CLIMATE CHANGE: A SIMPLE MATHEMATICAL MODEL OF THE MELTING ARCTIC. Stephanie Norwood & Iordanka N. Panayotova, Dept. of Mathematics & Computer Science, Virginia Wesleyan College, Norfolk, VA 23502. Due to global warming there is an accelerated melting of the Arctic ice caps. Observations show that summer sea ice cover has been disappearing at approximately 70,000 km^2 per year. While the shrinking of the Arctic sea ice is a serious problem, an even bigger problem is the thinning of the ice. Measurements from submarines indicate that the ice has thinned by about 40% over the last two decades. When the area of the ice decreases, it replaces an area of white, which reflects about 90% of the solar radiation, by water surface, reflecting less than 10% of the solar radiation. This effect can additionally raise the global average rate of warming and the melting Arctic will contribute to a global sea level rise. In this work, we created simple mathematical models to study the changes in the sea ice area and thickness. We assumed that the ice melts at a rate proportional to the area present at time t, and used the fact that the sea ice is disappearing at approximately 70,000 km^2 per year. Fourier's law of heat conduction was used to create a differential equation for the rate of the melting ice. Despite the simplicity, the models capture some of the main features of ice melting/growing. The summer sea ice extent will decrease twice for less than 50 years. The ice thickness grows as the square root of time, meaning that with the increase of the ice thickness, the growth rate slows down, and inversely, with the decreasing of the ice thickness the melting process speeds up. Both models predict that the effect of climate change on Arctic caps will be devastating, resulting in their disappearing in our lifetime.

MATHEMATICAL MODEL OF EBOLA OUTBREAK. Nicole Johnson & Iordanka N. Panayotova, Dept. of Mathematics & Computer Science, Virginia Wesleyan College, Norfolk, VA 23502. The Ebola Virus originates in West Africa. The Ebola Virus Disease (EVD) has become a crisis in West Africa, centralized around Liberia, Sierra Leone, and Guinea, and is a potential threat to other areas of the world as United States and European Nations. Because the Ebola virus spreads only through direct contact with bodily fluids and not via airborne means like the influenza virus, its spread is easier to control than the influenza virus. But since there is no vaccination currently available for EVD, only physical methods can be used to limit contact by the susceptible population with the living virus. The objective of this project was to create a mathematical model of the spread of Ebola outbreak. The model used time as independent variable and the number of susceptible people, number of infected, number of death, and number of recovered as dependent variables. System of differential equations describing the variation between the dependent variables was created. The contact rate, the death rate and control measures parameters have been derived using real data from the latest outbreak in 2014. The model assessed the impact transmission control measures, such as providing medical facilities, protective garments, cleaning detergents, bags, and training to the population, would have on an outbreak.

Particularly, the model showed that applying transmission control measures is a viable way to mitigate negative impact of the outbreak by decreasing the ultimate number of people infected and who die. Conclusions of this model were supported by the findings from the observational studies during 2014 outbreak in Sierra Leone and Liberia.

PREDATOR OR PREY: MATHEMATICAL MODEL OF THREE SPECIES INTERACTIONS IN CHESAPEAKE BAY. McKenzie Dowd & Iordanka N. Panayotova, Dept. of Mathematics & Computer Science, Virginia Wesleyan College, Norfolk, VA 23502. Chesapeake Bay, the largest estuary in the United States, is an extremely complex ecosystem. The fisheries of the Chesapeake Bay play a very important role in the ecosystem, but have declined significantly as a result of overfishing, habitat loss and deterioration in water quality. Fisheries in the Bay are managed as single species entities, yet the multi-species nature of the ecosystem is very important. In this project, we created a three-species mathematical model that simulates the prey-predator interactions of three different species of the Bay ecosystem; menhaden, striped bass, and sharks. The model shows that the behavior of all three species is actually defined by the parameters affecting the bottom prey, the menhaden, and the top predator, sharks. When the product of the natural growth rate of menhaden and the propagation rate of the sharks is equal to the product of the declining rate of the menhaden in the presence of predator and the death rate of sharks in the absence of their prey, all three species have periodic behavior over time with a common period. If one of these parameters changes the whole system behavior changes, all three populations either increase without limit, or decrease over time and the top predator will become extinct first. The middle species, that play the role of prey and predator, act merely as a conduit between the bottom prey and the top predator. It is interesting to point out that both menhaden and shark populations are declining over the last 30 years by the same percentage of about 86%. The results of this model show that predator-prey interactions are very important for the whole ecosystem and have to be taken into consideration by the Fishery management who use multi-species models when taking decisions.

INVARIANT AMPLITUDES FOR DECAY OF HIGGS PARTICLE TO THREE Z BOSONS: NON-DYNAMICAL METHODS TO DISTINGUISH SCALAR AND PSEUDOSCALAR DECAYS. Deva A. O'Neil[1], Howard E. Haber[2] & Sang Y. Kim[1], [1]Physics Department, Bridgewater College, Bridgewater, VA 22812 & [2]Santa Cruz Institute for Particle Physics, Santa Cruz, CA 95064. In the CP-conserving Two-Higgs Doublet Model, the Higgs field A^0 is described as a pseudoscalar, due to exhibiting odd parity in coupling to fermions. However, in the absence of fermionic couplings, its parity is not well-determined. The decay of the A^0 to a ZZZ final state was found to be useful as a parity test for the A^0 in its bosonic interactions. Using non-dynamical methods, scalars and pseudoscalars were shown to produce distinct invariant amplitudes in parity-conserving decays to ZZZ. While this provides a method for experimental probing of the parity of A^0, the results apply to any decay of a (pseudo)scalar to three identical massive vector bosons.

A ROTATING METRIC THAT ACCOUNTS FOR THE ENERGY OF THE GRAVITATIONAL FIELD. Joseph D. Rudmin, College of Integrated Science and Engineering, James Madison University, Harrisonburg, VA 22807. The metric for a rotating field is found by equating the Einstein Tensor of a Lorentz transformed metric to a Lorentz transformed Einstein tensor of a stationary isotropic metric. In general relativity, the Einstein Equation describes how energy density and momentum density curve space and time. The Einstein Equation equates the Einstein Tensor, which is a curvature tensor, to the stress-energy tensor, which is the density of energy and momentum. The Einstein Tensor for an isotropic metric at rest has two terms, one which looks like a charge density, and the other which looks like an energy density of a field. The first term is the density of ordinary energy and momentum, and the second is the energy density of the gravitational field. The metric for a rotating field is not at rest. Since both the metric and the Einstein Tensor are tensors, they both must transform as tensors: The Lorentz transformation and the calculation of the Einstein Tensor must commute. This commutation takes the place of equating the Einstein Tensor to zero in conventional general relativity. The resulting differential equations exactly determine the metric. These equations are solved as Taylor Series, using the Parker-Sochacki method.

POLARIZATION MEASUREMENTS OF NGC 7380 IN BOTH BROAD AND NARROW BANDS. M. A. Tate & G. A. Topasna, Dept. of Physics & Astronomy, Virginia Military Institute, Lexington, VA 24450. The wavelength dependence of polarization is described by the Serkowski law $p(\lambda)/p_{max} = exp[-K\ln^2(\lambda_{max}/\lambda)]$ where p_{max} is the maximum degree of polarization, λ_{max} is the wavelength of maximum polarization and K is typically taken to be a function of wavelength ($K \approx 1.86\lambda_{max}$). The Serkowski law is well-established for stellar observations using broadband filters. Previous observations of the isolated star HD 197770 using the VMI optical polarimeter have shown that it also accurately describes the wavelength dependence when using narrowband ($\Delta\lambda \sim 10$ nm) filters and that p_{max}, λ_{max}, and K were, for both narrow and broad bands, nearly identical or within instrumental error. We made new polarization measurements for selected stars in the cluster NGC 7380 in front of the emission nebula Sh2-142. Both narrowband and broadband filters were used and the wavelength dependence of polarization was plotted. A nonlinear least squares fit to the Serkowski law was used to determine p_{max}, λ_{max}, and K. By comparing the two filter sets we find that the difference in the maximum degree of polarization is $\Delta p_{max} < 0.3$ % and the percent difference in λ_{max} is less than 2%. However, fitted values of K in the narrow band were significantly higher (>45%) than those in the broad band. Therefore, while the determination of p_{max} and λ_{max} is fairly unaffected by the choice of filters used to measure stellar polarization in the presence of the nebula emission, the values of K appear to differ significantly.

Biology with Microbiology and Molecular Biology

SHIGA TOXIN PATHOGENESIS IN THE GASTROINTESTINAL TRACT. Abigail J. Lenz & Andrew J. Fabich. Dept. of Biology & Chemistry, Liberty Univ., Lynchburg, VA 24515. Enterohemorrhagic *Escherichia coli* (EHEC) is a gram negative bacteria that is the leading cause of infectious kidney failure worldwide; a primary mechanism of EHEC infection is Shiga toxin (stx), which is carried by Golgi phosphoprotein 4 (GPP130) and binds globotriaosylceramide (Gb3) receptors on the endothelial cell surface, initiating a cascade that ultimately leads to apoptosis. *Citrobacter rodentium* genetically engineered with stx (CR) has successfully been used in mice to model the effects of EHEC in humans. We show that competition drives the pathogenic effects of CR infection.

ENTRAINMENT OF SYNTHETIC GENE OSCILLATORS BY A NOSIY STIMULUS. N. C. Butzin, P. L. Hochendoner, C. T. Ogle, P. Hill & W. Mather, Dept. of Physics, Virginia Tech, Blacksburg, VA. Modulation of biological oscillations by external stimuli lies at the root of many phenomena, including maintenance of circadian rhythms, propagation of neural signals, and somatogenesis. While it is well established that regular periodic modulation can entrain an oscillator, a curious phenomenon is that a noisy (rugged) modulation can also robustly entrain oscillations. This latter scenario may describe, for instance, the effect of irregular weather patterns on circadian rhythms, or why irregular neural stimuli can still reliably transmit information. A synthetic biology approach has already proven useful in understanding the entrainment of oscillators by periodic signaling, which can mimic the response of a number of noisy oscillating systems: cell cycles, NF-*k*B response, etc. We similarly seek to use synthetic biology as a platform to understand how aperiodic signals can strongly correlate the behavior of cells. This study should lead to a deeper understanding of how fluctuations in our environment and even within our body may promote substantial synchrony between our cells. We investigate experimentally and theoretically the entrainment of an ensemble of synthetic gene oscillators by a noisy stimulus. Stochastic simulations suggested that a synthetic gene oscillator would be strongly entrained by two aperiodic signals: telegraph noise and phase noise. This simulation-based prediction was tested by a combination of microfluidic and microscopy using a real synthetic circuit in *Escherichia coli*. We use delayed feedback models to analyze these cells. We show that cells are entrained by two noisy signals: telegraph and phase noise. Cells are entrained when either signal period or amplitudes are varied.

EFFECT OF CONVERTING TO ORGANIC TURKEY REARING PRACTICES ON ANTIBIOTIC RESISTANCE OF ENTEROCOCCI FROM USED LITTER. Steven G. McBride, Lindsey Toothman, Pradeep Vasudevan & Joanna B. Mott. Dept. of Biol., James Madison Univ., Harrisonburg VA. 22807. Conventional turkey production employs antimicrobial compounds for prophylaxis, treatment, and growth promotion. Conversely, organically raised turkeys are not administered antimicrobial compounds. Increasing public interest in organic and antibiotic free foods has led to a growing

market for their production. In this study the prevalence of antibiotic resistance in *Enterococcus* spp. isolated from the turkey litter of adult tom turkeys after they were sent to market, was compared before and after the farm transitioned to organic rearing practices. *Enterococcus* spp. were isolated on m-EI agar and identified to species phenotypically. Susceptibility to 12 antimicrobial compounds was determined using the Kirby-Bauer disc diffusion technique. The proportions of resistant bacteria were compared using chi-square test and Fischer's exact test. Isolates from the litter of organic birds differed in species composition and resistance profiles from those isolated from the conventionally farmed litter. Isolates from organic litter exhibited a reduction in the percentage of isolates resistant to gentamicin (- 47%), tetracycline (- 42%), and doxycycline (- 25%). These results suggest that changing to organic rearing practices affects the antibiotic resistance of bacteria in turkey litter.

EFFECTS OF SYNTHETHETIC ANDROGEN ON P21 EXPRESSION IN MCF-7 CELLS. Tawany C. Almeida & Rosemary Barra, Department of Biological Sciences, University of Mary Washington, Fredericksburg, VA 22401. In the United States, breast cancer is the most prevalent form of cancer in women and is second only to lung and bronchial cancer as the leading cause of cancer death. A number of factors have been identified that increase the risk of developing breast cancer, including specific gene expression, age, estrogen exposure, and obesity. It has also been demonstrated by both *in vivo* and *in vitro* studies, that some breast cancer cells express both androgen and estrogen receptors. These studies suggest that breast cancer may be linked to a hormonal imbalance between estrogens and androgens. The physiological effects of androgens on breast cancer cells have not been clearly described. However, the hyperactivation of the mitogen-activated protein kinase (MAPK) pathway has been shown to result in a growth-inhibitory response. Recent studies have also shown that androgen receptor signaling/activation of the MAPK pathway is dependent on the cyclin dependent inhibitor, p21. For this study, we hypothesized that androgens would have an inhibitory effect on the growth of MCF-7, androgen receptor positive breast cancer cells, and that p21 would mediate this effect. In the first phase of this study, we determined the effects of androgens on cell viability using the MTT assay. At an androgen concentration of 10^{-6} M, the cell viability was decreased 12% in comparison to the control cells. A p21 ELISA assay was used to detect and quantify the level of p21 activity in MCF-7 cells treated with 10^{-6} M androgen. The results of three experiments indicated that p21 activity was increased 34.7% by exposing the cells to androgens for 24 hours. These preliminary studies suggest that p21 plays a role in the observed anti-proliferative effect, however additional studies are needed to confirm this observation and to elucidate the mechanism.

QUORUM SENSING EFFECTS BASIC BACTERIAL PHYSIOLOGY. R. A. Betar, R. N. Montalvo, A. J. Fabich PhD. Department of Biology, Liberty University, Lynchburg, VA 24502. Bacterial populations communicate to each other through Quorum sensing (QS). This form of communication is based on genetic induction by a two component regulatory system, which has been associated with the bacterial stress

response. The protein QseC is the receptor sensory kinase that phosphorylates the response regulator QseB and induces transcription of specific genes. QseC typically responds to autoinducers released from bacteria and also responds to intestinal to epinephrine and norepinephrine. QS is known to cause induction of both virulence and motility genes. Previous research has been performed in pathogens, associating QS with virulence. To understand the basis of QS more *E. coli* MG1655 wild type and *E. coli* MG1655?*qseC* were colonized within the murine intestine. The results indicated that without the sensory kinase, there was a competitive advantage for colonization. Since no one had previously measured bacterial physiology of *E. coli* MG1655?*qseC*, we measured basic physiology on the strain to determine the cause of the greater advantage on colonization. We found that QS is not limited to the induction of virulence and motility as shown in previous studies, and that downstream carbon metabolism is heavily influenced. Specifically, the *E. coli* MG1655?*qseC* strain has a quicker generation time than the wild type on both catabolite-repressing and non-catabolite repressing sugars.

STABLE ISOTOPE ANALYSES OF DIETARY DIFFERENTIATION AMONG FREE-RANGING SMALL RUMINANT BREEDS. Pieter A.P. deHart & Julie A. Lozier, Department of Biology, Virginia Military Institute, Lexington VA 24450. As society strives to adapt to a rapidly changing economic and environmental climate, families and farmers are exploring opportunities for increased self-reliance and sustainable practices. These explorations have been particularly evident in small- and medium-sized farms throughout the United States, as there have been systematic increases in abundance of free-ranging dairy goat (*Capra hircus*) and sheep (*Ovis aries*) production throughout the country. Concomitant with this growth have been new research efforts aimed at assisting producers in refining herds and their diets to increase output and efficiency. One popular approach has centered on both optimal breed selection and an increase in breed diversification. Little scientific evidence exists, however, on innate physiological differences of dietary uptake between breeds, which may dictate herd health, as well as milk, meat, and fleece quality. Given inherent differences in size, behavior, and diet selectivity between breeds, there are likely breed-specific and dietary-independent physiological differences dictating overall herd characteristics in both these species. To determine what specific differences may exist, and bridge a critical knowledge gap, we examined the carbon and nitrogen isotopic signatures from hairs of six breeds of dairy goats (n=123) and from six breeds of multi-purpose sheep (n=56) across a total of ten farms exhibiting similar vegetation profiles within Appalachian Virginia. Our results indicate that while the mean (±SD) values obtained for all breeds within each species varied widely, the differences between goat breeds ($\leq$2.3‰ δ^{15}N, $\leq$1.7‰ δ^{13}C) and sheep breeds ($\leq$2.8‰ δ^{15}N, $\leq$5.7‰ δ^{13}C) are much greater than those between farms ($\leq$£0.3‰ for both δ^{15}N and δ^{13}C). For goats, the expected ontogenetic differences yielded more exaggerated distinctions between breeds, with variations between kids of different breeds $\leq$3.8‰ and $\leq$2.2‰ for δ^{15}N and δ^{13}C, respectively. This variation in δ^{15}N and δ^{13}C of kids is likely due to differential protein investment in milk by does, which could have implications for milk production

rate and quality, and ultimately breed selection for specific environments. For sheep, greatest variation was apparent between genders, as males of most breeds had signatures differing by ~2.1‰ and ~1.7‰ for $\delta^{15}N$ and $\delta^{13}C$, respectively. These sex-mediated differences in sheep are likely driven by behavioral differences, and so producers selecting breeds which exhibit minimal gender differences could yield more consistent meat and fleece quality throughout the flock. This work suggests that future research on free-ranging ruminants, their diet, and health effects of dietary supplementation should be performed at breed-specific levels.

GENOME-WIDE RNA-SEQ ANALYSIS OF CHANGING GENE EXPRESSION IN BRAIN AND BLOOD IN AN ALZHEIMER'S DISEASE MOUSE MODEL. A. Házy, M. Dalton & G. D. Isaacs, Dept. of Biology and Chemistry, Liberty University, Lynchburg VA 24515. Previous studies have established a causative role for altered gene expression in development of Alzheimer's disease (AD). These changes can be affected by methylation and miRNA regulation. In this study, genome-wide expression changes in AD hippocampus and blood were determined by RNA-sequencing of mRNA from control and AD mice. Epigenetic changes contributing to AD were also investigated via qPCR to determine expression changes of miRNA known to change methylation status in AD. The qPCR data showed significantly increased expression of Mir 17 in AD. Sequencing data revealed 729 genes in hippocampus and 152 genes in blood showing significant differential expression (q value < 0.05). Changing genes in hippocampus were compared to changing genes in blood to identify 75 genes as candidates for development of an expression-based diagnostic blood test for AD.

ANATOMY OF AN INVASION: THE EFFECTS OF HOST PREFERENCE ON THE BIOGEOGRAPHY OF TICKS. Robyn M. Nadolny, Dept. of Biological Sciences, Old Dominion University, Norfolk, VA 23529. Ticks depend on the movements of their hosts to transport them across a landscape, and host specificity is key to any parasite's ability to disperse and invade new areas. Ticks that show preference for specific hosts may move across a landscape in different and potentially unexpected ways. We documented the northward expansions into Virginia of two tick species, *Ixodes affinis* and *Amblyomma maculatum,* both of which carry pathogens that have been linked to human and wildlife disease. To assess population connectivity and ancestry, we sequenced the 16S mitochondrial rRNA gene from a representative sample of individuals of both species from populations throughout the eastern US. We found that despite overlapping host preferences throughout ontogeny, each species exhibited very different genetic and geographic patterns of population establishment and connectivity. We suggest that tick life stage, host, and habitat preferences are all important in understanding and predicting tick range expansions.

Posters

GENETIC AND PHENOTYPIC CHARACTERIZATION OF TWO EXTANT RHOA ALLELES IN DROSOPHILA MELANOGASTER. Laura A. Johansen & Susan R.

Halsell, Dept. of Biol., James Madison Univ., Harrisonburg, VA 22807. *Drosophila melanogaster*, the fruit fly, is a powerful model for genetic studies into developmental biology. Function of the Rho signal transduction pathway is critical during development, including in humans. In *Drosophila*, mutant alleles coding for the RhoA protein have been implicated in causing morphogenetic errors in fruit fly embryos. These characterized *RhoA* mutant alleles are homozygous lethal with characteristic defects in head involution. Genetic and phenotypic characterization of the $RhoA^{3.5.1}$ and $RhoA^{4.4.2}$ alleles involved an examination of the severity of defects in homozygous embryos. Since $RhoA^{3.5.1}$ showed a complete loss of function as its lethality rate is 100% of all homozygous embryos and trended towards the more severe phenotype defects, it is likely that the mutation is consistent with previously found *RhoA* loss-of-function mutant alleles. For $RhoA^{4.4.2}$, the results strongly suggest it is a partial loss-of-function mutation known as a hypomorph. Homozygous $RhoA^{4.4.2}$ embryos showed only 58% lethality at the embryonic stage of development. However, when one of the $RhoA^{4.4.2}$ alleles is replaced with a deficiency that completely removes the entire *RhoA* gene, $RhoA^{4.4.2}$*/Df(2R)Jp8* embryos showed an increased embryonic lethality of 84%. This means that each $RhoA^{4.4.2}$ allele provides some functional protein, but when placed in trans to the deficiency encoding no protein, less than half of the protein is made, resulting in the more severe phenotype.

CELL PHONE INDUCED GENE EXPRESSION IN HUMAN GLIOBLASTOMA CELLS. Virginia L. King & Deborah A. O'Dell. Dept. of Biol., Univ. of Mary Washington. Fredericksburg VA 22401. The link between cell phone radiation and the production of brain cancers has not been firmly established, although many governments regulate the amount of radiation permitted in cell phones. Previous studies in Dr. O'Dell's lab indicate an increase in certain oncogenes and a decrease in certain tumor suppressor genes up to 24 hours after a 25 minute exposure to cell phone radiation, followed by a decline in expression by 36 hours, indicating that cell phone radiation can lead to cell cycle changes. Although the changes were reversed, they were not reversed back to pre-exposure levels. We were interested in determining the length of time it took to completely reverse gene expression changes induced by cell phone radiation. We exposed cultured glioblastoma cells to 25 minutes of continuous cell phone radiation. The cells were separated from the cell phone by skeletal, muscle and skin tissue approximating the human skull structure. Whole cell RNA was extracted from the cultured at 24 and 48 hours after exposure and the change in expression was measured using RT-PCR using a commercially available array assessing 84 oncogenes and tumor suppressor genes (Qiagen). The changes in gene expression were analyzed using 2^dCt to measure fold changes. Any gene which showed a change in expression >2 is considered to have significant changes in expression. These results confirm previous results that a brief exposure to cell phone radiation temporarily increases gene activity. These results also showed that cell phone radiation is not impeded by structures of the human head. The types of changes indicate that cell activity may be altered in such a way to promote a cancerous condition. This study was funded in part by the VA. Academy of Science and the Univ. of Mary Washington.

TRANSCRIPTIONAL REGULATORS OF EPIGENETICALLY ALTERED GENES IN ALZHEIMER'S DISEASE. John T. Lawson & Gary D. Isaacs, Dept. of Biol. and Chem., Liberty Univ., Lynchburg VA 24515. Most cases of Alzheimer's disease (AD) are sporadic-not clearly genetic in nature. Because of this, epigenetics, which deals with factors that modify DNA expression without altering the DNA sequence, may help explain how the environment could interact with genes to promote AD. Epigenetic changes have been observed in AD and the Isaacs lab at Liberty previously determined genes that increase in methylation (hypermethylated) and decrease in methylation (hypomethylated). Methylation can silence genes by inhibiting transcription factor binding. To look into what transcription factors may regulate these genes, bioinformatics methods and tools including the AME program from the MEME suite were used to test for enrichment of transcription factor motifs in promoters and "peaks" (areas of epigenetic changes) of genes that were differentially methylated in AD. Out of 591 motifs from the Jaspar and Uniprobe Mouse databases, 16 motifs were enriched in genes that were hypermethylated in AD and 8 motifs in genes that were hypomethylated in AD. Out of these, 14 of 16 motifs from hypermethylated genes and 8 of 8 motifs from hypomethylated genes were also specifically enriched in the "peak" regions of epigenetic change in each promoter compared to adjacent regions in the same promoters. The transcription factors for the enriched motifs, many of which were involved in processes that could be relevant to AD, may be able to provide a link between epigenetic changes and changes in gene expression in AD as well as offer prospects for future research. (Supported by: the Jeffress Memorial Trust, the Virginia Academy of Science, and the ARDRAF grant from the Virginia Center on Aging).

SIGNIFICANT UP-REGULATION OF MIR-17 IN AN ALZHEIMER'S DISEASE MOUSE MODEL. M. R. Dalton, A. D. Házy & G. D. Isaacs, Dept. of Biol. and Chem., Liberty University, Lynchburg VA 24515. Previous work by our group has demonstrated a correlation between AD pathology and changes in epigenetic markers, including cytosine methylation of gene promoter regions. Several genes determined to have AD-related changes in methylation code for miRNA, which is known to regulate gene expression at a post-transcriptional level. Research suggests that miRNA play a key role in AD development by alteration of gene products and transcription factors, particularly in that of amyloid-ß (Aß) production and apoptosis of postmitotic neurons. This analysis shows a significant up-regulation of demonstrated epigenetically modified miR-17 in the hippocampi of transgenic AD mice when compared to that of non-AD mice. MiR-17 belongs to the polycistronic cluster miR-17-92 and is believed to be involved in normal neuronal cell proliferation and ultimately the regulation of Beclin-1, which has been shown to modulate amyloid beta accumulation in mice.

VALIDATION OF PREDICTED TRANSCRIPTION FACTOR BINDING SITES IN ALZHEIMER'S DISEASE. Bria E. Johnston & Rachel C. Bordelon, Dept. of Biology and Chemistry, Liberty University, Lynchburg VA 24515. Alzheimer's Disease (AD) is a neurodegenerative disorder affecting over five million Americans as of 2015. Symptoms include severe memory loss, confusion, and gradual loss of the ability to

self-care. While the underlying causes of the disease are yet unknown, what is clear is that there is no single mutation that causes AD. Rather, changes to the genome that affect gene expression but do not alter DNA sequence may be more likely to blame. These epigenetic changes include the chemical modification of bases, such as the methylation of certain cytosine bases. Methylation within the promoter region of a gene can change the expression levels of that gene by preventing transcription factors from binding and recruiting RNA polymerase. Using preliminary data from another student generated using various bioinformatics programs, the transcription factor binding sequences within the promoter regions of eight genes of interest will be predicted. Whether these sequences actually bind to the corresponding transcription factors will be tested using an electrophoretic mobility shift assay (EMSA), commonly used to show DNA-protein interaction. Once these sequences are known, the methylation status within the transcription factor binding site can be compared between the AD state and wild type. For a given gene, if the methylation state changes between healthy and diseased state, the expression of that gene is likely changing as well, potentially contributing to AD pathology.

CORRELATION OF METHYLATION ASSAY AND BISULFITE SEQUENCING DATA TO DETERMINE THE EPIGENETIC REGULATION OF MIR-17 IN AN ALZHEIMER'S DISEASE MODEL. John D. Arza, Nathan J. MacGilvary & Gary D. Isaacs, Liberty University. Previous research done by our team indicated that there are epigenetic modifications on genes coding for miRNAs in an Alzheimer's disease (AD) model. miRNAs are involved in the post-transcriptional regulation of genes and may play a role in the pathology of AD. miR17-1 showed epigenetic significance from a methylation sensitive microarray analysis. However, the base pair resolution of these epigenetic changes has not been achieved. This study incorporates bisulfite sequencing to analyze the promoter region of miR17-1 for site-specific CpG methylation to further the understanding of AD pathology. In addition, this method makes up for the weaknesses of the methylation microarray in order to give a more holistic picture of the genomic epigenetic changes in AD.

GENERAL METHOD FOR VALIDATION OF PRIMER PAIRS FOR MEASURING INFLAMMATORY GENE EXPRESSION IN NAFLD SUBJECTS BY REAL-TIME Q-PCR. Anna Zhang[1], Edgar Rodriquez[2], Ancha Baranova[2,3], & Aybike Birerdinc[2,3], [1]Chemistry (Biochemistry) Department, College of Science, George Mason University, Fairfax, VA, [2]Betty and Guy Beatty Center for Integrated Research, Inova Health System, Falls Church VA and [3]Center for the Study of Chronic Metabolic Diseases, School of Systems Biology, George Mason University, Fairfax, VA. Real-time polymerase chain reaction (q-PCR) is a popular tool used in a variety of settings to amplify, detect and quantify specific nucleotide sequences, or genes. In order to achieve reliable and reproducible results from q-PCR, it is important to take initial steps to ensure specificity of primer pairs used to initiate the amplification of nucleotide sequences. Primer validation utilizes qPCR and gel electrophoresis to ensure primer specificity. Primer pairs were synthesized using Primer-BLAST tool provided by

NCBI, and validated for the following target genes: *CTGF* (connective tissue growth factor), *IL13* (interleukin-13), *IL17* (interleukin-17), *CSF2* (colony stimulating factor-2) and *CSF3* (colony stimulating factor 3). All targeted genes when elevated, with the exception of *IL13*, are noted to correlate with markers of inflammation and have strong association with the advanced progression of non-alcoholic fatty liver disease (NAFLD) based on previous studies. Prior to designing specific primers, a literature search was done for genes with more than one transcript variant in order to determine the most common transcript variants discovered in visceral adipose tissue. For one such gene, *CSF3*, transcript variant 1 was determined to be the common variant found in adipose tissue. This project aims to document the materials and methods used for primer validation.

THE EXPRESSION OF A DOUBLE GREEN FLUORESCENT PROTEIN-NUCLEAR LOCALIZATION SIGNAL FUSION PROTEIN IN TRANSFECTED HUMAN EMBRYONIC KIDNEY CELLS. Alexander Bond, Kristina Krumpos, Deborah Zies & Stephen Gallik, University of Mary Washington. Green Fluorescent Protein (GFP) is a preferred reporter protein for cellular localization studies, but for nuclear localization studies, a fusion protein containing multiple copies of GFP must be used to eliminate simple diffusion as a mechanism through which the protein can enter the nucleus. Our long-term goal is to create a plasmid expression vector containing four copies of the GFP gene linked to a single monopartite nuclear localization signal (4GFP-1NLS). The specific objective of the research study reported here is to create an intermediate plasmid, containing two copies of the GFP gene, from which the 4GFP-1NLS plasmid could be eventually produced. Using site-directed mutagenesis techniques, the parent plasmid used in this study, the pCMV/myc/nuc/GFP pShooter plasmid (Life Technologies, Inc.), was modified to create 2 intermediate plasmids, one serving as a vector and the other serving as a source for a single copy GFP insert. The restriction enzyme *PstI* was then used to open the vector and isolate the insert. Attempts at ligating the insert into the vector have been unsuccessful. It is hoped that future attempts at the ligation will be successful, leading to the eventual production of the final 4GFP-1NLS plasmid. Once produced, the final plasmid could be used to study various aspects of NLS-dependent nuclear import.

SUPPRESSION OF PYRUVATE KINASE DELETION PHENOTYPES IN *CRYPTOCOCCUS NEOFORMANS*. Nicolas Terreri[1], Joshua Sellwood[1], John R. Perfect[2], and Michael S. Price[1,2], [1]Dept. of Biology and Chemistry, Liberty University, Lynchburg, VA, [2]Div. of Infectious Diseases, Duke University Medical Center, Durham, NC. *Cryptococcus neoformans* is a fungal pathogen that affects immunocompromised individuals such as AIDS patients. With the high prevalence of HIV in Africa, *Cryptococcus neoformans* and relative *Cryptococcus gattii* cause over 600,000 deaths every year just in Africa alone. Unlike many fungal pathogens, *Cryptococcus* migrates from the lungs, usually after causing pneumonia, to the brain into the cerebrospinal fluid (CSF). Once in the brain, it causes fungal meningitis and encephalitis which are life threatening diseases [3]. Carbon utilization is an important

part of the persistence of *Cryptococcus neoformans* because glucose utilization is required for CNS disease, and deletion of pyruvate kinase (*PYK1*) inhibits glucose utilization and CNS disease. *pyk1?* deletion mutants have been identified that are able to grow on glucose. We are identifying the gene(s) responsible for this phenotype rescue, which appears to be correlated with increased hyphal growth likely due to activation of the MAT locus located on Chromosome 5.

ESTABLISHMENT OF A CELL CULTURE SYSTEM FOR MEASURING THE EXPRESSION OF THE LONG NON-CODING RNA GAS5. J. Shahid[1], K. Solocinski[2], M. L. Gumz[2] & D. Zies[1], [1]Department of Biological Sciences, University of Mary Washington and [2]Department of Medicine, University of Florida College of Medicine. Aldosterone, a primary regulator of blood pressure in mammals, functions by complexing with the mineralocorticoid receptor and altering the expression of blood pressure associated genes. It is my hypothesis that Gas5, a newly discovered long non-coding RNA, is also a negative regulator of the aldosterone response. The overall goal of this project is to test this hypothesis by treating mouse IMCD3 cells with aldosterone and measuring changes in Gas5 mRNA expression by real-time PCR. Through my research experience at the University of Florida (UF) in summer 2014, I was able to learn about long noncoding RNAs, aldosterone, transporter proteins, cell signaling pathways in the kidneys and the molecular techniques used to study them. I gained hands-on experience managing and treating cell cultures in order to perform RNA isolations, RT-PCR, and semi-quantitative and real-time PCR and also western blots. My specific goal here, at UMW, has been to establish the use of these skills and extend the work started at UF. Here, I show results from successful RNA isolation from aldosterone treated IMCD3 cells and preliminary real-time PCR experiments. The establishment of these protocols will help future students investigate the link between Gas5 and Aldosterone. If Gas5 is involved in regulating the aldosterone response then understanding more about its expression may reveal its effects in blood pressure regulation and facilitate the treatment of cardiovascular disease.

TXL INDUCED APOPTOSIS IN JURKAT E6-1 CELLS. Claire R. Harrington & Rosemary Barra, Depart. of Biological Sciences, University of Mary Washington, Fredericksburg, VA 22401. The herbal dietary supplement, Tian Xian Liquid (TXL), has been reported to be an effective treatment for some forms of cancer. The mechanism of this effect is unknown, however, studies using a related herbal extract, Tien-Hsien liquid, showed an increase in apoptosis in cancer cells. The activation of p53 is a major regulator of cellular apoptosis. In this study, the anti-proliferative effects of TXL were determined by utilizing a MTT Assay. An ELISA assay was subsequently used to quantify p53 levels in TXL-treated cells. TXL, at concentrations ranging from .002 to .2 mg/mL, showed significant anti-proliferative effects in a dose-dependent manner on transformed cells. As the concentration of TXL increased, the number of viable cells decreased. At .2 mg/mL, the viability expressed as a percent of control values was 54.5%. There was an increased level of p53 activity in the TXL-treated cells. Interestingly, the cells treated with .002 mg/mL of TXL showed the greatest

absorbance, indicating the greatest activity of p53 in those cells, compared to the control and the higher concentrations of TXL. This may be due to the fact that there are a greater number of viable cells at lower concentrations of TXL, allowing the p53 levels to be observed more readily. This is preliminary data and more research is needed to confirm the role of p53 in the anti-proliferative effects of TXL.

INVESTIGATING PHENOTYPIC DIFFERENCES BETWEEN STP1 K/O AND WT *ARABIDOPSIS THALIANA* IN RESPONSE TO VARIOUS SALT CONCENTRATIONS. Katie McCullar, Dustin Phillips, Maria Wilkins & Janet Daniel, Department of Biology, James Madison University, Harrisonburg, VA 22807. *Arabidopsis thaliana* is a commonly used model organism in the study of plants and is described as a glycophytic plant. In this experiment, the role of sugar transport protein-1 (STP1) in relation to salt resistance is investigated by observing phenotypic differences in the growth of wild type (WT) and STP1 k/o plants when exposed to varying concentrations of sodium chloride using hydroponics and agar plates. The hydroponics system is used to expose the plants to 0mM or 50mM concentrations and measurements are taken of root length, stalk length and number of leaves at four weeks. The average root lengths of STP1 k/o were longer than WT at 50mM after four weeks when grown using hydroponics. We also investigated a dose response using agar plate concentrations from 0-200mM. Root length was not correlated with NaCl concentration. While increased average root lengths were seen at 25mM and 100mM NaCl, at concentrations greater than 100mM, both WT, and STP1 k/o decreased in average root lengths. Overall, STP1 k/o average root lengths grown on plates were longer than WT root lengths, at two and four weeks. In total, results suggest that the STP1 k/o plant exhibits an alternate phenotype when grown in higher NaCl concentrations. This may indicate that STP1 k/o phenotype includes a resistance to increased salt concentrations.

DETERMINATION OF THE IMPACT OF *PYK1* DELETION ON INTERACTIONS OF *C. NEOFORMANS* WITH THE HOST IMMUNE SYSTEM. Elizabeth Rasmussen[1], Yansirre Aviles[1], Michal Olszewski[2], and Michael Price[1], [1]Dept. of Biology & Chemistry, Liberty University, Lynchburg. VA, [2]Div. of Pulmonary and Critical Care Medicine, University of Michigan, Ann Arbor, MI. *Cryptococcus neoformans* is an important fungal pathogen of immunocompromised individuals. During initial infection, *C. neoformans* colonizes the airspaces of the lungs, resulting in pneumonia, and subsequently migrates to the central nervous system (CNS). There is also epidemiological evidence for dormancy of cryptococcal infections. To greater understand fungal carbon utilization (particularly gluconeogenesis and glycolysis) during colonization of these fundamentally different niches within the host, mutants were created at key points in these carbon metabolic pathways. Our objective is to develop a model that will allow for the effective studying of dormancy in this important human pathogen by quantifying cytokine expression in macrophages exposed to these pyruvate kinase mutants that fail to elicit inflammation in the lung.

OPTIMIZING METAGENOMICS ANALYSIS. Vhuthuhawe T. Madzinge & Andrew J. Fabich, Dept. of Biology and Chemisty, Liberty Univ., Lynchburg, VA 24515. *Escherichia coli* is a micro-organism that is common in the gastrointestinal tract. It is found in normal microbiota. While most *E. coli* are harmless, some are equipped with toxins that are harmful to humans. The focus of this study in this experiment uses non-pathogenic *E.coli* studied in streptomycin-treated mice. *E.coli* was used as a model to observe the changes that are likely to occur in the GI when it is introduced in streptomycin-treated mice. *E.coli* was chosen because previous studies have shown it to become an efficient colonizer. Such advantageous colonization is achieved by its ability to compete for nutrients efficiently and maintain a growth rate of 2-hours per turnover of the intestinal contents. These advantageous abilities are influenced by the deletion of *flhDC* operon, also known as the master regulator of flagella synthesis. Its deletion saves energy and thus causes an up-regulation/hyper-expression of carbon and energy metabolizing genes therefore increasing the population of *E.coli*. However, how do these changes affect the community of the normal microbiota? Is this advantageous or disadvantageous? Does this improve or decrease the health of the streptomycin-treated mice? First, knowing what the microbial community that interact with *E.coli* are made of will assist in answering some of these questions. Streptomycin-treated mice colonized with different *E. coli* demonstrated similar metagenomic signatures with notable differences in the Bifidobacteria. Studying these interactions will help us understand the value of bacterial interaction in mammals.

INDUCING *CITROBACTER RODENTIUM* VIRULENCE IN STREPTOMYCIN-TREATED MICE. Kaitlyn A. Shondelmyer and Andrew J. Fabich, Dept. of Biology and Chemisty, Liberty Univ., Lynchburg, VA 24515. *C. rodentium* causes disease in conventional mice; however, it does not in streptomycin-treated mice. We know, therefore, that colonization is not sufficient for pathogenesis, so there must be other facultative anaerobes driving pathogenesis. Competition with certain *E. coli* strains causes pathogenesis by an unknown mechanism. If the competition-induced disease state is similar to disease caused by *C. rodentium* in conventional mice, inducing pathogenesis via competition will be relevant to EHEC modeling. Streptomycin-treated mice colonized with *C. rodentium* and laboratory strains of *E. coli* did not induce pathogenesis. However, pathogenesis returned with *C. rodentium* colonized with either human commensal or probiotic *E. coli*.

TAU AND BETA-AMYLOID INTERACTIONS IN ALZHEIMER'S DISEASE. Tyrrell C. Graham & Deborah A. O'Dell, Dept. Biological Sciences, UMW, Fredericksburg, VA 22401. In Alzheimer's Disease, changes in the phosphorylation of Tau protein and the presence of b-amyloid plaques are seen. The stimulus for changing Tau phosphorylation is unknown. The effect of the presence on beta-amyloid aggregates on the phosphorylation state of Tau was examined by exposing cultured neurons to beta-amyloid aggregates and using immunohistochemistry. Microscopic examination of cells showed that cultured cells exposed to aggregates had increased levels of pThr231 Tau protein compared to control cells. This suggests that the

presence of beta-amyloid plaques stimulates the changes in the phosphorylation of Tau. This work was supported by an Undergraduate Research Grant from UMW.

RHO-GDP DISSOCIATION INHIBITOR AFFECTS GROWTH AND AFLATOXIN PRODUCTION IN *ASPERGILLUS FLAVUS*. Stephen Matherlee[1], Claudia Bernaschina[1], Gregory OBrian[2], Gary A. Payne[2], and Michael S. Price[1, 2], [1]Dept. of Biology & Chemistry, Liberty University, Lynchburg. VA, [2]Dept. of Plant Pathology, NC State University, Raleigh, NC. Regulation of aflatoxin (AF) production is complex, involving transcriptional and post-transcriptional regulation focused mainly through the pathway specific transcriptional regulator *aflR*. An investigation into the nature of the transcriptional regulation of AF production by comparing conducive and non-conducive culture conditions revealed a clade of genes with a similar transcription profile to that of *aflR*. One of these genes, a putative Rho-GDP dissociation inhibitor, was characterized by gene deletion and shown to regulate AF production in *Aspergillus flavus*. The protein encoded by this gene, Afrdi1, showed 45% identity to Rdi1p in *S. cerevisiae*. The Δ*Afrdi1* mutant exhibits a severe growth defect on minimal medium, a moderate growth defect on complete medium, and a temperature sensitive phenotype. Moreover, the Δ*Afrdi1* mutant produces 97.3% less toxin than wild type. Inferences from *S. cerevisiae* reveal a possible link between AfRdi1 and RasA, which has been shown to regulate sterigmatocystin production in *A. nidulans*.

Biomedical and General Engineering

FEMTOSECOND LASER USE IN MEDICAL THERAPEUTICS: KEY ADVANTAGES AND LIMITATIONS OF NONLINEAR OPTICAL TISSUE INTERACTIONS. William R. Calhoun III[1,2] & Ilko K. Ilev[2], [1]Virginia Commonwealth University, Richmond VA 23298 and [2]Department of Biomedical Physics, Office of Science and Engineering Labs, U.S. Food and Drug Administration, Silver Spring MD 20993. Some of the most commonly performed surgical operations in the world, including laser-assisted in-situ keratomileusis (LASIK), lens replacement (e.g. cataract surgery), and keratoplasty (cornea transplant), now employ Femtosecond Lasers (FSLs) for their extreme precision, low energy and ablation characteristics. The application of FSLs in medical therapeutics is a recent development, and although they offer many benefits, FSLs also stimulate nonlinear optical effects (NOEs), many of which were insignificant with previously developed lasers. In order to improve the understanding of FSL-tissue interactions related to NOEs stimulated during laser beam propagation though corneal tissue, research investigations were conducted to determine how corneal tissue properties including corneal layer, collagen orientation and collagen crosslinking, and laser parameters including pulse energy, repetition rate and numerical aperture affect second and third-harmonic generation (HG) intensity, duration and efficiency. The results of these studies revealed that all laser parameters and tissue properties had a substantial influence on HG. The dynamic relationship between optical breakdown and HG was responsible for many observed changes in HG metrics. The results also

demonstrated that the new generation of therapeutic FSLs has the potential to generate hazardous effects if not carefully controlled. This work was supported by the Oak Ridge Institute for Science and Education.

SOFT ELECTRODE SYSTEMS CAPABLE OF INTEGRATING ON THE AURICLE AS BRAIN-COMPUTER INTERFACE. Dong Sup Lee & Woon-Hong Yeo, Department of Mechanical & Nuclear Engineering, Virginia Commonwealth University, Richmond VA 23284. Non-invasive electrodes for recording of electroencephalograms on the scalp offer the diagnosis of neurological disorders and brain-computer interfaces. However, the existing devices using conductive gels are not usable for more than a few days due to side effects such as the skin irritation and irreversible degradation of electrical properties at the skin interface. To overcome the limitations, we introduce a set of electrodes and interconnects composed by a soft, foldable collection of open fractal mesh that adequately mounts on the complex surface topology of auricle and mastoid for high performance and long-term monitoring of electroencephalograms. Computational and experimental studies constitute the fundamental aspects of the bending and stretching mechanics suitable on highly irregular and textured surfaces. Cell level tests and thermal imaging studies demonstrate the biocompatibility and confirm wearability throughout daily activities including exercise, sleeping, and bathing. Experiment includes a text speller via steady-state visually evoked potential-based brain-computer interfaces.

FIBRONECTIN FIBRILLOGENESIS MEDIATES TGF-β1-INDUCE EMT IN MAMMARY EPITHELIAL CELLS. Lauren A. Griggs[1], Roshni Malik[1], Nadiah Hassan[1], Brittany A. Martinez[1], Lynne W. Elmore[2] & Christopher A. Lemmon[1], [1]Department of Biomedical Engineering, [2]Department of Pathology, Virginia Commonwealth University, Richmond VA 23284. Epithelial to Mesenchymal Transition (EMT) is a biological process characterized by a phenotypic switch in epithelial cell sheets into motile and invasive mesenchymal cells. During cancer progression, carcinoma cells seize the EMT regulatory circuity to initiate metastasis. This work investigates the role of the microenvironment in the induction of EMT. We examine the relationship between assembly of the extracellular matrix protein fibronectin (FN) into insoluble fibrils and the occurrence of EMT. We believe that increased tissue stiffness drives FN assembly, which exposes cryptic binding sites for various growth factors, such as Transforming Growth Factor-Beta1 (TGF-β1), and creates a high concentration of these growth factors at the cell surface, which in turn drives EMT. When mammary epithelial cells were co-treated with the FN assembly inhibitor and TGF-β1, EMT was notably inhibited. Addition of soluble FN to culture medium in a dose response alone was unable to induce EMT. Furthermore, increasing cell contractility increased FN assembly, but did not cause cells to undergo EMT, suggesting that growth factor localization to FN was required for EMT. On the other hand, inhibition of contractile forces decreased TGF-β1 induced FN assembly and blocked EMT. This work highlights novel targets in the tumor microenvironment for cancer therapy.

EFFECT OF VISUAL BIOFEEDBACK ON GAIT BALANCE SYMMETRY DURING ELLIPTICAL TRAINER EXERCISE. Trisha J.Massenzo[1] & Peter E. Pidcoe[2], [1]Department of Biomedical Engineering, Virginia Commonwealth University, Richmond VA 23284 and [2]Department of Physical Therapy, Virginia Commonwealth University, Richmond VA 23298. The aftereffects of a stroke can greatly influence parameters of gait, such as decreasing cadence, decreasing balance and stability and increasing the time spent on the non-paretic limb. Modern rehabilitation techniques are transitioning from compensatory actions to constraint-induced therapy. This widely implemented technique promotes neuroplasticity by constraining use of the paretic limb to perform daily activities of living. Both manual therapy and robotics can be implemented during this therapeutic approach to promote brain remodeling. Although manual therapy and robotics are widely used, there are a few disadvantages. Manual therapy poses a high physical demand on therapists, which may directly limit duration of therapy due to fatigue. Robotics offers a solution to this problem, but comes as a costly alternative and limits independence of the patient while gait training. In consideration of the benefits and disadvantages of these therapeutic approaches, a low-cost visual biofeedback system was constructed to allow users to independently adjust kinetic postural parameters. A pilot study was performed on a sample set of healthy participants to determine the effect of visual biofeedback. Four visual representations were also developed and were tested to determine which produced the best performance determined by index of symmetry values. Results proved visual biofeedback during kinetic weight training to be effective and found that one visual representation performed significantly better than the other three representations.

ELECTROPSINNING OF ARABINOXYLAN AS A NOVEL NANOFIBER SCAFFOLD. Donald C Aduba, Jr.[1], W. Andrew Yeudall[2] & Hu Yang[1,2], [1]Department of Biomedical Engineering, Virginia Commonwealth University, Richmond, VA 23284 and [2]Massey Cancer Center, Virginia Commonwealth University, Richmond, VA 23298. Research strategies in developing polysaccharide carbohydrate biomaterials for wound healing have steadily grown over the last decade. Arabinoxylan (AXF) is a carbohydrate polymer derived from cereal grains. However, their potential for clinical applications has yet to be fully realized. It is a polysaccharide comprised of a linear xylose backbone with arabinose units that are ester linked to ferulic acid. AXF is hydrophilic and possesses tunable swelling properties for fluid absorption. Polysaccharides have also been shown to increase macrophage proliferation necessary to ingest bacteria, debris and other infection causing agents. Therefore, AXF may be a suitable polymer to develop a wound dressing material for wound healing applications. This study aims to demonstrate the feasibility of electrospinning AXF to nanofibers and investigate the physical and biocompatible properties of the resulting nanofiber constructs. Gelatin (GEL) was blended with AXF to facilitate nanofiber formation and provide a natural polymer host tissues can readily accept after injury. Blends of GEL to AXF were successfully electrospun and characterized in terms of nanofiber morphology, tensile properties, pore size, degradation, molecular

composition and fibroblast cellular response. The work shows the potential of this novel scaffold for wound dressing development.

DESIGN AND CREATION OF A NOVEL DEVICE TO INDUCE VERGENCE EYE MOVEMENT TO QUANTITATIVELY STUDY THE DIFFERENCE AMONG PATIENTS WITH MTBI. Jacob Jaminet & Paul A. Wetzel, Virginia Commonwealth University, Richmond, VA 23220. Mild traumatic brain injury (mTBI) can affect different areas of the brain including those that are necessary for sight. The vergence eye system is the visual system responsible for depth perception. In order to study the effects of mild traumatic brain injury on vergence eye movements, a novel device was created. A mirror galvanometer is used to reflect a laser spot along a thin membrane plane. The laser spot moves along the visual midline of the viewer to a depth between 10 cm and 100 cm. A previously used program was used to control the mirror galvanometer so that a variety of movements could be programmed into the device. These movements cause the eyes to rotate 10.7° from midline. This device will be used to induce vergence eye movements that can then quantifiably measure the difference in convergence, accommodation, and pupillary constriction. This device will be used to identify the severity of mTBI between patients.

LICHEN INSPIRED SOLAR ENERGY SYSTEM. Jerney B. Davis & Jacquelyn K. Nagel, Department of Engineering, James Madison University, Harrisonburg VA 22807. The Climate Adaptable Solar Energy (CASE) System, as designed by a prior engineering capstone team, is a design inspired by lichen and applies biological concepts of protection and energy conversion to achieve adaptability. Adaptability addresses the performance reduction due to changing environmental conditions. Lichen is a composite organism of algae and fungus. Dye sensitized solar cells (DSSC) are an organic and sustainable method of obtaining electrical energy from light, and mimics algae in lichen. This research aims to vet the previous team's DSSC design for the CASE system. Four different DSSC designs were constructed and tested in various conditions to measure the efficiency in converting electrical energy, protection for the dye, and compact design. Preliminary results indicate that connection to the cells is more important than surface area exposed to the sunlight, and the cells incorporating Parafilm as a protective cover and alligator clips provide the most efficient and consistent voltage. The Parafilm and alligator clip design will be used in future experiments with the CASE system to improve future sustainable energy options.

ARABINOXYLAN FOAMS FOR WOUND DRESSING APPLICATIONS. Donald C Aduba, Jr.[1], W. Andrew Yeudall[2] & Hu Yang[1,2], [1]Department of Biomedical Engineering, Virginia Commonwealth University, Richmond, VA 23284 [2]Massey Cancer Center, Virginia Commonwealth University, Richmond, VA 23298. Fabrication of an ideal wound dressing material is critical in managing healing post-injury. Wound dressing materials have been developed to help treat acute, moderately exudating wounds by creating a moist microenvironment conducive to tissue regeneration while preventing infection at the injury site. An ideal wound healing

material must possess the following properties to help aid wound management. It must be an occluder and have good biocompatibility. It should have mechanical strength for insulation, wound protection and exudate removal from the injury site. Lastly, it must be absorptive, impermeable to bacteria and inexpensive. Many current wound dressing materials on the market possess the aforementioned properties but none have used arabinoxylan as a base material. Arabinoxylan should be considered as a wound dressing because of its high porosity and swelling properties which allow easy absorption and retention of wound exudate. This allows the injury site to stay moist. Similar carbohydrate based polymers as arabinoxylan have also shown an ability to modulate immune response which is critical during the inflammation stage of wound healing. The goal of this study is to investigate and highlight the material and biocompatible properties of arabinoxylan foams as a potential wound dressing material. D.A. is a recipient of SREB-State Doctoral Fellowship.

Posters

SUSTAINABLE MANUFACTURING THROUGH BIO-INSPIRED DESIGN. Jacquelyn K Nagel[1], Chris Graves[1], Austin Underhill[1], Katie McCullar[2] & Katie Kelly[3], [1]Dept. of Engineering, [2]Dept. of Biology, [3]Dept. of Integrated Science & Technology, James Madison Univ., Harrisonburg VA 22807. Bio-inspired design, or biomimicry, is an approach to innovation by taking nature's patterns, forms, functions, processes, and materials and using them to develop engineering solutions. Biological systems exhibit multi-functionality from form and not material which offers inspiration for product life-cycle management. The goal is to better understand the connection between form and function as found in nature to re-design semi-recyclable products. Through application of bio-inspired design, to the manufacturing and disposal lifecycle phases, product recyclability is increased through minimization of material diversity while still achieving desired functions. One inspiring biological morphology that has been utilized across multiple biological kingdoms and in this research is variations in hardness and flexibility found in alternating layers that are used to provide strength, durability, distribution channels, and protection. Another inspiring morphology considered in this research is found on the neck membrane of the exoskeleton of a dragonfly, which consists of intricate folding that provides the functions of stiffness, elasticity, and low friction smoothness which increases maneuverability of the dragonfly's head. These multi-function forms have resulted in the redesign of a semi-recyclable product fabricated using additive manufacturing to create a product that is made from a single material yet still achieves all necessary functions.

Botany

AN ANALYSIS OF INFRASPECIFIC VARIATION WITHIN *ELEOCHARIS* TENUIS (CYPERACEAE). Lane D. Gibbons & Conley K. McMullen, Dept. of Biol., James Madison Univ., Harrisonburg VA 22807. The presence of subtle and often

vague variations in morphology that convolute specific and subspecific boundaries within the genus *Eleocharis* R.Br. (Cyperaceae) has resulted in lasting taxonomic uncertainty. As with many species of *Eleocharis*, taxonomic issues within the *E. tenuis* complex are made more difficult due to an array of diminutive morphological characters typical of the genus. As currently circumscribed, the varieties of *E. tenuis* present considerable levels of infra- and interspecific variation between the varieties of *E. tenuis* (Willd.) Schult. and its close congeners *E. compressa* Sullivant and *E. elliptica* Kunth. This suite of plants exhibits various morphological character states intermediate to one or more taxonomic entities which, has resulted in a provisional treatment of the group that remains to be elucidated. Multiple authors have added confusion to the complex by proposing various hypotheses for the infra- and interspecific relationships of *E. tenuis*. Though some proposed changes are notable and widely discussed, researchers have not yet generated the taxonomic data necessary to conclude such discussions. To evaluate fully infra- and interspecific relationships within the *E. tenuis* complex and elucidate species relationships in *Eleocharis*, a rigorous analysis of morphological variation within the species *E. tenuis* intent on determining the true presence and relative strength of intermediate characters as well as their correlation to taxonomic entities is currently in progress.

CLEISTOGAMOUS POLLINATION IN SUBTERRANEAN SPATHES OF *COMMELINA BENGHALENSIS* (COMMELINACEAE). Camille Fagan & W. John Hayden, Dept. of Biol., Univ. Richmond. *Commelina benghalensis* (Tropical Spiderwort) is an Old World species currently expanding its range in North America as a troublesome agricultural weed. We studied the anatomy of its subterranean cleistogamous flowers with the goal to understand better the reproductive process undertaken by these unusual structures. Only the three anterior stamens of cleistogamous flowers bear functional pollen grains, the three posterior stamens are non-functional. Tapetum is amoeboid and functional anthers bear a well-developed endothecial layer. The two anterior carpels each bear two ovules but the posterior carpel bears a single ovule. Ovules are orthotropous. In cleistogamous flower buds the style is straight; however, at the stage comparable to anthesis in a chasmogamous flower, the style elongates in a helical fashion as described in previous literature. Our observations suggest that helical style growth is an adaptation to facilitate rupture of anther sacs thus bringing pollen grains into contact with stigmas. Pollen tubes were observed within the acellular transmitting tissue of older styles.

ANATOMY OF HOMEOTIC MALE TO FEMALE INFLORESCENCES OF *ACALYPHA HERZOGIANA* (EUPHORBIACEAE). Carlee Evans, Joie Ha, & W. John Hayden, Dept. of Biol., University of Richmond. Whereas wild type *Acalypha herzogiana* produces terminal spikes bearing inconspicuous staminate flowers, cultivated forms produce terminal spikes of showy red pistillate flowers, putatively the result of a homeotic male to female mutation. We studied flower development in cultivated *A.herzogiana*; for comparison, ordinary male and female flowers of *A.wilkesiana* were also studied. The showy spikes of *A.herzogiana*, as is typical of the

genus, consist of a central axis bearing cyme-like clusters of flowers in the axils of inconspicuous bracts. Floral meristems first initiate four sepals, which subsequently enclose four (or more) primordia, initial stages of which we interpret to be consistent with stamen primordia. However, unlike typical stamens, these primordia expand laterally, eventually filling the space between the sepals, at which point ovule-like structures become detectable. Ongoing studies will focus on the transition from early stages resembling staminate flowers through the mature structure of homeotic pistillate flowers.

EFFECT OF LEAF AGE ON ANTIOXIDANT CONTENT IN *SALVIA OFFICINALIS* AND *LAVANDULA ANGUSTIFOLIA*. W. H. Deaver, W. J. Geyer & M. H. Renfroe, Dept. of Biol., James Madison Univ., Harrisonburg VA 22801. *Salvia officinalis* and *Lavendula angustifolia* are herbs that are known to have beneficial levels of antioxidants, which the human body uses to counteract harmful reactive oxidative species. Top, middle, and bottom leaves were sampled from the plants in order to test for differences in antioxidant values as aging in leaves progresses. Previous studies in the effects of foliar aging on antioxidant levels have shown a tendency for the newer leaves towards the top of the plants to have higher antioxidant levels. An ABTS decoloration assay was used to measure antioxidants extracted from fresh leaves of these two herbs. Acquired data was analyzed using a one-way analysis of variance followed by a Dunnett's T3 test to determine significance of differences of means at a 95% confidence interval. Analysis of fresh weight and dry weight values for both plants showed a significant difference in means for both hydrophilic antioxidants and total antioxidants within the plants. The most mature leaves contained the greatest concentration of hydrophilic antioxidants. Youngest leaves contained the least concentration of hydrophilic antioxidants. However, lipophilic antioxidants were not statistically significant and demonstrated more uniform levels throughout both plants. Our findings contradict previous studies and shed light on the unique distribution of antioxidants between newer and younger leaves of *S. officinalis* and *L. angustifolia* as well as raising consumer awareness about antioxidant dietary values.

ANALYSIS OF LIPOPHILIC AND HYDROPHILIC ANTIOXIDANTS IN COMMON CULINARY HERBS AND SPICES. C. R. Thiel, T. J. Mullins & M. H. Renfroe, Dept. of Biol., James Madison Univ., Harrisonburg VA 22801. Lipophilic and hydrophilic antioxidant contents were analyzed for basil, Mediterranean basil, parsley, cilantro, rosemary, gourmet rosemary, rubbed sage, oregano, chives, and thyme. Extracts were analyzed using an ABTS decoloration assay and reported as trolox equivalents. Among the dried spices that were tested, chives, parsley, and cilantro contained relatively low concentrations of hydrophilic antioxidants. Oregano and Mediterranean basil contained intermediate concentrations of hydrophilic antioxidants, and sage, rosemary, thyme, and basil contained high concentrations of hydrophilic antioxidants. Rosemary contained significantly more hydrophilic antioxidant than any other tested herb. When tested for lipophilic antioxidants, Mediterranean basil, basil, parsley, chives, cilantro, and oregano had relatively low

concentrations of antioxidant content. Thyme and sage had intermediate content, and rosemary and gourmet rosemary had the highest lipophilic antioxidant content. These results may be especially useful to dieticians preparing specialized diets for clients with particular health needs.

EFFECTS OF WEIR ESTABLISHMENT ON VEGETATION SURROUNDING LAKE TECUMSEH IN VIRGINIA BEACH, VA. Julie M. Slater[1], Willard Smith[2] & Robert B. Atkinson[1], [1]Department of Organismal & Environmental Biology, Christopher Newport University, Newport News, VA 23606 & [2]U.S. Fish & Wildlife Service, Virginia Field Office, Gloucester, VA 23061. Lake Tecumseh (also known as Brinson Inlet Lake) is a shallow mesotrophic lake in Virginia Beach, VA within the watershed of Back Bay, a nationally significant estuary. In 2011, the US Fish and Wildlife Service established two submerged weirs on the lake in order to reduce silt discharge into the Back Bay estuary; however, regulatory authorities were concerned higher water levels resulting from weir operation could lead to shifts in the composition of the adjacent forested wetland community. The purpose of this study was to identify effects of the weirs on vegetation in and around the lake. In 8 10-m^2 plots (for trees) and 24 1-m^2 (for herbs) we monitored tree mortality, average percent herbaceous cover, percent open water, plant species richness, and percent canopy closure annually from 2009 to 2014; and bald cypress (*Taxodium distichum*) tree cores were collected in fall 2014. No directional shifts in the wetland plant community composition or tree ring widths were observed in wetlands adjacent to the lake.

THE EFFECT OF SALINITY AND ELEVATION ON TREE RING WIDTH OF LOBLOLLY PINE (*PINUS TAEDA*) AT FOUR TIDAL WETLAND SITES ALONG THE YORK RIVER ESTUARY, VIRGINIA. Brittany D. Bowen & Robert B. Atkinson, Dept. of Organismal & Env. Biol., Christopher Newport Univ., Newport News, VA, 23606. Loblolly pine, *Pinus taeda* L., is a dominant species in coastal plant communities throughout the southeastern US and occurs at elevations that are subject to the effects of rising sea level. The purpose of this study was to evaluate the effect of elevation and salinity on annual growth of 40 *P. taeda* trees located at super tidal (low elevation) and non-tidal (high elevation) positions at four sites along a salinity gradient present on the York River Estuary, Virginia. Tree cores were collected from 10 trees at each site using an increment borer and were dried, mounted, and measured. Elevation was measured at each tree using a Real Time Kinematic (RTK) Global Positioning System. No clear trends for the effect of elevation were noted. For trees at lowest elevation, ring widths of the first ten years were found to be significantly different among the four sites ($p = 0.02$), with numerically lowest widths associated with highest salinity. The results of this study suggest that local elevation and position along the salinity gradient may influence stress exposure and alter structure in coastal forested communities. Special acknowledgments to the Rouse-Bottom Fellowship Program and the GK-12 Fellowship Program.

SAPLING RESPONSE TO BEAVER PREDATION IN A CREATED FORESTED WETLAND IN LOUDOUN, VA. B. Gerovac, E. Wright & R. B. Atkinson, Department of Organismal & Environmental Biology, Christopher Newport University, Newport News, VA 23606. Wetlands are known to be created by the American Beaver (*Castor canadensis)* via dam building and by anthropogenic activities, such as the creation of mitigation wetlands in accordance with the Clean Water Act of 1972. Beaver activities which influence the development of mitigation created wetlands, such as changes in hydrology or herbivory on planted trees, may hinder tree establishment in mitigation sites. In 2009, 17 plots consisting of three or four subplots were established in a mitigation site located at the eastern edge of Loudoun County. Each subplot was randomly planted with 7 tree species and 3 stock types (21 experimental units) with a total of 1092 trees. Survival and morphometric measurements, including stem diameter, canopy size, and tree height, were collected annually and in the spring of 2014 when girdling and/or stem removal by beaver were first discovered. Of the seven planted tree species, *Salix nigra*, though not the most prevalent species by 2014, did exhibit the greatest beaver predation (53%). *Platanus occidentalis* exhibited the lowest frequency of damage (3%). These findings are consistent with previously published literature demonstrating beaver selectivity for species of the genus *Salix* as well as other works that describe beaver preference being independent of tree species abundance.

THE FLORA OF VIRGINIA: THE FLORA APP AND NEW DIRECTIONS FOR THE PROJECT. Bland Crowder, Flora of Virginia Project, Richmond VA 232180512. The Flora Project was formed in 2001 to oversee production of the *Flora of Virginia,* published in 2012. In addition to authors Alan Weakley, J. Christopher Ludwig, and John Townsend, nearly 100 people worked in research, writing, advising, outreach, illustrating, and fund-raising. The *Flora* could not have been possible without the support of our designated partners, the Virginia Natural Heritage Program, the Virginia Academy of Science, the Virginia Native Plant Society, the Virginia Botanical Associates, and Lewis Ginter Botanical Garden, Richmond. Our phase-two mission is education, but it includes many kinds of students, K–12, college-level, and adult (each also diverse). It includes outreach, to increase awareness of the Project and the need for environmental stewardship. And it includes creation of our Flora App. The App will put the contents of the *Flora* into a truly portable format—smart phones and tablets—but it will be more than an eBook. The *Flora's* descriptions have been converted into a database with which six other environmental data sets will be merged. It will provide dichotomous keys, as in the book, but the new streamlined, graphic key will be a hallmark. The App will attract new users, like students in grades 6–12 who might otherwise use the *Flora* only as limited handouts, but also, via connection to social media (e.g., Facebook, Instagram), it will appeal to children as young as 6 in a way that parallels a popular computer game—but focusing on actual living organisms: Virginia plants.

THE FLORA OF VIRGINIA PROJECT: OVERVIEW OF EDUCATIONAL MODULES FOR COLLEGE STUDENTS AND ADULT LEARNERS. Marion B. Lobstein, Professor Emeritus, Northern Virginia Community College. The *Flora of Virginia* was published in December 2012 and the second printing with corrections in December 2013. The Foundation of the Flora of Virginia Project continues to pursue goals of the Flora Project. One of these goals is the development of teaching and learning modules at the K-12, undergraduate, and adult education levels. General background on the importance of education efforts pertaining to use of *the Flora of Virginia* and the efforts of the Education Committee of the Foundation of the Flora of Virginia Project was briefly discussed. This presentation outlined the following six modules under current development for undergraduate and adult education: overview of the layout of the *Flora of Virginia*, how to use the dichotomous keys of the *Flora*, taxonomy and how to use and interpret the synonymy used in the *Flora*, what is a plant and overview of basic botany of vegetative and reproductive structure as well as life cycles of groups covered in the *Flora*, characteristics of major plant families included in the Flora, and habitat information and how to use the information in the *Flora* chapter "Nature of Virginia Flora." Members of the Botany Section were encouraged to consider reviewing these modules for use at the undergraduate level and to complete a questionnaire indicating interest in assisting in this review process.

TREE GROWTH IN CREATED PIEDMONT WETLANDS IN RELATION TO VERTICAL VEGETATION STRUCTURE. Eli Wright & Robert Atkinson, Department of Organismal & Environmental Biology, Christopher Newport University, Newport News, VA 23606. In Virginia the most frequently destroyed wetland type is freshwater forested wetlands with many permitted projects requiring 2:1 mitigation. Success of created forested wetland mitigation sites is dependent in part on criteria related to tree growth, but the effect of interspecific competition on growth is poorly understood. In February of 2009, 1,596 trees composed of 7 species and 3 stock types were planted in 76 subplots across 3 constructed mitigation bank sites. Three morphometric growth parameters were collected annually through 2014. In summer of 2014, the extent of vertical vegetation densities was characterized within four strata for both planted saplings and colonizing herbaceous vegetation by utilizing a 2-meter tall vertical cover board divided into four, 0.5 m quadrants. Results indicate a negative linear correlation between increased extent of herbaceous vertical vegetation and tree growth. The strongest relationship observed ($r^2 = 0.2357$) occurred when the extent of strata co-occupation between tree canopy and herbaceous vegetation was characterized. These results suggest that competition between saplings and herbaceous vegetation for light, and possibly for other resources including nutrients and water, is likely influencing tree growth.

USING ARCGIS TO EVALUATE COMPETITION IN CREATION OF FORESTED WETLANDS IN VIRGINIA. P. Foote, E. Wright, & R. Atkinson, Department of Organismal and Environmental Biology, Christopher Newport University, Newport News VA 23606. The successful creation of forested wetlands is an important part in

the mitigation process of wetland permitting under the Clean Water Act. Tree establishment has often been cited as the most challenging objective. The purpose of this study was to assess the interspecific shade competition effects that could alter growth of planted trees within a created wetland utilizing the geographic software package, ArcGIS. In February 2009, 1596 trees representing 7 species and 3 stock types were planted in 76 subplots across 3 constructed mitigation bank sites in Loudoun County, Virginia. Height of surviving trees were measured each August since planting with average vegetation height and maximum vegetation height being measured at all planting sites during summer 2014. ArcMap 10.2 was utilized to georeference each tree location within a defined coordinate system to create graphic visualizations of relative height and growth of each planted tree and competing vegetation. Graphical outputs comparing average vegetation heights with height of planted trees successfully facilitated observations of trends heretofore only shown statistically; however, few other known relationships were graphically represented, indicating that GIS may have limited application in assessing interspecific competition in created forested wetlands.

Posters

REGENERATION AND RECRUITMENT IN A HEMLOCK-HARDWOOD FOREST AT SHENANDOAH RETREAT, VA. M. Phillips, J. Kincaid, & A. Landes, Env. Studies Program, Shenandoah Univ., Winchester, VA 22601. *Tsuga canadensis* (Eastern hemlock) dominates portions of eastern forests in North America but its distribution and abundance is changing as the result of the nonnative hemlock wooly adelgid (HWA, *Adelges tsugae*). Loss of *T. canadensis* may substantially alter ecosystem composition, structure, diversity, and function. The goal of this research is to characterize tree regeneration and recruitment in a hemlock-hardwood forest prior to significant change in forest composition and structure. A 20x50 meter plot consisting of 10x10 meter quadrats was established. Within each quadrat, all seedlings, saplings, trees and snags were counted and identified; cores extracted by increment borers were taken from all *T. canadensis* stems in the sample plot; tree rings were visually counted and dated. The forest is currently dominated by *T. canadensis*. Size and age structures indicate pulses of regeneration, but waning recruitment for *T. canadensis*. Lack of recruitment, largely resulting from observed HWA-induced mortality, suggests this forest will soon experience significant shifts in species composition and structure. The forest will likely experience increases in species such as *Acer rubrum*, *Quercus prinus*, and *Q. rubra*. Establishment of *Ailanthus altissima* is also cause for concern because this exotic tree easily displaces native vegetation in canopy gaps such as those created by *T. canadensis* mortality. As this forest shifts in composition and structure, we can also expect changes in the hydrology and ecology of the adjacent stream. Information presented by this research provides a baseline for forest monitoring and management efforts at Shenandoah Retreat, Virginia.

RADIAL GROWTH OF ATLANTIC WHITE CEDAR UNDER CONTRASTING HYDROLOGICAL CONDITIONS IN THE GREAT DISMAL SWAMP. K. M.

Kowalski & R. B. Atkinson, Dept. of Organismal & Env. Biol., Christopher Newport Univ., Newport News, VA, 23606. Atlantic white cedar, *Chamaecyparis thyoides*, is an obligate wetland tree that once dominated the Great Dismal Swamp (GDS). However, the species now exists in small, scattered stands. Portions of GDS contain ditches which have lowered the local water table. The purpose of this study is to assess radial growth of cedar in saturated and drained soils within a single system, the GDSNWR. Two perpendicular core samples were collected from ten mature cedars in the saturated site. One cross section sample was collected from ten downed cedar in the drained site. Samples were air dried before sanding with progressively finer sandpaper. Ring widths were measured using a sliding stage microscope connected to a computer with MeasureJ2X software. Mean ring width of the saturated site (2.35±2.06 mm) differed from the drained site (2.80±1.61 mm) ($p<0.001$). The widest and narrowest mean annual ring widths occurred in 1949 (4.16 mm) and 2008 (1.0 mm) for the saturated site and 1975 (3.95 mm) and 1930 (1.05 mm) for the drained site (respectively). Results suggest that cedars grown in divergent hydrological conditions within the same swamp system have dissimilar patterns of radial growth. These data may be useful in evaluating historic hydrologic conditions in regions of swamps where historic hydrologic data may be lacking. Special acknowledgment to the NSF GK-12 program.

ATTEMPTING TO OVERCOME "PLANT BLINDNESS": THE EFFECTS OF PARTICIPATING IN PEOPLE-PLANT INTERACTION ACTIVITIES ON COLLEGE STUDENT ATTITUDES AND INTEREST IN PLANTS. Lisa D. Williams, Dept. of Biol., Northern Virginia Community College, Annandale, VA 22003. New lecture materials and lab exercises for a mixed-majors general biology course focusing on people-plant relationships were developed. Students were initially surveyed regarding their interest in, knowledge of, and motivation to learn about plants. During the non-treatment unit, students participated in a traditional lecture method of instruction and lab exercises on plant structure and assessed thereafter. Topics covered during the treatment unit included medicinal plants and relationships amongst plants, soil, water and people. Plant examples were used to illustrate ecological principles. The lecture method, two short assessments, two out-of-class assignments, a drawing exercise, and creation of a woody plant portfolio were used to capture student interest. Students also participated in lab exercises on medicinal properties of plants and tea brewing and tasting. No change was found in student interest in plant-related topics over the course of this project. Student ability to identify common woody plants and vines significantly improved after developing the plant portfolio. Instructor motivation to teach this course was low-to-moderate at the beginning of the project but highly motivated after this project. A new botany course intended for non-science majors has been proposed using many of the materials and tools from this project.

Chemistry

SYNTHESIS OF METAL ORGANIC FRAMEWORKS AND THEIR ACTIVATION KINETICS. Barbara A. Reisner & W. Tyler Price, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg VA 22807. Metal organic frameworks derived from the hydrotris(1,2,4-triazolyl)borate ligand were synthesized from water, dimethylformamide (DMF) and isopropanol (IPA). $Na[BH(C_2H_3N_3)_3]\cdot$solvent (solvent = H_2O, DMF, IPA) crystallize as a porous framework with the distorted primitive cubic (pcu) topology. Solvent molecules occupy the framework pores. The solvent of crystallization can be removed by heating. Isothermal thermogravimetric analysis shows that solvent loss is consistent with a 1-D diffusion mechanism. Variable temperature powder X-ray diffraction (PXRD) data show some loss of crystallinity upon desolvation, indicating some framework decomposition. These materials adsorb water from the atmosphere. The structures of $Na[BH(C_2H_3N_3)_3]\cdot$solvent, their thermal behavior, stability and the kinetics of solvent loss of will be reported.

EVALUATION OF NAPHTHALIMIDE-TAGGED RUTHENIUM (II)-ARENE COMPLEXES AS POTENTIAL ANTICANCER AGENTS. Kesete Y. Ghebreyessus[1], Ashley N. Peralta[1], Meena Katdare[2], Krishnan Prabhakaran[2], & Shanthi Paranawithana[1], [1]Department of Chemistry, & [2]Skin of Color Research Institute, Hampton University, Hampton, VA 23668. New ruthenium (II)-arene complexes bearing ligands that incorporate a biologically active 1,8-naphthalimide moiety have been synthesized and characterized by NMR, IR, and electrospray (ESI-MS) mass-spectrometer. The anticancer activities of the ligands and their corresponding ruthenium (II)-arene complexes were further evaluated *in vitro* against CRL7687 (human melanoma skin cancer) and CA-M75 (normal skin melanocyte) cell lines. All of the compounds exhibit significantly high anticancer activity, with IC_{50} values of <1mM. The high anti-proliferative activity of the new ruthenium (II)-arene complexes against the human melanoma skin cancer cell line has indicated their potential for further development as anticancer drugs. Furthermore, as DNA is considered to be one of the main biological targets for ruthenium(II)-arene complexes, their interaction with DNA were followed by UV-Vis and fluorescence spectroscopy, and gel electrophoresis assay. The results of the absorption and fluorescence titrations, and gel electrophoresis assay suggest that these new complexes bind to DNA moderately, presumably interacting through an intercalative mode. (Supported by the Hampton University Faculty Research Fund and NSF CREST center).

WinPSSP: A REVAMP OF THE CRYSTAL STRUCTURE DETERMINATION PROGRAM PSSP WITH EDUCATIONAL PERSPECTIVES. S. Pagola[1], A. Polymeros[2] & N. Kourkoumelis[3], [1]Applied Science Dept., College of William & Mary & Applied Research Center, 12050 Jefferson Avenue, Newport News, VA, 23606, [2]Department of Physics, University of Ioannina, 45110, Ioannina, Greece, [3]Department of Medical Physics, Medical School, University of Ioannina, 45110, Ioannina, Greece.

PSSP is a direct-space methods program for the crystal structure solution of molecular solids from X-ray powder diffraction. PSSP uses the integrated intensities of the powder diffraction peaks extracted in a Le Bail fit of the data, the geometry of the molecules from databases or molecular geometry optimizations and the simulated annealing algorithm to locate the molecules (asymmetric unit) in the lattice. *WinPSSP* is based on the *PSSP* source code. A new GUI (graphical user interface) suitable to familiarize undergraduate college students to crystal structure solution from powders has been added, and work on advanced features for non-routine problems, such as crystal structure solution of co-crystals and other materials with more than one crystallographically independent fragment in the asymmetric unit is in progress. Our goals are: (1) to optimize the code for faster runs in windows-based operating systems, and (2) to facilitate additional educational features to introduce the crystallographic and diffraction nomenclature in undergraduate courses.

COMPARISON OF NEGATIVE ION ELECTROSPRAY IONIZATION EFFICIENCIES FOR A DIVERSITY OF SMALL ACIDIC MOLECULES WITH WIDELY VARYING pK_A'S. James M. Mattila, Shelsea A. Hurdle & Christine A. Hughey, Dept. of Chemistry & Biochemistry, James Madison University, Harrisonburg VA 22807. Negative ion electrospray (ESI), an ionization technique that selectively ionizes acidic molecules by deprotonation, has not been studied as extensively as positive ion ESI. As a result, our long-term goals are to elucidate the mechanisms of ionization and to develop a model that predicts ESI response for a diversity of small acidic molecules with a wide range of acidities. To date, negative ion ESI studies have largely focused on two compound classes: phenols and benzoic acids. Here we measure the ionization efficiencies of ~100 compounds by triple quadrupole mass spectrometry. The compounds were systematically selected among *n*-carboxylic acids, benzoic acids, phenols, thiophenols, acetanilides, indoles and steroids. The pK_a's for compounds studied ranged from -0.78 to 20. Within each class, compounds substituted with electron-withdrawing groups (EWGs), such as CF_3, NO_2 and CN, generally exhibited higher responses than compounds with electron donating groups (EDGs), such as $–OCH_3$ and NH_2. Compounds with SH and $NH(CO)CH_3$ exhibited higher than expected responses. This larger data set further supports our initial hypothesis that functional groups that withdraw electrons from the benzene ring through induction and/or resonance stabilization makes it easier to remove the proton during ionization. NSF CHE-1307226 supports this work.

FORMATION OF NANOPARTICLES USING GREEN TEA EXTRACT. Michelle K. Waddell[1], Jermarion Griffin[2] & Amira Manes[3], Department of Chemistry, [1]Hampton University, [2]Kecoughtan H.S. Hampton VA, & [3]King's Fork H.S. Suffolk VA. Pollution of the world oceans by oil has become a major environmental problem. As a result, numerous methods are employed to remove these contaminants. Surfactants are used in various stages of oil spill clean-up by the petroleum industry. The critical micelle concentration (cmc) of surfactants in solution must be reached to achieve maximum absorption. However, there is a concern about the wide spread use of

surfactants due to their ability increase the diffusion of other environmental contaminants. Nanoparticles that incorporate a minimum concentration of surfactants which can effectively disperse oil in aqueous media would be an innovative advancement for the petroleum industry. This research project will occur in two phases. The first phase involves synthesis of iron magnetic nanoparticles coated with capping agents and ionic surfactants. Organic capping agents (green tea extract) and surfactants will serve a dual purpose. First, it will protect the easily oxidized iron center and assist in micelle formation of the nanoparticles. Secondly, the ionic surfactants will form emulsions with organic contaminants in aqueous media. Due to the magnetic characteristic of these nanoparticles, they will be used to remove organic contaminants noninvasively. A series of studies were to be conducted on the effectiveness of forming iron nanoparticles in various solvents and different pH levels (5, 6, 7 and 8) using tetrabutylammonium iodide or lecithin as a surfactant. The results of this research will be presented in this paper. (Supported by: NSF HBCU-UP ACE Nano HU HRD-1238838).

OPTIMIZING THE RATIO OF GREEN TEA TO SILVER NITRATE IN THE FORMATION OF SILVER NANOPARTICLES. Charles M. Bump, Brandon Peck & Kayla Davis, Department of Chemistry, Hampton University 23668. Nanoparticle synthesis requires the reduction of a metal salt to the elemental form of the metal in the presence of a "capping agent" that prevents aggregation of the metal in an amorphous mass. Green tea has been advanced as an environmentally friendly and fast-acting reducing agent while simultaneously serving as the capping agent. We report the amount of silver ion that can be converted to silver nanoparticles from a fixed amount of green tea.

ASSESSING THE ACTIVITY OF ANTIBACTERIAL POLYMERS. O. Oyesanya, Department of Chemistry, Norfolk State University, Norfolk VA 23504. Quaternized poly(4-vinylpyridine) (P4VP) and poly(4-vinylpyridine-*co*-styrene) (P4VP-S) are polymers with antibacterial properties against both Gram-positive and Gram-negative bacteria. The syntheses of the two polymers were carried out using controlled free-radical polymerization in the presence of benzoyl peroxide (BPO) and 2,2,6,6-tetramethylpiperidine-*N*-oxyl (TEMPO) followed by quaternization with 1-bromobutane. Polymers were characterized by nuclear magnetic resonance (NMR) spectroscopy, Fourier transform infrared (FTIR) spectrophotometry, and ultraviolet-visible (UV-Vis) spectroscopy. Differences in the antibacterial activity of the two polymers were investigated due to differences in the number of pyridinium groups on polymers. Antibacterial assessments were conducted by interaction of P(4VP-BB) and P(4VP-S-BB) with Gram-positive bacteria (*Staphylococcus aureus* and *Enterococcus faecalis*) and Gram-negative bacteria (*Escherichia coli* and *Pseudomonas aeriginosa*) in aqueous solutions. Results reveal that the polymers are significantly effective against the test bacteria.

SOLVENT EFFECTS ON THE LINEAR PROPERTIES OF A SERIES OF CENTROSYMMETRIC D-Π-D ARYL STYRYL ORGANIC SEMICONDUCTORS. E. M. N. Ndip[1] & C. E. Dula,[2] [1]Department of Chemistry & Biochemistry, Hampton University, Hampton, VA 23668 [2]Washington University School of Medicine, The Edward Mallinckrodt Department of Pediatrics, St. Louis, MO 63110. This work is part of our ongoing investigation on the design, synthesis, and laser spectroscopic characterization of variously bridged aryl styryl heterocyclic systems for molecular electronics. We have investigated solvent effects on the linear absorption spectra, λ_{max} (bandgap,ΔE), transition dipoles, and oscillator strengths of a series of furan, thiophene, and pyrrole vinylene bridged donor-π-donor aryl styryl systems at the semi empirical level using ZINDO-CI methodology. The solvents used in these studies included: acetonitrile, chloroform, methanol and toluene. The difference in absorptions wavelengths between gas phase and solvated model sytems vary from ±20 nm for the thiophene systems to ±15 nm for the furans and ±10 nm for the pyrrole systems. Solvent effects are less noticeable in the azo-bridged systems than in the vinylene-bridged systems. Support for this work was provided through Hampton University's NSF CREST CLaSS (Materials and Modeling IRG) grant (HRD-0734635).

CAN DSC BE USED TO DETERMINE THE ENTHALPIES OF FORMATION FOR THE 3d TRANSITION METAL OXALATES? R. Snell-Feikma & T.C. DeVore, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg VA 22807. On paper, the thermal decomposition of first row transition metal oxalates occurs in one step to produce well established products so it should be possible to use these reactions to determine the enthalpies of formation for these compounds. In practice, secondary reactions between the gaseous and solid products or between the gaseous products often occur producing a mixture of products. Attempts to fully oxidize the products by doing the decomposition in static air also failed to give consistent values. However, adding a flameless combustion catalyst (CuO) and using slow scans (2 K min^{-1}) in static air produced values for the enthalpies of formation that agreed to within 1% of the more reliable values reported previously.

Posters

FABRICATION OF MAGNETIC IRON NANOPARTICLES FOR OIL SPILL REMEDIATION BY FACILE MICROWAVE PROCESS. Breyinn N. Loftin, & Michelle K. Waddell PhD, Dept. of Chemistry, Hampton University, Hampton VA 23668. Recently, innovative nanotechnology approaches have gained attention for oil spill remediation. Magnetic nanocomposites have added magnetic properties that allow for the recovery of the deployed nanomaterial. Using nanomaterials for oil spill remediation offers a more cost and time efficient method. Nanomaterials are also more feasible than using sorbent materials and bioremediation. The superparamagnetic properties of iron nanoparticles make these materials ideal for use in oil spill remediation. In this presentation, the fabrication of magnetic iron nanoparticles by

facile microwave process is demonstrated. The microwave approach is more effective for large-scale production of high quality nanoparticles. The procedure consisted of making a precursor solution to be used in the microwave reactions. The precursor was obtained by using $FeCl_3 \cdot 6H_2O$ and HCl with a series of capping agents lecithin, green tea extract, pure tannic acid, and poly(bisphenol A carbonate). The capping agent combines with lecithin to form micelles around the iron core to form the nanoparticles. A progression of microwave trials were ran in order to observe any effects on the formation of nanoparticles. The resulting products were characterized using UV-Vis spectroscopy. Iron nanoparticles usually absorb light in the 400-600nm region. Results indicated that nanoparticles are present in the reaction mixture of the tannic acid.

UNIQUE CHARACTERISTICS OF POLYOXOMETALATES AND THEIR SYNTHESIS. M. Smith, S. Puckett, O. Wampler, J. D. Powell, School of Natural Sciences & Mathematics, Ferrum College, Ferrum VA 24088. Polyoxometalates are clusters of highly oxidized early transition metals covalently bonded to oxygen atoms and sometimes other heteroatoms. These molecules usually contain a caged structure that encloses a smaller molecular ionic unit. They most commonly contain molybdenum and tungsten, which when combined with other metals give a wide variety of physical and chemical properties. Their complex caged structures can be rearranged by adjusting concentration, pH, and counter ions. Because of their high molar mass, polyoxometalate compounds are best characterized in the crystalline state by FT-IR and single-crystal x-ray diffraction. UV-visible spectrophotometry and electrochemistry provide supplementary characterization in solution. Lacunary polyoxometalate structures can be formed by the removal of at least one metal vertex from the cage. The remaining ions retain a high negative charge which makes them highly reactive towards metal ions and other Lewis bases. Sample reactions were observed through a series of tests on solutions containing different polyoxometalate ions. Synthesis and characterization of new polyoxometalates may produce compounds with unique chemical and physical properties for future applications.

Computer Science

A STUDY ON THE CHALLENGES OF BUILDING A TRUSTWORTHY NETWORK. Yen-Hung Hu, Department of Computer Science, Norfolk State University, Norfolk VA 23504. Building a trustworthy network faces several severe challenges adhering to the current computing infrastructure (e.g., computer architectures, network architectures, operating systems, communication protocols and applications, and so on.). Since hardware and software of a network system are from various vendors and manufacturers, it is very difficult to assess trustworthiness of any system without proper criteria and methods. Meanwhile, misconfigurations of hardware and software by end-users will worsen this issue even though such hardware and software are well prepared by following appropriate industrial security guidelines. Therefore, concerns regarding criteria and methods for assessing trustworthiness should

be defined and identified first. Although the concept has been discussed more than ten years and several researchers have studied the implementation of trustworthy systems, we have observed that there is no mature approach for building a trustworthy network. There is no absolute trust between any two network components and external security mechanisms must be embedded to force this trust. In order to have a trustworthy network, we believe, security, privacy and reliability of every major network component must be enforced. For instance, if there is no trusted mechanism for protecting data transactions across different network components, a network cannot be relied on performing trustworthy computing. In this paper, we investigate the criteria and methods for building a trustworthy network and develop a trustworthy network model that is both scalable and interoperable with existing and future network architectures.

A VISUALIZATION TOOL FOR MONITORING, PREDICTING AND MITIGATING NETWORK INTRUSIONS. Yen-Hung Hu, Department of Computer Science, Norfolk State University, Norfolk VA 23504. There currently exist thousands of network attacks worldwide. Along with the explosive growth of the Internet and wireless services, the impact of network attacks has been increasing dramatically. Attacks may be denial of service, viruses or worms, port scanning, and so on. Many network intrusion detection systems have been proposed or introduced in recent years. They can be partitioned into two complementary types: misuse detection and anomaly detection. In both detection approaches, traffic classification has been the main issue affecting their performance. Traffic classification algorithms distinguish types of traffic used for various intrusion detection systems to identify flows. Since there is no single traffic classification algorithm that can be effectively applied to all traffic types, we will need to use a set of traffic classification algorithms to identify all different and complex types of traffic present in today's Internet traffic. However, high resource overhead and false positive rates will be the major challenges for potential systems and users. In this paper, we introduce our investigations and results for guiding the design and development of an Integrated Visualization Platform for Monitoring, Predicting, and Mitigating Network Intrusions which can be used to: 1) Assess network activities, 2) Depict normal and malicious network activities maps, 3) Predict future trends of network intrusions, and 4) Monitor network intrusions and mitigate their negative impacts.

Posters

A COMPARATIVE STUDY OF OPTIMIZATIONS TO THE BINARY SEARCH ALGORITHM. Elizabeth E Cho & Robert M Marmorstein. Dept. of Computer Science, Longwood University, Farmville VA 23909. The binary search algorithm is one of the fundamental algorithms used in computer science. It is an extremely efficient and ubiquitous algorithm for locating data in a list. Several optimizations to binary search exist which improve its efficiency on certain kinds of data. One of these

optimizations is interpolation search in which the value of the data item is used to predict its location in the list. However, the performance of these algorithms depends heavily on the distribution of the data. In this study, we compare the performance of binary search and interpolation search on data which fits several different discrete random probability distributions.

Education

THE DEVELOPMENTOF AN INSTRUMENT TO MEASURE STUDENTS' ATTITUDES TOWARD SCIENCE FAIRS. Kurt Y. Michael & Claudia A. Huddleston, School of Education, Liberty University, Lynchburg VA. 24515. Every year, thousands of students participate in science fairs, however, little is known about their attitudes toward science fairs. The purpose of this study was to develop an instrument that measured students' attitudes toward science fairs and determined the instrument's validity and reliability. The instrument was field-tested using 110 students in southwest Virginia. The instrument originally consisted of 45 questions. After applying a principal component factor analysis, the instrument loaded on two domains, enjoyment and value. Each domain consisted of five questions. The internal consistency for the overall instrument was calculated using Cronbach's alpha and showed good internal consistency of 0.94. Correspondingly, the sub-scale enjoyment yielded a value 0.89 and the sub-scale value yielded a value 0.90, indicating good internal consistency. Further analysis was conducted using demographic information and the results revealed a significant difference on attitudes toward science fairs based on gender. A significant difference between males ($M = 23.0$, $S.D. = 7.06$) and females ($M = 26.2$, $S.D. = 7.38$) was found, $t(98) = 2.04$, $p = 0.04$, whereas eta squared equaled 0.12 demonstrating a large effect size. Overall, females had a more positive attitude toward science fairs than males.

APPLICATION OF SIMULATION – BASED APPROACH IN PHYSICAL CHEMISTRY INSTRUCTION. Edmund M. N. Ndip, Department of Chemistry & Biochemistry, Hampton University, Hampton, VA 23668. The majority of professionals in the STEM disciplines are well versed in the content of their respective disciplines. There is general consensus that learning is best achieved by doing. Each scientific discipline and sub-discipline poses problems for the learner. Physical chemistry – the sub-discipline of chemistry that deals with the mathematical and theoretical foundations of all the chemical sciences is no different. A fundamental difficulty is the abstract nature of its concepts. Simulation based approach is a technique used to replace real experiences with guided ones often requiring active participation by the learner. Simulation based activities have been implemented to facilitate instruction in areas requiring higher mathematical skills through a combination of object oriented programming using VenSim PLE, numerical simulations using Excel, quantum mechanical modeling/calculations and visualization

techniques. The combination of simulations and wet experiments provides students avenues for developing higher order skills. Students completed term projects using this approach to more complex problems in kinetics, thermodynamics and quantum mechanics and spectroscopy. Additionally, students used simulations to interpret and explain results obtained in physical chemistry laboratory activities such as infrared spectra of organic compounds, and absorption spectroscopy of dyes.

COUPLING EXPERIMENT WITH DFT CALCULATIONS: ON THE ROAD TO DISCOVERY. Thomas C. DeVore, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg VA 22807. The rapid advances in the computational capabilities of personal computers now makes it easy and relatively inexpensive to include theoretical calculations into the chemistry curriculum. These calculations can be added to the curriculum by tacking them onto an existing laboratory exercise, integrating them into the exercise, or by using them as the exercise. The well-known rotational analysis of HCl-DCl is used to illustrate how calculations can be added to an exercise. Two NMR experiments based on measurements for methanol [MeOH] are presented to illustrate integration of calculations into the exercise. Measured chemical shifts for MeOH liquid and vapor are compared to shifts calculated for MeOH, MeOH dimer, and MeOH ringed trimer to offer insight intothe changing chemical shift for the OH proton. The example for the stand alone exercise presented is an investigation of the low and high spin electron configurations for several atoms. These calculations allow the student to "discover" the Aufbau Principle and Hund's Rule. All calculations presented were done using the DFT-B_3LYP method with a 6-311G^{++} (3df, 3pd) basis set.

SCIENCE ON A SPHERE: AN ETHICS LEARNING TOOL. J. S. Boles, University of Wisconsin-Madison & E. G. Maurakis, Science Museum of Virginia & Biology Dept., University of Richmond. Finding effective ways to educate the general public about environmental ethics and the decision making process used by scientists and ethicists has been an important goal for informal science education institutions. The goal of our pilot presentation was to use NOAA Science on a Sphere (SOS®) technology to teach the general public about environmental ethics decision making processes. Using SOS® data visualizations such as global shipping routes, global air traffic patterns, and woody biomass, the presentation conveyed the interconnectedness of the global biosphere. These examples were coupled with a discussion of the individual's role in these issues to demonstrate that each audience member has an impact and can use the same ethical decision making process in their own environmental decisions. Delivered to 19 staff members and museum guests, the presentation was followed by a seven question survey that asked if the presentation changed what they learned and how they think about decision making. Preliminary results show that while 89% of audience members previously considered other people and the environment in their decision making, 76% learned something new. Additionally, nine audience members said the presentation changed the way they will

think about decision making and ethics in the future. Results also indicated the SOS® technology was successful teaching new concepts to the audience, some of whom had prior knowledge of the concepts of environmental ethics in decisions making. Based on pilot study results, SOS® can be used as an informal ethics learning tool for the general public. Travel funds provided by University of Wisconsin Genetics Department.

CREATING ENGAGING STEM OPPORTUNITIES FOR YOUTH OUTSIDE OF SCHOOL. Charles L. English, Dir. Playful Learning & Inquiry, Science Museum of Virginia, Richmond VA. 23220. The Science Museum of Virginia has developed and implemented a program designed to inspire youth towards learning more about STEM and how their academic work ties to relevant aspects of their lives. STEM, far too often, means little more than science or math classes for many youth without tangible connections to projects, activities or even career options. Educators at the Science Museum of Virginia have created a project-based program aimed at engaging youth in a variety of settings from Boys & Girls Clubs to schools, YMCAs and libraries. The program helps youth build and create solutions to open-ended problems, engaging them in a way that is unique to their school setting. It also helps participants to bridge their knowledge and skills from different disciplines into a STEM themed project so STEM seems more tied to other aspects of their educational experiences. STEM careers are also related to the hands-on projects in order to broaden youths' perspectives on STEM opportunities they may wish to investigate further. Use of undergraduate facilitators also supports a near-peer mentor piece that which helps create a dialogue with the middle school aged participants. (Supported by Altria Group, The Custis Westham Fund of the Community Foundation, the Institute of Museum and Library Services, Pauley Family Foundation, The Cameron Foundation, John Randolph Foundation, The Cognizant Technology Solutions Charitable Fund, Wells Fargo Foundation and Moses D. Nunnally, Jr. Charitable Lead Unitrust.)

THE MIX: EXPLORING PROJECT BASED AND INFORMAL LEARNING WITHING A TEEN-CENTRIC LEARNING LAB ENVIRONMENT. Matthew L.M. Baker, Outreach Education, The Science Museum of Virginia, Richmond, VA 23220. The MiX, a tech-based, maker space at The Science Museum of Virginia, was formed in 2014 to offer teens a safe and open learning environment to promote creativity, exploration, and iteration. In October 2013, a Teen Advisory Council of ten students was formed in order to involve teens in the creation of the space. Teens helped determine the type of programming they wanted to participate in, designed The MiX membership card, and created promotional videos and materials for the space. Today, The MiX consists of eighty-eight members, with more teens joining weekly. Teens now participate in monthly workshops, video filming and broadcasts, and show off their work during a monthly open house on the last Saturday of every month. The MiX has become a successful hub for project based and informal learning as evidenced through the growing number of members, workshop participation increase, and burgeoning

partnerships within the Richmond community and beyond. Additionally, The MiX is a member of the YOUmedia Learning Labs community, which consists of twenty-nine similar sites across the United States. This community helps determine best practices, shares resources and ideas, and helps like-minded practitioners create similar spaces. The MiX was made possible by generous grant support from The Institute for Museum and Library Services and The MacArthur foundation.

LEARNING WHAT THEY LEARN – ASSESSING OUT OF SCHOOL TIME PROGRAMMING. Erika R. Carson, The Science Museum of Virginia, Richmond VA 23220 & Northcentral University, AZ 86314. Children can learn so much from informal and non-formal STEM learning experiences. However, measuring what students have learned from these experiences continues to be a challenge for so many afterschool, out-of-school, museum, etc. program providers. Non-formal STEM programs and Informal Science Institutions (ISI) struggle between keeping kids excited about science, and teaching them science content without mimicking what children experience in the classroom, for better or for worse. These program providers tend to want to steer clear of tests and surveys that feel like tests for fear of losing participants. There are strategies however, for learning what these kids learn - assessments can be simple, fun, and/or innovative. Through the use observations, name tag information, participant interviews of each other, "game show" competitions, etc. we have been able to collect information about our participants understandings before, during, and after participating in our programs. Non-traditional approaches to assessment can help us learn what they learn.

Posters

ASSESSMENT OF A SECONDARY SCIENCE STEM FIELDTRIP THAT PAIRS A TREATMENT PLANT TOUR WITH A HANDS-ON NATURAL WETLAND TOUR IN EASTERN VIRGINIA. K. N. Morris, D. F. Timmer, & R. B. Atkinson, Organismal & Environmental Biology Dept, Christopher Newport University. This project evaluated changes in confidence and content retention in middle school students before and after participation in a tour of a wastewater treatment plant and a natural tidal wetland. Learning styles vary between students and traditional classroom-based approaches to teaching may not optimally support learning. During the wetland tour students rotated through three stations that focused on flora, fauna, and water quality ecosystem services in contrast with waste water treatment plant processes. Student confidence improved by 3.8 points based on attitude questions and average correctness on content questions also improved by 0.46 points. Sex and science career interest were also assessed and students interested in a career in science performed higher in both attitude and content scores than any other group; however no trends were detected based on sex of the participant. Results of this and ongoing formative assessment will be used to enhance student experiences.

Environmental Science

AN INTEGRATED ECOLOGICAL AND WATER QUALITY ASSESSMENT OF THE HEADWATERS OF THE NORTH FORK SHENANDOAH RIVER. Bryce D. Yoder, Jesse B. Parker, Douglas S. Graber Neufeld & James M. Yoder, Department of Biology, Eastern Mennonite University, Harrisonburg Virginia 22802. This study is part of an ongoing collaborative project developed by Eastern Mennonite University and various partners to address watershed health in the primarily agricultural community of Bergton, Virginia. Short-term goals of this project are to establish baseline measurements for water quality parameters and determine relative contributions of tributaries to overall nutrient and sediment levels within the watershed. Storm events were found to cause spikes in nutrient, sediment, and bacteria levels. On average across sites, sediment levels increased from 10 mg/L to 285 mg/L, fecal coliform increased from 50 cfu/ 100ml to 372 cfu/ 100ml and nitrate levels doubled from 1.2 mg/L to 2.71 mg/L after storm events. This suggests that the streams in the study area are not able to manage the hydrologic stress of storm events, resulting in bank erosion and general stream instability as well as nutrient and bacteria input from runoff. Baseline total coliform levels averaged about 1500 cfu/ 100ml, a concentration far above the DEQ recommended amount of 235 cfu/ 100ml. Macroinvertebrate biotic indices, while overall indicating good to excellent conditions, were more stressed in reaches where livestock exclusion was not being implemented (VSCI of 65.75 compared to 83.94). Turtle surveys indicated relatively low wood turtle abundance and no evidence of a currently reproductive population. Continued baseline data collection and long-term monitoring will help evaluate the effectiveness of future stream restoration efforts and livestock exclusion practices.

BASELINE WATER MONITORING PROGRAM IN RESPONSE TO POTENTIAL HYDROFRACKING. Hannah M. Daley[1], Janaya M. Sachs[1], Tara Kishbaugh[1]& Douglas S. Graber Neufeld[2], [1]Dept. of Chemistry & [2]Dept. of Biology, Eastern Mennonite Univ., Harrisonburg VA. 22802. Stream and well water samples near a potential hydrofracking site in Bergton, VA. were collected from 2011 to present. Temperature, pH, conductivity, and TDS (Total Dissolved Solvents) data was used to determine a baseline sample dependent on seasonality. Barium and Strontium concentrations of the samples were measured through atomic absorption spectroscopy. It was found that, on average, Bergton, VA wells had 0.29 ppm and 0.23 ppm of Barium and Strontium, and Bergton, VA streams had 0.14 ppm and 0.05 ppm of Barium and Strontium, respectively. Barium in Bergton, VA. wells was significantly greater than in streams ($p < 0.05$). All of the samples measured, so far, have been well below the EPA limit for Barium and Strontium concentration of 2.0 g/mL and 4.0 g/ml, respectively. Barium in Bergton, VA was found to be significantly lower than other stream baseline samples in the Shenandoah Valley region ($p < 0.05$), which may be due to differences in geology, such as the presence of limestone. Strontium levels showed no significant difference throughout the Shenandoah Valley region. Bergton, VA

samples were also compared with samples in Doddridge County, WV, where hydrofracking is widespread, and although no significant differences were found in Barium and Strontium concentration, the Doddridge County samples appeared to have more variance. If hydrofracking began in Bergton, VA, the established baseline and observations from other areas could be used to indicate hydrofracking fluid leaking into the surrounding waters.

COMPARATIVE ANALYSIS OF NON-TIDAL, MITIGATED, FORESTED WETLANDS IN VIRGINIA PIEDMONT AND INNER COASTAL PLAIN. J.B. Radolinski & M.L. Bass, Department of Earth & Environmental Sciences, Univ. of Mary Washington, Fredericksburg, VA, 22401. Three constructed non-tidal palustrine forested wetlands (PFO) and one natural PFO were compared based on vegetative proliferation and soil physiochemical characteristics. Vegetation parameters included woody stem counts, a list of total wetland flora, Basal Area (BA), and Diameter at Breast Height (DBH) measurements. Soils were flooded using enriched freshwater and measured colorimetrically for N exchange/release and P sorption/desorption, in order to approximate biogeochemical nutrient cycling as a result of prolonged inundation. All wetland soils released N (2.65-13.6 mg NH_4-N/m^2). P sorption/desorption ranged from -4.35 mg PO_4-P/m^2 (desorption) to 16.6 mg PO_4-P/m^2 (sorption). The natural wetland (PNWL) supported significantly larger trees (DBH=13.1±1.29 cm) (BA=9.93 $cm^2 m^{-2}$) (ANOVA, $F_{3,12} = 9$, $p<0.0001$), the lowest density of woody stems (1102±440 ws ha^{-1}), the lowest species richness (S=14), while also containing the most soil organic matter and phosphorus through a depth of 30 cm. Overall, the 19 year old SMWL differed significantly from PNWL with a high density of smaller trees (4095±1951 ws ha^{-1}) (p=0.046) (DBH=0.99±0.43 cm) and sandy entisols showing a reduction in soil quality with depth. Underdeveloped, anthropogenically altered soils (udorthents) found in SMWL and beaver activity have likely limited success for this constructed PFO. Findings suggest that special attention be paid to initial soil conditions during construction. This study also underlines the complexity of flood-induced nutrient cycling in hydric soil, especially relevant as sea level rise and increased precipitation may result in more flood-prone wetlands in many transitional fluvial systems.

SEASONAL WATER QUALITY DEGRADATION, WILDLIFE, AND PROTECTED AREAS IN SOUTHERN AFRICA. J. Tyler Fox[1] & Kathleen A. Alexander[1,2], [1]Department of Fish & Wildlife Conservation, Virginia Polytechnic Institute & State University, Blacksburg, VA 24061 & [2]CARACAL: Centre for Conservation of African Resources, Kasane, Botswana. Sustainable management of dryland river systems is often complicated by extreme variability of precipitation in time and space, especially across large catchment areas. Because of the extensive provision of ecosystem services and high subsistence value of southern African dryland rivers and wetland systems, there is a critical need to better understand the interdependent drivers of regional water quality changes. Using field transect data, GIS and remote sensing analysis, and spatiotemporal modeling, we examined seasonal variation of the fecal indicator

bacteria, *Escherichia coli,* and total suspended solids (TSS) in the Chobe River in relation to land use and hydrology. Our results suggest that direct deposition of fecal material in the Chobe River by wildlife, as well as accumulation feces in the landscape and subsequent flushing by rainfall and seasonal floods, are significant drivers of water quality declines in this dryland system. Park land use (p = 0.0009) and the presence of river floodplain (p = 0.016) were significantly associated with higher *E. coli* concentrations, and locations where *E. coli* was highest corresponded spatially with areas of high wildlife biomass.

DISTRIBUTION OF BACKGROUND TRACE INORGANIC MERCURY WITHIN TERRESTRIAL ECOSYSTEMS IN ROCKINGHAM CO., VA. Greg E. Mansour, Gail M. Moruza & Dean Cocking, Department of Biology, James Madison University. Despite the fact that there are no major anthropogenic sources of Hg in Rockingham County, there is still a presence of background mercury in A horizon soil, ~0.04 - 0.05 µg Hg•gdw^{-1}. and O horizon duff 0.02 µg Hg•gdw^{-1}. The overall study examines two sites located ~5 km NE and SW of Harrisonburg City for low-level Hg contamination within soil, duff, air, and various macro-invertebrate species. Both sites contain intermediate aged deciduous forest vegetation. Airborne Hg (dissolved, vapor, particulate and that in small organic matter fragments) was collected using passive samplers constructed from inverted plastic petri dishes containing a layer of TangleTrap®. Soil and duff samples were collected manually as were the macroinvertebrates discussed in the next paper. Soil, biotic tissue, and TangleTrap® gel were then digested in hot concentrated sulfuric and nitric acid and analyzed using a Perkin Elmer Flow Injection Atomic Absorption Spectrophotometer (FIMS). The NULL hypothesis was that there would be no difference in the Hg concentrations at the two sites. Detectable Hg was found at both and the NULL hypothesis was rejected for airborne Hg and accepted for the O and A horizon layers. These data were compared with a 2010-12 preliminary study and confirmed similar results for soil but differing results for the airborne sample. This is not unexpected because the years differed in many temporal aspects (e.g. weather) and Air Indices of µg Hg•m^2-surface•day^{-1} of exposure are expected to vary yearly. Detectable low level Hg is present as a potential source for biological uptake at both sites.

DISTRIBUTION OF TRACE INORGANIC MERCURY WITHIN INVERTEBRATE COMPONENTS OF TERRESTRIAL ECOSYSTEMS IN ROCKINGHAM CO., VA. Gail M. Moruza, Greg E. Mansour & Dean Cocking, Department of Biology, James Madison University. Ecosystems in the Shenandoah Valley of Virginia are not directly exposed to major known sources of mercury (Hg) contamination. Therefore, Harrisonburg, located in Rockingham County, was assumed to be suitable as a low level control site in comparison with locations in Waynesboro, VA (48 km distant), which were exposed to industrial Hg contamination in the mid-1900's. Subsequently, the presence of low level background Hg has been demonstrated in Rockingham County. This study examines the total Hg content associated with macroinvertebrate

taxa within the two successional forest sites located within Rockingham County described in the previous presentation. A variety of groups of organisms were digested in hot concentrated nitric and sulfuric acid and analyzed for total Hg concentrations using a Perkin Elmer flow Injection Spectrophotometer dedicated to Hg Analysis. The NULL hypothesis was that, where detectable Hg was present, it would not differ between the replicate sites. Several groups, including house flies, hornets, stink bugs, cockroaches, pill bugs, carion beetles, and hymenopterans contained 0.03 - 0.09 µg $Hg \bullet gdw^{-1}$ (ppm) and the NULL hypotheses were accepted for the Hg containing replicates. They were very similar for the individual species. Others, including Japanese beetles, ants and shield beetles, had concentrations from 0.1 - 0.4 µg $Hg \bullet gdw^{-1}$ and differed at the sites. Higher trophic level daddy long-legs and spiders, contained ~0.23 µg $Hg \bullet gdw^{-1}$. Hg is associated with these organisms, but this study does not confirm whether the association is superficial or internal.

USING STATE-OF-THE-ART MARK-RECAPTURE TECHNIQUES TO CREATE A CONSERVATION ACTION PLAN FOR ENDANGERED FRESHWATER MUSSELS. Alaina C. Esposito[1], Patrice M. Ludwig[1], Lihua Chen[2] & Christine L. May[1], [1]Department of Biology, James Madison University & [2]Deptartment of Mathematics & Statistics, James Madison University. The critically endangered James Spinymussel (*Pleurobema collina*) is a species of unionid freshwater mussel endemic to the James and Dan River basins. In the last 20 years *P. collina* has experienced a substantial decline and currently only occupies 10% of their original habitat, however little information is currently known about this species to assist in conservation. A 230-meter reach of transitional habitat in Swift Run was selected for repeat observations to estimate detection probabilities using a Capture-Mark-Recapture framework. In June 2014, visual scouting began to locate and tag *P. collina* (as well the as other mussel species found) with 12mm Passive Integrated Transponders tags. Repeat surveys were conducted on a bi-weekly basis to relocate all tagged individuals, record their current position and visibility on the surface, as well as relevant habitat characteristics that may have influenced their behavior or detectability. Results show that most *P. collina* are visually detectable <7% of the time, and that water depth, season, mussel size and community composition are significant predictors of detection probabilities. Additionally, modeling simulations have identified how to increase adult survival to 87.5% from manipulating glochidia and juvenile mortality rates. This information has been synthesized into field-usable information and helped create the backbone of a conservation action plan.

CONSERVING ENDANGERED FRESHWATER MUSSELS THROUGH COURSE-EMBEDDED RESEARCH. C. L. May, Department of Biology, James Madison University, MSC 7801, Harrisonburg, VA 22807. Freshwater mussels are among the most endangered animals in North America. Developing conservation strategies for them is complicated by the fact that they are cryptic, rare and poorly understood organisms. Our research team is integrating field studies and artificial stream channel

experiments with mathematical and statistical models to fill important knowledge gaps that can aid in their recovery. The novelty of our approach is using a series of linked courses that provide authentic research experience for both undergraduate and graduate students. Our presentation will use a case example of the federally endangered James Spinymussel and a team of students doing course-embedded research in Population Ecology, Mathematical Models in Biology, and independent research credits. Field studies are utilizing state-of-the art mark-recapture methods to quantify detection probabilities, population size and mortality rates. Artificial stream channel experiments are exploring environmental conditions that effect surface expression, and therefore the probability of detecting the species when it is present. Both approaches are integrating with mathematical and statistical models which are united into a conservation action plan.

Posters

MODELING HABITAT USE FOR THE ENDANGERED JAMES SPINYMUSSEL (*PLEUROBEMA COLLINA*): AN APPROACH FOR SETECTING RARE CRYPTIC ORGANISMS. Dorottya K. Boisen, Dakota M. Kobler, Katie M. Sipes, Alaina C. Esposito, Patrice M. Ludwig & Christine L. May, Department of Biology, James Madison University, Harrisonburg VA 22807. Freshwater mussels are keystone species in their ecosystems, and their filter feeding ameliorates water quality in downstream areas. Over 70% of freshwater mussel species worldwide are listed as vulnerable or more greatly threatened. The James Spinymussel (*Pleurobema collina*) is a species of top priority for conservation in Virginia. Due to limited research, cryptic appearance and behavior, and small population sizes, freshwater mussel conservation efforts have been hindered. A mark and recapture study has tracked approximately 20 James Spinymussels and 60 Notched Rainbow (*Villosa constricta*) mussels marked with Passive Integrated Transponder (PIT) tags at Swift Run in the summer of 2014. Multiple mussel recapture histories provide data about habitat use, stream-bed surface expression, and inform source sink models. We will present our work on this integrated approach to understanding rare cryptic organisms. This research is funded by the Jeffress Memorial Trust.

Medical Sciences

DESIGN AND SAR STUDY OF SMALL MOLECULE CTBP INHIBITORS. S. Korwar[1], B. L. Morris[2], S. R. Grossman[2] & K. C. Ellis[1,2], [1]Department of Medicinal Chemistry & [2] Massey Cancer Center, Virginia Commonwealth University. This project involves developing small molecule inhibitors of C-terminal Binding Protein (CtBP) which act as anti-cancer agents. CtBP is a transcriptional co-repressor of several tumor suppressor genes. It is over expressed in many colon, breast, and ovarian cancer tumors. CtBP has a catalytic site in which the co-factor NADH and substrate 4-

methylthio-2-oxobutyric acid (MTOB) bind. At higher concentrations, MTOB has been found to inhibit CtBP (IC_{50} = 300 μM). Based on the pi-interactions observed in CtBP-MTOB co-crystal structure, the methylthio- group of MTOB was replaced by a phenyl ring to give phenylpyruvic acid (PPA), which was found to be active (IC_{50} = 116 μM).This further led to the synthesis of non-reducible ketone isosteres of PPA, of which the hydroxy imine analog (HIPP) was the most potent compound (IC_{50} = 0.24 μM). Compounds containing various substituents such as hydroxy-, fluoro-, chloro-, methoxy- and methyl- at the 2, 3 and 4 positions of HIPP were then synthesized. The synthesis of these compounds was achieved in two steps. The first step involved condensing the corresponding aldehyde with hydantoin or 1,4-diacetylpiperazine-2,5-dione, followed by hydrolysis under basic or acidic conditions respectively to give the corresponding α-ketoacid. These α-ketoacids were converted to oximes in a one-step reaction. The α-ketoacids and oximes were tested against recombinant CtBP. The oximes of 4-chlorophenylpyruvic acid (IC_{50} = 0.18 μM) and 3-chlorophenylpyruvic acid (IC_{50} = 0.17 μM) were the most potent compounds in this series. All the compounds were further tested in HCT-116 cells using MTT assay.

ROLE OF TOLL-LIKE RECEPTOR 4 IN ENTERIC GLIA. S. Bhave, P. Brun, M. Kang, W.L. Dewey & H. I. Akbarali, Department of Pharmacology & Toxicology, Virginia Commonwealth University, Richmond, VA 23298. Toll-like receptors (TLRs) are a class of pattern recognition receptors that play an important role in mediating inflammatory responses to pathogens. TLR4 recognizes lipopolysaccharide (LPS), a membrane component of gram negative bacteria. In the gastrointestinal tract, basal activation of TLR4 by LPS has a protective role. However, a compromised gut epithelial barrier leads to enhanced entry of bacterial proteins such as LPS into the lamina propria, leading to neuronal toxicity. Enteric glia are important for the maintenance of neuronal integrity. In the present study we determined the activation of enteric glia in response to low and high concentrations of LPS. LPS dose-dependently increased mRNA expression of IL-6 and TNF-α with 0.1 μg/ml inducing a 25-fold and 10-fold IL-6 and TNF-α mRNA expression, respectively. A 100-fold higher concentration of LPS (1-100 μg/ml) lead to expression of connexin-43 hemichannels and induced ATP release indicative of cell damage. Whole cell voltage clamp studies showed that high concentration of LPS also increased ATP-induced inward currents with a corresponding increase in P2X1, 2, 3, 4, and 7 receptor mRNA expression. Thus, low concentrations of LPS induce cytokine release whereas high concentrations of LPS induce ATP release and P2X receptor activity and further enhance the release of pro-inflammatory cytokines. Understanding the role of P2X in LPS induced enteric glia activation and associated inflammation will point to new therapeutic targets to control gut inflammation while still maintaining the beneficial effects of basal TLR4 signaling. (Supported by DK046367, DA024009)

COMPUTATIONAL DESIGN OF DIRECT ALLOSTERIC THROMBIN INHIBITORS. D. K. Afosah[1,2], S. Verespy[2,3], R. Karuturi[1,2], & U. R. Desai[1,2],

[1]Department of Medicinal Chemistry & [2]Institute for Structural Biology & Drug Discovery, Virginia Commonwealth University, Richmond VA 23219 & [3]Department of Chemistry, Virginia Commonwealth University, Richmond VA 23284. Heparin mimetics present a valuable way of preventing the side effects associated with the use of heparin in thrombotic diseases. Sulfated benzofuran dimers (SBDs), which directly inhibit thrombin by an allosteric mechanism have previously been developed by our group. Considering that the crystal structure of the thrombin–SBD complex remains unsolved to date, we employed molecular modeling to help understand the SAR of these compounds and advance the design of these inhibitors. Using GOLD, a genetic algorithm-based docking and scoring program, a diverse virtual library of SBD analogs were screened to identify potential analogs as thrombin inhibitors. This was followed by chemical synthesis and biological evaluation of the most promising agents. Molecular modeling predicted that benzylated 5-sulfate and phenethyl 5-sulfate containing benzofurans were likely to exhibit higher potency due to pi–pi ligand–protein interaction. Yet, the putative designed inhibitors did not exhibit inhibition potency as predicted. Yet, interestingly majority of these analogs displayed maximal efficacy of only 50-60%, which is different from those reported in the literature. Partial inhibition of thrombin is likely to reduce the risk of bleeding, which typically accompanies inhibitors that completely inhibit this key coagulation factor. Further work is underway to identify the structural basis for the submaximal inhibition of thrombin by these benzofuran analogs.

ESTIMATES OF METABOLIC EXPENDITURE CAPACITY IN CHRONIC LIVER DISEASE (CLD) PATIENTS CAN DIFFER WIDELY BETWEEN CARDIOPULMONARY EXERCISE TESTS (CPET) OF PERFORMANCE AND SELF-REPORTS OF ACTIVITY. Jillian K. Price[1,2,3], Carey Escheik[3], Patrick Austin[3], Lynn Gerber[2,3] & Zobair M. Younossi[3], [1]Department of Rehabilitation Science, George Mason University, [2]Center for Chronic Illness & Disease, George Mason University, [3]Beatty Liver & Obesity Research Program, Inova Health System. The potential impact of chronic liver disease (CLD) on cardiopulmonary function has not been well characterized. Cardiopulmonary exercise testing (CPET) is a strongly validated means of assessing cardiopulmonary function and performance. The Human Activity Profile (HAP) is a questionnaire developed to detect subtle changes in functional level whose scores can be converted to metabolic equivalent (METs) estimates of energy expenditure and has been well-validated in a variety of clinical populations. A convenience sample of 10 subjects seeking treatment at a tertiary liver disease center were recruited to completed the HAP and a modified Bruce CPET [70% male, age 50.4 ± 9.3 years, 3 NAFLD, 7 HCV (4 naïve, 2, relapse, 1 sustained virologic response-SVR), body mass index (BMI) 30.2 ± 6.8]. VO2 Max-derived calculations of metabolic equivalents (METs) differed significantly from self-report-based METs. Maximum METs estimates ranged from 94 to 176% of performance VO2Max. All but one subject overestimated their METs capacity during self-report. All subject self-reports of average daily activity METs expenditure were higher than their anaerobic threshold

(24-213% higher). The general population-derived METs estimate for the HAP requires modification for a CLD population.

CB1 HETEROZYGOUS MICE REVEAL IN VIVO EFFICACY DIFFERENCES OF PHYTO AND SYNTHETIC CANNABINOIDS. T. W. Grim[1], B. F. Thomas[2], J. L. Wiley[2], S. S. Negus[1], & L. H. Lichtman[1], [1]Department of Pharmacology & Toxicology, Virginia Commonwealth University, Richmond, VA 23298 & [2]Research Triangle Institute, Raleigh-Durham, NC 27709. Within the last decade, myriad synthetic cannabinoids (SC) have been detected in abused herbal preparations. Most SCs activate the CB1 receptor to a much greater degree than the phytocannabinoid r^9-tetrahydrocannabinol (THC), rendering them considerably more dangerous. Here, we utilize CB1 (+/+), (+/-), and (-/-) mice to assess these differences in efficacy to produce CB1-mediated catalepsy, hypothermia, and antinociception, and we hypothesize that the potency to produce these effects in CB1 (+/-) will decrease relative to wild-type mice as efficacy decreases with little or no effect in CB1 (-/-) mice. When potency ratios were calculated between CB1 (+/+) and (+/-) mice across each endpoint, these experiments produced a rank order of A-834,735D > WIN55,212-2 > CP55,940 > JWH-073 > CP47,497 > THC. This result aligns with in vitro assays investigating functional activity of these ligands at CB1.

MARBLE BURYING: NOVEL MEASURE OF MURINE NEUROPATHIC PAIN DEPRESSED BEHAVIOR. Jenny L. Wilkerson[1], Ken Hsu[2], Micah Niphakis[2], Mario van der Stelt[3], Benjamin Cravatt[2] & Aron H. Lichtman[1], [1]Dept. Pharmacology & Toxicology, VCU, Richmond, VA 23298, USA [2]The Skaggs Institute, TSRI, La Jolla CA 92037, USA & [3]Leiden Instit. of Chem & NL Proteomics Centre, Leiden, NL. Pathological pain states represent one of the most common reasons to seek medical attention. Most preclinical assays measure behaviors that are evoked by a nociceptive stimulus. Limitations of these endpoints include difficulties in distinguishing between motor impairment and analgesia, as well as the conceptual issue of whether they adequately model clinical symptoms. In the present study, we modified the marble burying test to explore pain-depressed digging behavior in the chronic constriction injury of the sciatic nerve (CCI) neuropathic pain model. We compared the effectiveness of a panel of analgesic drugs (i.e., morphine, valdecoxib, gabapentin), and cannabinergic drugs and a non-analgesic (i.e, diazepam) in reversing CCI-induced decreases in marble burying versus reversing CCI-induced increases in mechanical allodynia and thermal hyperalgesia. Each of the analgesics dose-responsively reversed CCI-induced depression of marble burying as well as CCI-induced allodynia and thermal hyperalgesia. In contrast, diazepam further reduced marble burying, but did not affect pain-stimulated measures. The present results indicate that marble burying represents a simple assay to assess pain-depressed behavior.

α4 nAChRs AND SEPTUM ERK SIGNALING REGULATE AGE-ASSOCIATED CHANGES IN ANXIETY-LIKE BEHAVIOR. Claire I. Dixon[1], Shawn M. Anderson[1],

Alexandra M. Stafford[1], Petra Scholze[2] & Darlene H. Brunzell[1], [1]Dept. of Pharmacology & Toxicology, Virginia Commonwealth University, Richmond VA 23298, United States & [2]Medizinische Universität Wien, Zentrum für Hirnforschung, A-1090 Wien, Austria. Pharmacological inhibition of α4β2 subunit containing nicotinic acetylcholine receptors (α4β2*nAChRs) reduces anxiety-like behavior in rodents. As expression of α4β2*nAChRs declines with age, the present study assessed how reduced expression of these nAChRs during adulthood (ADULT; 6-8 mo.) and aging (AGED; 22-24 mo.) affects anxiety behavior in wildtype (WT) and α4 subunit null mutation heterozygous (α4HET) mice. AGED and α4HET ADULT mice showed reduced anxiety-like behavior, whereas AGED α4HET mice showed increased anxiety-like behavior. Antagonism of α4β2*nAChRs with dihydro-beta-erythroidine (DHβE) increased anxiety-like behavior in ADULT α4HETs. Western blot analysis revealed that AGED WT and ADULT α4HET mice showed elevated levels of septal pERK that were inversely correlated with anxiety behavior. These findings suggest that reduced expression of α4β2*nAChRs that may occur with normal aging supports anxiolysis-like phenotype but that inhibition of this pool of receptors may increase anxiety-like behavior in individuals that have a poverty of α4β2*nAChR expression.

ACTIVATION OF a6*NACHRS IS SUFFICIENT FOR NICOTINE REWARD IN MICE: PUTATIVE INVOLVEMENT OF THE NUCLEUS ACCUMBENS SHELL. Alexandra M. Stafford & Darlene H. Brunzell, Department of Pharmacology & Toxicology, Virginia Commonwealth University, Richmond, VA 23298. Nicotine, a primary addictive component in tobacco, binds to nicotinic acetylcholine receptors (nAChRs), producing its rewarding effects. Rodent studies have shown that activation of β2*nAChRs (*denotes assembly with other subunits) promotes nicotine reward. However, less is known regarding the subunit make-up of β2*nAChRs that regulate reward. β2 primarily assembles with the a4 and L97\f"Symbol"\s106 subunits. a4β2*nAChRs are ubiquitously expressed throughout the brain, while a6β2*nAChRs are selectively expressed in catecholaminergic nuclei such as the ventral tegmental area and projection terminals in the nucleus accumbens (NAc), which are implicated in nicotine's rewarding properties. The goal of this study was to investigate the contribution of α6β2*nAChRs to nicotine reward. We showed that a6β2*nAChR gain-of-function (a6L9S) mice, whose α6β2*nAChRs are hypersensitive to nicotine, exhibit enhanced nicotine conditioned place preference (CPP) compared to wild-type (WT) mice, suggesting that activation of α6β2*nAChRs is sufficient to promote nicotine reward. Further, we showed that antagonism of α6β2*nAChRs in the NAc shell with α-conotoxin MII blocked nicotine CPP in WT mice. Overall, these studies suggest that activation of α6β2*nAChRs on terminals in the NAc shell promotes nicotine reward.

Posters

LEPTIN EXPRESSION IN ADIPOSE AND SKELETAL MUSCLE OF MORBIDLY OBESE PCOS AND NON-PCOS WOMEN. M-A Orciga[1], K. Yao[1], Z. Younoszai[1],

A. Baranova[1,2], Z. Younassi[1,3] & A. Birerdinc[2,3], [1]Betty & Guy Beatty Center for Integrated Research, Falls Church, VA 22042, [2]Center for the Study of Chronic Metabolic Diseases, Falls Church, VA 22042 & [3]GMU-Inova Translational Research Institute, Fairfax, VA 22030. Polycystic ovarian syndrome (PCOS) is one of the most common reproductive disorders of the modern world afflicting an estimated 10% of women of reproductive age. An estimated 30-40% of women with PCOS are obese, and 70% of all PCOS cases are found to have some level of insulin resistance (IR) regardless of weight. Understanding IR and the role it plays in pathogenesis of PCOS is inherent in improving treatment and diagnosis of this disorder. To evaluate IR, we examined the role of leptin, a key insulin modulator mainly produced by adipocytes, in morbidly obese, BMI-matched patients with PCOS (n=16) and those without PCOS (n=17). There was a non-statistical trend of higher leptin expression in non-PCOS (NP) patients than in PCOS (P) patients ($p>0.05$). However, in the non-PCOS, non-diabetic (NPND) group a statistically significant 26-fold increase ($p<0.05$) in gene expression of leptin is seen as compared to the non-PCOS diabetics (NPD), with this trend disappearing in the PCOS group. These results suggest that leptin expression is affected by PCOS state when comparing diabetics versus non-diabetics, which should be further evaluated in future studies.

TOLERANCE OF PROXIMAL THYMINE GLYCOL IN DNA DOUBLE-STRAND BREAK REPAIR BY NONHOMOLOGOUS END JOINING. D. Bafail, S. L. Chalasani, M. Almohaini, L.F. Povirk, & K. Akopiants, Department of Pharmacology & Toxicology & Massey Cancer Center, Virginia Commonwealth University, Richmond VA 23298. DNA double strand breaks (DSBs) are extremely toxic to cells because they can lead to genomic rearrangements and even cell death. Two main pathways can repair DSBs: the homologous recombination repair (HRR) pathway and the non-homologous end-joining (NHEJ) pathway. NHEJ is the primary pathway overall and predominant pathway in G1. In the present study NHEJ was assessed using substrates with complex DSB, specifically DSB accompanied by thymine glycol (Tg) at the end (Tg1), 2nd (Tg2) 3rd (Tg3) and 5th (Tg5) positions from the broken end. Experiments were done using XRCC4-like factor (XLF)-deficient cell extracts, with or without the addition of XLF and/or Artemis, EndoIII and ddTTP, or using purified NHEJ protein Ku and XRCC4/Ligase IV with or without XLF. Our results indicated that cell extract could ligate the plasmid with Tg located at third base and fifth the DSB with high efficiency but ligation was severely inhibited when Tg was located at first or the second position from DSB ends. The joining of the Tg5 plasmid was lower than Tg3 with higher efficiency of base excision repair. On the other hand, end joining by the purified proteins was proportional to the thymine glycol position from the DSB end. While XLF was required for ligation of Tg1 and Tg2 by the purified proteins, there was some repair in Tg3 and Tg5 substrates even in its absence. The extracts did not show ligation of the substrates in the absence of XLF.

CAFETERIA STYLE DIET IMPAIRS MEMORY AND INCREASES RISK OF METABOLIC SYNDROME. M. L. Knabe, C. Curtiss, K. S. Sarfert & S. N. Blythe, Dept. of Biology, Washington & Lee University, Lexington VA 24450. Increasing evidence suggests that excess energy intake and obesity are associated with cognitive dysfunction. Although many studies utilize a Western-style diet to examine the effects of diet-induced obesity on cognitive impairment, we believe the Cafeteria-style diet (CSD) more accurately represents the varied and energy-dense diet that contributes to hyperphagia and obesity in humans. This study aimed to investigate the physiological and behavioral effects of CSD consumption on juvenile rats. Twenty-two male Sprague-Dawley rats were divided into control (n=11) and CSD (n=11) groups from weaning. Diet exposure continued for 10 weeks, during which all animals were given ad libitum access to standard rat chow and water. The CSD animals were offered two alternating energy-dense diets, which included various cookies, chips, processed meats, and sweet drinks. During diet exposure, the rats were subjected to Novel Object Recognition, Novel Place, Novel Context, and Morris Water Maze tasks to assess hippocampal-dependent memory performance, as well as an open field task to assess hyperactivity. Following sacrifice, fat pads, livers, aortas, and brains were excised for post-mortem studies. Cognitive tests revealed that CSD rats had compromised spatial and episodic memory. Tissue analysis demonstrated that CSD rats were composed of more fat than control rats, despite comparable total body weight. These data suggest that exposure to energy-dense CSDs leads to memory impairment and the replacement of lean muscle with fatty visceral tissue, potentially contributing to the development of metabolic syndrome and neurological disorders.

AUGMENTATION OF T CELL FUNCTION AS A SELECTION CRITERIA FOR CHEMOTHERAPEUTIC STRATEGIES IN TREATMENT OF MELANOMA. Se W. Jeong, Dan Gioeli, Michael Weber, Alex McClanahan, Devin Roller & Timothy N.J. Bullock, Department of Pathology, University of Virginia, Charlottesville, VA 22908. Metastatic melanoma has a very poor prognosis. PLX4032 (Vemurafenib) is a specific inhibitor that targets a B-Raf gene mutation that is present in more than half of the melanoma patients. Unfortunately, the tumors escaped the therapy by activating other signaling pathways. To address this adaptive resistance, synthetic lethality screens were used to identify small molecule inhibitors (SMI) that synergized with PLX4720, in a panel of melanoma cell lines. As recent studies have indicated that the effectiveness of numerous chemotherapies is dependent upon the recruitment of an adaptive immune response, we probed how these combinations of chemotherapies impacted T cell function and cytokine expression. Two of six inhibitors were found to be overtly detrimental to T cell responses. In contrast, three inhibitors were found to augment varying aspects of T cell responses (frequency and function) and promoted function of T cells from human tumor samples. The activity of the SMI correlates with the expression of checkpoint molecules such as TIM3 and LAG3, but not PD1. Our data indicate that the immunomodulatory capacity of SMIs should be screened as a selection

criterion for single agent therapy and as a component of combination immunotherapies, and suggest opportunities for synergistic chemo-immunotherapeutic clinical trials.

OBESITY AND ADIPOKINE SIGNALING IN CHILDREN AND ADOLESCENTS: THE EFFECTS OF CHRONIC INFLAMMATORY SIGNALING IN OVERALL HEALTH AND GROWTH. Tooba Khan[1], Ancha Baranova[2] & Aybike Birerdinc[2], [1]Dept. of Biology, George Mason Univ., & [2]School of Systems Biology, College of Science, George Mason Univ., Fairfax VA. 22030. NAFLD is one of the most widely increasing diseases in the world today and it is increasing rapidly in children as young as 3 years old. There are many different symptoms of NAFLD but obesity appears to be the most common amongst all. The purpose of this research was to study the prevalence of obesity in children. PubMed was used for this research and the terms used were: 'pediatric NAFLD,' 'Obesity', 'NASH', 'metabolic syndrome' 'and 'adipokine signaling', 'obesity and pregnancy', 'obesity and depression', and 'obesity and mental disorders'. The search was limited to the past 10 years and excluded animal studies. The search resulted in 447 articles out of which 59 were used. In 2007, the International Diabetes Federation defined NAFLD in children aged 6-10 years who were obese and had family histories of cardio metabolic diseases and children aged 10-16 years who were obese and met the criteria for triglycerides being >150 mg/dL. Obese children with symptoms of NAFLD who turn into obese adults tend to have more chances of developing T2DM, hypertension, and atherosclerotic cardiovascular disease. In the US, 17% of the children have type I NASH while 51% have type II NASH and 16% have simple steatosis.8% of the children have advanced fibrosis while 3% have liver cirrhosis. Generally, 85% of the obese children in the US tend to turn into obese adults.

PROFILING FIBROTIC GENES IN VISCERAL ADIPOSE TISSUE (VAT) AMONG PATIENTS WITHIN THE SPECTRUM OF NAFLD. Kameron Tavakolian, Ancha Baranova, Zobair Younossi & Aybike Birerdinc, School of Systems Biology, College of Science, George Mason University and Fairfax VA 22030 & the Beatty Liver & Obesity Research Program, Falls Church VA 22042. Non-alcoholic fatty liver disease (NAFLD) occurs when fat is deposited in the liver, not as a result of alcohol consumption. NAFLD is a spectrum of diseases ranging from relatively benign fatty liver, to non-alcoholic steatohepatitis (NASH). While studies have suggested a role for proinflammatory and profibrotic in the development of NAFLD and NASH, very few of the aforementioned studies have analyzed the expression of genes encoding these profibrotic with varying degrees of hepatic fibrosis (under the NAFLD spectrum) in the visceral adipose tissue (VAT). The aim of this study is to select and validate a panel of biomarkers of inflammation and fibrosis and correlate their gene expression in VAT with the degree of severity of NASH. Primer design and validation is often an underappreciated step in projects involving qPCR, particularly in studies when it is unclear if said genes are indeed expressed. The first major result of this study was validation of the designed primers (n=8) for genes related to both the fibrotic signaling

process and inflammation. IL13RA2 and COL1A2 were found to amplify the intended target products (gel electrophoresis confirmed). CCL11, AGT, and CSF1 show perfect melt curves, however subsequent gel electrophoresis shows amplification of multiple products indicating non-specific binding or the presence of different versions of the genes. IL5, CSF2, and CSF3 have shown abnormal melt curves, again suggesting either differential expression of gene isotypes.

Natural History and Biodiversity

RESPONSES OF THE CATALPA SPHINX AND ITS PRIMARY PARASITOID TO HIGH AND LOW LEVELS OF IRIDOID GLYCOSIDES. Jessica L. Bray[1], M. Deane Bowers[2] & Karen Kester[1], [1]Dept. of Biology, Virginia Commonwealth University, Richmond VA 23298 & [2]Dept. of Ecology & Evolutionary Biology, University of Colorado, Boulder CO. Caterpillars of the catalpa sphinx, Ceratomia catalpae, feed exclusively on Catalpa, which contains the iridoid glycosides catalpol and catalposide. Many catalpa trees are heavily infested and defoliated by catalpa caterpillars each year whereas others are untouched. Most populations of catalpa sphinx caterpillars are heavily parasitized by a parasitic wasp, Cotesia congregata, but some populations remain unparasitized. We hypothesized that iridoid glycoside levels would vary among trees and that insect responses to relatively high or low levels of these chemicals could explain these patterns of herbivory and parasitism. Iridoid glycoside levels varied among trees and trees with relatively high levels of iridoid glycosides were more heavily defoliated. Catalpa moths preferred to oviposit on trees with high iridoid glycoside levels in choice oviposition assays. Caterpillars displayed no preference for high or low iridoid glycoside leaf discs in choice feeding assays. Searching times of C. congregata on high and low iridoid glycoside leaf discs did not differ in no choice searching assays. Results indicate that observed variability in herbivory among trees can be explained by moth oviposition preferences for trees with relatively high levels of iridoid glycosides.

BEHAVIORAL RESPONSES OF MALE PARASITIC WASPS TO PLANT CUES WITH RESPECT TO HOST-PLANT COMPLEX ORIGIN. Megan Ayers & Karen Kester, Dept. of Biolology, Virginia Commonwealth University, Richmond VA, 23284. The role of plant cues in host location by female parasitic wasps has been well studied; however, very little is known about the use of plant cues by males in mate location. Female *Cotesia congregata* display inherent responses to plant cues that can be modified by post-emergence experience. We hypothesized that males would exhibit similar inherent and modifiable responses to plant cues. Further, we hypothesized that males originating from one of two host-plant complexes, *Manduca sexta* on tobacco or *Ceratomia catalpae* on catalpa, would display different responses to tobacco or catalpa. In no-choice assays, searching responses of both males and females to a non-host plant increased sharply at Day 2 and remained stable through Day 4. In no-choice assays

with tobacco and catalpa, males searched longer on catalpa but their responses were not modified by post-emergence experience. In choice assays, naïve males did not display an orientation preference; however, males given a post-emergence experience with their natal host-plant preferred their natal host-plant complex. Overall, results indicate that post-emergence experience with the natal host plant can facilitate assortative mating on the natal host plant.

THE EFFECTS OF URBANIZATION ON BIRD PARASITISM RATES BY VARIOUS TICK SPECIES. E. L. Heller, C. L. Wright, H. D. Gaff & E. L. Walters, Department of Biological Sciences, Old Dominion University, Norfolk, VA 23529. Coastal Virginia is home to one of the largest urban areas within the Atlantic Flyway, a migration pathway used by at least 500 species of birds. By sampling birds at 5 sites across an urbanization gradient, we tested the effect of increasing urbanization on prevalence of ticks parasitizing birds under two alternative hypotheses: (1) host constraint hypothesis-ticks exhibit lower host specificity in more urbanized areas and (2) environmental constraint hypothesis-birds in more urbanized areas exhibit lower tick burden. We sampled birds using mistnets from August 2012 to August 2014. The proportion of birds parasitized by ticks was significantly (ANOVA, $F=6.221$, $df=2$ $p=0.001$) related to level of urbanization and in general, birds from rural and suburban sites were more heavily parasitized by ticks. This study has the potential to demonstrate how urbanization can influence avian host choice in ticks and the corresponding relationship between urbanization and pathogen prevalence.

Posters

POTENTIAL IMPACTS OF CHANGING CLIMATE ON WINTERING BIRD POPULATIONS OF CENTRAL PIEDMONT VIRGINIA. Eric Salamon, Christopher Labosier & Sujan Henkanaththegedara, Department of Biological & Environmental Sciences, Longwood University, Farmville VA 23909. Previous research has shown that many wintering bird species in Piedmont Virginia is declining over the past 60 years. Forty two out of 76 species analyzed (55%) using Christmas Bird Count data show significant population declines in Central Piedmont. One of the possible causes for these declines is changes in regional climate over the last century. We explored the correlations between long-term population trends of Northern cardinal, Mourning dove and Carolina chickadee, with long-term trends of regional climate variables. We acquired climate data for 1950-2015 from National Climatic Data Center and ran linear regression models to isolate any significant correlations between bird population trends and long-term climatic trends. The climate variables include minimum, average and maximum monthly temperatures, precipitation for months of October, November and December, first frost day, and storm frequency. We found a significant trend for October minimum temperature and a significant correlation between October minimum temperature and decline of Northern cardinals. Future research involves expanding the analysis for more wintering bird species.

POTENTIAL IMPACTS OF INVASIVE CRAYFISH ON NATIVE PIEDMONT CRAYFISH (CAMBARUS SP. C) - INSIGHTS FROM LABORATORY EXPERIMENTS. James Wilson, Patricia Hale, Bryan Ditursi, Jackson Wagstaff & Sujan Henkanaththegedara, Department of Biological & Environmental Sciences, Longwood University, Farmville VA 23909. Invasive species are identified as the second greatest cause for imperilment of native species in the United State. In Virginia, there are 137 known invasive taxa, including three invasive crayfish species, and about 50 species of native crayfish. Invasive crayfish can dramatically alter shallow water habitats and cause population declines of native species. We assessed the potential impacts of invasive Virile crayfish (*Orconectes virilis*) on native Piedmont crayfish (*Cambarus sp. C*), focusing on interspecific competition for food and shelter, and survival in sympatry. Native and invasive crayfish were acclimated in a 37.9 L glass aquaria with a central glass divider for 72 hours. Then a food pellet was introduced into the middle of the aquarium after removing the glass divider and feeding and agnostic behavior of both species were monitored. Further, daily monitoring of individual survival of both species was performed for 8 days, and percentage survival was estimated. Feeding trials suggest that native Piedmont crayfish can detect food quickly and "win" the competition for food. However, sympatric survival trails suggest that there is a negative impact of the presence of invasive signal crayfish on survival of native Piedmont crayfish (i.e. a 25% drop of native survival). Future research focuses on scaling up the experiments with mesocosm experiments to generate more realistic information.

INVESTIGATING THE EFFECT OF LARVAL DIET QUALITY ON ADULT BODY SIZE AND MALE HORN MORPHOLOGY IN THE BEETLE *ONTHOPHAGUS TAURUS*. Adrienne J. Muetterties & Patrice M. Ludwig, Biology Department, James Madison University, Harrisonburg, VA. The aim of this experiment is to test the extent to which two resources, commonly used by the sexually dimorphic burrowing dung beetle *Onthophagus taurus*, differ in their effects on adult body size and male horn development. This experiment is based on those done by Moczek (1998) and Hunt and Simmons (2004). Pairs of beetles were placed in breeding tubes with thawed dung, and the brood balls were collected and weighed. With the use of digital imaging and ImageJ, horn length and thorax width were measured for each emerging offspring. Statistical analyses (Mann-Whitney-Wilcoxon, regression, and Chi Square) tested the following hypotheses: there is a difference in the number and mass of brood balls that produce live offspring; there is a difference in the thorax size and horn length of resulting male offspring based on resource quality. Results showed a significant difference between brood ball mass and the type of dung, and additionally a significant difference between the brood ball mass and the sex of the resulting offspring. The Chi Square test revealed that frequencies for emerging offspring were significantly different between the two treatments. Finally, regression analysis showed no significant correlation between brood ball mass and thorax width and horn length. The results of this work implicate that the form in which the resource is available may affect parental

energy investment in offspring, which may in turn affect the sex of the offspring. (Supported by: Betty Jo Loving Butler '58 Endowment for Undergraduate Research Scholarship and Farrell Summer Research Scholarship Award).

THE GLOBAL DISTRIBUTIONS OF HEPATITIS B VIRUS INFECITON, ITS VIRAL GENOTYPES, AND VACCINE COVERAGE: UPDATED HBSAG SEROPREVALENCE ESTIMATES AND ANALYSIS OF DETERMINANTS. John Kim, Max Marzouk, Lei Wang, Peter Masschelin, Ancha Baranova & Aybike Birerdinc, Dept. of Biol., George Mason Univ., Fairfax VA. 22030. Hepatitis B virus infection leads to cirrhosis of the liver and hepatocellular carcinoma (HCC). Despite the discovery of effective vaccine in 1969 against the hepatitis B virus, HBV infection remains a major global health problems with significant amount of prevalence rates throughout different regions of the world. The virus is currently classified into 10 genotypes (A-J) and several subgenotypes. The most severe liver disease predominate in regions with high hepatitis B surface antigen (HBsAg) seroprevalence levels; the most common indicator of HBV infection. In order to precisely assess current and future burdens to global health, we provide updated HBsAg seroprevalence and models illustrating the global distributions of Hepatitis B infection. Distributions of HBV genotypes and national vaccine coverage rates are also integrated into the model. A systematic review of HBsAg seroprevalence between 2005 to 2015 was conducted. World Health Organization reports and recent literature reviews were used to model vaccine coverage and genotype distribution. Data was only collected from articles that meet inclusion and exclusion criteria. HBV prevalence, vaccine coverage, and genotype distribution can be used to prioritize the regions that are in need of help.

PRELIMINARY CHECKLIST OF THE ANTS (HYMENOPTERA: FORMICIDAE) OF VIRGINIA. Kal Ivanov, Department of Recent Invertebrates, Virginia Museum of Natural History, Martinsville VA, 24112. No single treatment of family Formicidae in Virginia has ever been attempted, and the 121 ant species reported from the state, to date, are found scattered throughout the literature. These numbers represent a rather stark underestimation of the number of species expected to occur in the state given the diversity of ecoregions and habitats found in Virginia, and especially when viewed in the light of some recent updates to the ant lists of several neighboring regions. Here I present the first checklist of the ant species known to occur in the state, based primarily on literature records. In addition, I offer new data from materials in the Virginia Museum of Natural History and the Virginia Polytechnic Institute and State University research collections, as well as a small number of recently collected specimens. Currently a total of 124 ant species, including 10 exotics, are reliably reported from the state. These species represent most of the North American groups, lacking only the more tropical members of Cerapachyinae, Ectatomminae, and Pseudomyrmecinae. The most speciose genus in the state is *Formica* (17 spp), followed by *Strumigenys* (13), *Camponotus* (11), *Lasius* (11), and *Aphaenogaster* (9). I also provide distributional information for the few newly recorded species, and I offer brief comparison to species

lists for surrounding states. Increase in collecting effort, coupled with examination of museum specimens is needed to bridge the gap between our current understanding of the ant diversity and distribution in the state and the true diversity of Virginia's myrmecofauna.

WEST VIRGINIA ROCK VOLES. Ralph P. Eckerlin[1], Walter Bulmer[1], Alfred L. Gardner[2] & Suzanne C. Peurach[2]. [1]Natural Sciences Division, Northern Virginia Community College, Annandale, VA 22003, [2]USGS Patuxent Wildlife Center, National Museum of Natural History, Smithsonian Institution, PO Box 37012, Washington, DC 20013. The Rock Vole, *Microtus chrotorhhinus*, is distributed in eastern North America from southern Canada southward in the United States in the Appalachian Mountains to Tennessee. There are few records of the Rock Vole in West Virginia where it is listed as a state imperiled species. We had previously collected one individual on a talus slope at high elevation (ca.1120m) in Pocahontas Co. in the Monongahela National Forest. Beginning in October 2013, using Sherman live traps, we have attempted to collect Rock Voles at that location and learn more about the population size and extent of the population. We have tried a ½ hectare grid and multiple transects through the talus slope at 75-100m intervals. In 450 trap nights we captured only 2 Rock Voles. The two capture sites were about a kilometer apart. Thus, based on these preliminary data, we think the extent of the Rock Vole population is large but the population density is low. Ecological associates captured were *Blarina brevicauda* (14), *Sorex fumeus* (16), *Peromyscus maniculatus* (36), *P. leucopus* (3), *Synaptomys cooperi* (1), *Myodes gapperi* (13), *Napaeozapus insignis* (3), and *Mustela frenata* (1).

FIRST SPECIMENS OF *PEKANIA* (*MARTES*) *PENNANTI* (FISHER) FROM VIRGINIA. Nancy D. Moncrief[1] & Michael L. Fies[2], [1]VA Museum of Natural History, Martinsville, VA 24112 & [2]VA Dept. Game & Inland Fisheries, P.O. Box 996, Verona, VA 24482. Fishers (*Pekania [Martes] pennanti*) are believed to have occurred in portions of western Virginia before being extirpated in the late 1800s. However no specimen of *P. pennanti* from Virginia has ever been reported in a museum collection, and we were unable to find any museum records for specimens from Virginia, despite extensive electronic searches of museum databases in August 2014 and January 2015. Here we document the presence of this species in Virginia with verified photographic records and with voucher specimens deposited in the Mammal Collection of the Virginia Museum of Natural History. These animals probably have dispersed from populations that are expanding from western Maryland and northeastern West Virginia, following translocation of fishers to northeastern West Virginia in 1969. This report provides a benchmark for future studies of the distribution and abundance of fishers in Virginia.

Psychology

THE EFFECTS OF PSILOCYBIN ON THE BRAIN AND THE ROLE OF THE DEFAULT MODE NETWORK: A POTENTIAL TREATMENT FOR DEPRESSION. M. N. Huss, R. W. Campbell, & D. W. Harrison, Department of Psychology, Va. Polytechnic Inst. & State Univ., Blacksburg VA 24061. Psilocybin, the active agent in *Psilocybe* mushrooms, has shown to be a useful therapeutic agent for several brain disorders and is now being investigated as a potential treatment for depression. Current treatment for depression is slow to action and at times is completely ineffective. Thus, the Monoamine Theory of Depression is most likely oversimplified and many researchers have begun to study depression in regards to the Neurotrophic Theory of Depression. It has also been found that the Default Mode Network (DMN) is hyperactive in depression. The DMN is a set of anatomically distinct brain regions that consistently are more active during self-referential processing and internal cognitions. This is consistent with the observation that often people with depression report constant rumination of the self, personal past experiences, and plans for their future. In recent studies, psilocybin has shown to have a significant effect on perception of self and life including elevated mood, reduced stress, increased life-satisfaction, and other anti-depressant effects. Interestingly it has also shown to suppress DMN activity therefore inhibiting constant self-referential processing. Consequently, psilocybin is now being investigated for its potential as a treatment for depression. The exact mechanisms of psilocybin's quick and long-lasting therapeutic effects as well as appropriate methods of administration are yet to be determined and warrant further study.

THALAMIC PAIN SYNDROME: CASE PRESENTATION, TREATMENT, AND FUTURE DIRECTIONS. Kelly M. Corwith, Ransom W. Campbell & David W. Harrison, Department of Psychology, Va. Polytechnic Inst. & State Univ., Blacksburg VA 24061. Thalamic Pain Syndrome (TPS) is a neurologic condition that is both complex and difficult to treat. Thalamic pain syndrome (TPS), also known as Dejerine Roussy syndrome, is a subset of central pain syndrome. It is generally caused by damage to the thalamus from a thalamic stroke, although other causes can lead to this syndrome. Characteristics of TPS include, but are not limited to, severe pain contralateral to the site of thalamic damage, often presenting with feelings of hyperesthesia, allodynia, numbness, and tingling. A review of the literature on the thalamus, TPS, case presentations, as well as current and future proposed treatments has been created in hopes of creating a larger awareness of this syndrome as well as promoting ways to help those suffering from it. Discussion of case presentations involving typical damage to a 63 year old male, atypical damage to a 23 year old female, as well as atypical symptom presentation in a 76 year old male, current treatments such as simple pharmaceutical based regimes, proposed comprehensive treatment plans for patients and their families, and newer proposed treatments such as electroacupuncture and deep brain stimulation are the focus of this review. A concise paper on the current research on TPS may help those suffering, their families,

physicians, neuropsychologists, and students fully understand this syndrome and the progressions being made to help. Lastly, another benefit of this review is the correlations for treatments that may help those suffering from other chronic pain syndromes/disorders.

Posters

FORCASTING ERRORS IN STUDENT MEDIA MULTITASKING DURING HOMEWORK COMPLETION. Christopher A. Baker, Brittany E. Noah, Charles C. Calderwood, Jeffrey D. Green, Jennifer A. Joy-Gaba & Jaclyn M. Moloney, Department of Psychology, Virginia Commonwealth University, Richmond VA 23284-2018. Many students report that they multitask with media while doing homework, but we know very little about why they engage in these behaviors, when considering that they are damaging to their homework performance. We conducted a study to explore the nature and accuracy of students' predictions regarding media multitasking during homework completion. Sixty-one participants from an undergraduate psychology class predicted their mood and performance if they were and were not allowed to multitask. Participants then worked on their homework in the lab while providing mood ratings. We also obtained student permission to access homework grades. It was found that students predicted they would experience lower negative mood and performance if allowed to media multitask, but overestimated the impact of media multitasking on negative mood.

Statistics

SIMPLE GRAPHS IN POLICY PERSUASION: EXAMPLES FROM HARRISONBURG VIRGINIA AND THE U.S. SENATE. Panayotis Giannakouros[1], Lihua Chen[2], [1]Center for Computational Mathematics & Modeling, James Madison University, Harrisonburg VA, 22801, [2]Department of Mathematics & Statistics, James Madison University, Harrisonburg VA, 22801. The American Statistical Association's Ethical Guidelines for Statistical Practice call upon statisticians to "improve the public climate for, understanding of, and respect for the use of statistics throughout its range of applications." This includes supporting sound statistical practice toward serving the needs of society. In this regard, challenges can range from distrust of statistics to an over-reliance on technical procedures that can distort how problems are analyzed or can present a false sense of authority. This talk reports on a research program addressing such challenges by promoting, particularly to policy oriented economists, sensitivity to the philosophy of science and emphasis of the role of communication and data analysis to steer toward a sound and effective balance in statistical practice. We illustrate by showing how simple graphs have been provided by us in this spirit to support policy decisions in Harrisonburg Virginia and others to advocate for policy on the floor of the U. S. Senate.

THE APPLICATION OF LAST OBSERVATION CARRIED FORWARD (LOCF) IN THE PERSISTENT BINARY CASE. Jun He, Donna McClish, Department of Biostatistics, Virginia Commonwealth University, Richmond, VA 23298. In randomized clinical trials, patients often drop out before study completion, resulting in missing data. Last Observation Carried Forward (LOCF), a common method of imputation, assumes that after the point of dropout the last observed outcome is used in place of missing observation. We investigate this methods performance in analyzing persistent binary outcomes (once it occurs it will not change in the future). We ran a simulation study to see the effect of dropout rate and type of dropout (random or associated with treatment arm) on Type I error for the LOCF method of analysis. We also compared LOCF results to two versions of complete case analysis - Complete1 (excluding all observations with missing data), and Complete2 (excluding missing data when the event hasn't been observed to occur, but carrying forward observations if the event is observed to occur). LOCF was also applied to a real dataset – mammography rates in the Women Improving Screening through Education and Risk Assessment (WISER) clinical study, which had a high dropout rate. 1) If the dropout rates were equal, the three analysis methods all had appropriate Type I error; 2) If the dropout rates were unequal, the Type I error was much greater than 0.05 in both LOCF and Complete2 analysis; 3) Regardless of dropout rates, the estimated mean event rate was underestimated in the LOCF analysis and overestimated in the Complete2 analysis, while Complete1 analysis had the closest estimated mean event rate to the Full dataset. In the WISER study, we found that LOCF method underestimated final event rate.

MODELING CENSORED DISCRETE SURVIVAL TIME IN HIGH-DIMENSIONAL SETTINGS. Kyle Ferber, Kellie J. Archer, Department of Biostatistics, VA Commonwealth University, Richmond, VA 23298. The defining characteristic of high-dimensional data is that the number of subjects, n, is much smaller than the number of features, p. The design matrix will be singular in these situations, so standard regression techniques such as ordinary least squares are not appropriate. Regularization, also referred to as penalization, introduces bias into the parameter estimates in exchange for a reduction in variance, resulting in more stable estimates. This has been shown to be an effective method for modeling high-dimensional data. The generalized monotone incremental forward stagewise (GMIFS) algorithm is capable of fitting a penalized ordinal response model to high-dimensional data. Furthermore, a forward continuation ratio model with a complementary log-log link is appropriate for modeling discrete survival data in high-dimensions. We altered the log-likelihood of this model to account for the presence of censored observations and used the GMIFS algorithm to fit a model to predict short-, intermediate-, and long-term survival in patients diagnosed with acute myeloid leukemia (AML). The dataset contained $p = 270$ covariates including clinical data as well as proteomic data from $n = 191$ patients diagnosed with AML. We tested the performance of our method by examining the prediction accuracy of the fitted model in terms of resubstitution error and cross validation. The results demonstrated that our model is effective for modeling discrete survival time.

SEMIPARAMETRIC SINGLE-INDEX MODELING FOR SPATIALLY CORRELATED DATA. Hamdy. F. F. Mahmoud, Inyoung, Kim, Department of Statistics, Virginia Polytechnic Institute & State University, Blacksburg, VA 24061. In this paper, we propose two semiparametric single index models for spatially correlated data. One additively separates the nonparametric function and spatially correlated random effects, while the other does not separate the nonparametric function and spatially correlated random effects. We estimate these two models using two algorithms based on Markov Chain Expectation Maximization algorithm. Our approaches are compared using simulations, suggesting that the semiparametric single index nonadditive model provides more accurate estimates of spatial correlation. The advantage of our approach is demonstrated using the mortality data of seven cities, South Korea from January, 2000 to December, 2007.

BAYESIAN INFERENCE OF MULTILEVEL MODEL WITH SPATIALLY VARYING COEFFICIENTS. H. Moradi Rekabdarkolaee, Department of Statistical Sciences & Operations Research, Virginia Commonwealth University, Richmond, VA, 23284-3083. In spatial data analysis, sometimes we face to cases which the data are nested in different geological category, thus has intra class correlation. In addition, the response variable and covariates in first level are depend to second level variables, so we face to a multilevel problem. This setting is a generalization of linear models which along with modeling of response variable, the coefficients will be modeling too. In this study, we introduce an extended multilevel spatial model in which the coefficients are also spatially varying. Hence, it could provide more flexibility in modeling. The analysis is performed under a Bayesian paradigm and the MCMC method is developed to carry out posterior analysis. The proposed methodology is illustrated through an application to a data set of canopy vegetation percentage of Plour region at north of Iran.

GENERALIZING MCFADDEN'S CONDITIONAL LOGIT MODEL WITH GAUSSIAN COPULA. Arjun Poddar, N. Rao Chaganty, Department of Mathematics & Statistics, Old Dominion University, Norfolk VA 23529. Conditional logit model is a widely popular method to analyze discrete choice data. Originally publicized by McFadden (1974), this model assumes that the random components of the underlying utility functions follow independent Gumbel distributions. However, in practice the independence assumption may be violated and a more reasonable model should account for the dependence. In this research we use the Gaussian copula with compound symmetric correlation matrix to construct a general multivariate model for the joint distribution of the utilities. The induced dependence on the utilities and the choice probabilities are studied using analytic expressions and simulations. For regression with consumer and product specific covariates, we derive expressions for the likelihood function, score functions and the Fisher information. We use numerical methods and computer code to obtain the maximum likelihood estimates and standard errors.

Comparison of our model with other competing methods and practical applicability is illustrated using real world consumer preference data.

SIMULATING DEPENDENT BINARY DATA WITH RANDOM EFFECTS. Aobo Wang, Roy T. Sabo, Department of Biostatistics, Virginia Commonwealth University, Richmond, Virginia 23298-0032. Dependent binary data can be simply simulated using the multinomial sampling method. We extend this method to simulate dependent binary data with clustered random effect structures. Several distributions are considered for constructing random effects among cluster-specific parameters and effect sizes, including the normal, uniform and beta distributions. We present results from simulation studies to show proof of concept for the multinomial sampling method in creating data sets of repeated-measure binary outcomes with clustered random effect structures in various scenarios. The simulation studies show that multinomial sampling method can be successfully adapted to simulate dependent binary data with desired random effect structures.

COMPOSITIONAL DATA ANALYSIS. Theodore Chang, Department of Statistics, University of Virginia, Charlottesville, VA 22904-4135. Suppose we have a sample of rocks and $x_1,..., x_p$ is the weight of p minerals within the rock. Usually we assume that $x_1 + ... + x_p$ represents the total weight of a sample element, so x_p might be 'other'. Then $x_1,..., x_p$ are called the 'open' variables. Let $y_i = x_i / (x_1 + ... + x_p)$ denote the proportions, or 'closed' variables, such that $y_1 + ... + y_p = 1$. This is an example of compositional data. Another example might be data on time allocation: e.g. x_1 is the time spent eating, x_2 the time spent watching TV, etc.. John Aitchison (JRSS B 1982) proposed an approach to analyzing this type of data. We examine the geometry of moving from open to closed variables and, in that light, the mathematical attractiveness of the Aitchison approach.

Structural Biology, Biochemistry, and Biophysics

BIOPHYSICAL CHARACTERIZATION OF NATURALLY OCCURING TITIN M10 MUTATIONS. Michael W. Rudloff, Alec N. Woosley & Nathan T. Wright. Department of Chemistry & Biochemistry, James Madison University, Harrisonburg, Virginia 22807. The giant proteins titin and obscurin are important for sarcomeric organization, stretch response, and sarcomerogenesis in myofibrils. The extreme C-terminus of titin (the M10 domain) binds to the N-terminus of obscurin (the Ig1 domain) in the M-band. The high-resolution structure of human M10 has been solved, along with M10 bound to one of its two known molecular targets, the Ig1 domain of obscurin-like. Multiple M10 mutations are linked to limb-girdle muscular dystrophy type 2J (LGMD2J) and tibial muscular dystrophy (TMD). The effect of the M10 mutations on protein structure and function has not been thoroughly characterized. We have engineered all four of the naturally occurring human M10 missense mutants and

biophysically characterized them *in vitro*. Two of the four mutated constructs are severely misfolded, and cannot bind to the obscurin Ig1 domain. One mutation, H66P, is folded at room temperature but unfolds at 37 °C, rendering it binding incompetent. The I57N mutation shows no significant structural, dynamic, or binding differences from the wild-type domain. We suggest that this mutation is not directly responsible for muscle wasting disease, but is instead merely a silent mutation found in symptomatic patients. Understanding the biophysical basis of muscle wasting disease can help streamline potential future treatments.

MOLECULAR DYNAMICS STUDIES OF THE UBIQUITIN CONJUGATION MECHANISM. Serban Zamfir & Isaiah Sumner, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg, Virginia 22807. Post-translational modification of proteins can have drastic effect on their structure and function. One such modification involves the attachment of a small protein, ubiquitin. An important function of ubiquitination is to signal proteins for cellular degradation. This process occurs in three enzymatic steps. In the second step, ubiquitin transfers to a conjugating enzyme, called E2, which then transfers ubiquitin to a lysine in the target protein. However, the mechanistic details for this final transfer remain obscured. Although it is clear that ubiquitin does bind, there are no studies that show exactly how this happens. The two most favored proposals involve a step-wise mechanism with a tetrahedral oxyanion intermediate and concerted mechanism. This work probes the accuracy of the oxyanion hypothesis. In particular, if the oxygen on the observed carbonyl carbon can form a stable hydrogen bond with the hydrogen on the nitrogen of the asparagine side chain, then oxyanion intermediate is plausible. By using molecular dynamics (MD), combined with umbrella sampling, a free energy profile of the formation of the breaking and forming of the hydrogen bond is constructed to see if its creation is thermodynamically favorable. Furthermore, information about the hydrogen-bonding environment in the active site is extracted.

STRUCTURAL BASIS OF PHOSPHOINOSITIDE (PIP) RECOGNITION BY THE TIRAP PIP-BINDING MOTIF. Daniel G. S. Capelluto[1], Xiaolin Zhao[1], Shuyan Xiao[1], & Geoffrey Armstrong[2], [1]Department of Biological Sciences, Virginia Tech., Blacksburg VA. 24061 & [2]Department of Chemistry & Biochemistry, University of Colorado, Boulder CO 80309, USA. Toll-like receptors (TLRs) provide early immune system recognition and response to infection. TLRs activated by pathogens initiate a cytoplasmic signaling cascade though adaptor proteins, the first being the modular TIR domain-containing adaptor protein (TIRAP). TIRAP contains a C-terminal TIR domain, which is responsible for association with TLRs and other adaptors. Membrane recruitment of TIRAP is mediated by its N-terminal PIP- binding motif (PBM). Upon ligand-mediated activation, TLRs are recruited to the PIP-enriched regions where TIRAP resides. To understand the mechanism of membrane targeting of TIRAP and the basis for its regulation, we functionally and structurally characterized its PBM. TIRAP PBM adopts a folded conformation in membrane mimics, such as

dodecylphosphocholine micelles, and binds PIPs. Structural rearrangements of TIRAP PBM were influenced by membrane interaction, with monodispersed PIPs inducing helical structure in the peptide. In contrast, monodispersed phosphatidylinositol and inositol trisphosphate did not promote structural changes in TIRAP PBM. NMR spectra reveals that TIRAP PBM binds PIPs in a fast exchange regime with a moderate affinity through two conserved basic regions. Solution NMR structure of TIRAP PBM shows a central short helix, and paramagnetic studies indicate that this region is close to the micelle core. Thus, we proposed that two sets of basic residues contact both the head group and the acyl chains of PIPs, whereas the central helix is responsible for membrane insertion.

CHODNROCYTES: A SHOCKING REVELATION. Anthony J. Asmar, Michael W. Stacey, & Frank Reidy, Research Center for Bioelectrics & Department of Biological Sciences, Old Dominion University, Norfolk, VA 23508. Ion channels are typically associated with excitable cells such as neurons and muscle (skeletal and cardiac). However, chondrocytes also utilize ion channels, so to what extent are they electrically active? Chondrocytes are the cells that produce and maintain the extracellular matrix in cartilage. They are able to endure a variety of mechanical and biochemical stresses using ion channels. In this study, we establish a gene expression profile of ion channels in chondrocytes. Although many ion channels have been uncovered previously, we detected several more from various gene families. Not only do we observe a diverse population of channels, but we found the ion channel expression profile of chondrocytes to be similar to cardiomyocytes.

ADAPTING HYPERTHERMOPHILIC PROTEINS INTO SWITCH-BASED BIOSENSORS. Jonathan D. Dattelbaum, University of Richmond, Department of Chemistry, Richmond, VA 23173. The analytical detection of small molecules is an important theme in the molecular life sciences. Our studies here focus on the design of reagentless fluorescence protein biosensors using two members of the periplasmic binding protein superfamily recently identified from the hyperthermophile, *Thermotoga martima*. This Gram-negative bacterium is found primarily in hot springs and hydrothermal vents. Proteins isolated from *T. maritima* are thus likely to exhibit a high degree of physicochemical stability, making them useful targets for manipulation and utilization in biosensor design. Using site-directed mutagenesis, we created single cysteine variants of TmArgBP (*T. maritima* arginine binding protein) and TmMBP (*T. maritima* maltose binding protein). Thiol-reactive fluorophores were covalently attached to the protein and used to probe ligand binding. Changes in fluorescence were used to determine dissociation constants that typically range in the low micromolar level. Because these proteins exhibit large conformational alterations upon ligand binding, we propose a theoretical framework that provides a rational approach to the design of switch-based biosensors. Stable protein biosensors may provide a sensitive and specific platform for small molecule testing, particularly in complex cellular matrices.

HOFMEISTER ION AND CO-SOLVENT EFFECTS ON THE STRUTCURE, AGGREGATION, AND SOLVATION OF RECA. Taylor P. Light, Karen M. Corbett, Michael A. Metrick & Gina MacDonald, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg VA 22801. RecA is an *Escherichia coli* protein that catalyzes the strand exchange reaction utilized in DNA repair. Previous studies have shown that the presence of salts influence RecA activity, aggregation, and stability. Here we utilized attenuated total reflectance Fourier-transform infrared (ATR-FTIR) spectroscopy and circular dichroism (CD) to further investigate how various Hofmeister salts and co-solvents alter RecA structure, aggregation, and solvation. Spectroscopic studies performed in water and deuterium oxide suggest that salts alter amide I (or I') and amide II (or II') vibrations arising from the protein backbone. Specific IR vibrations that may arise from protein-solvent interactions were identified. IR vibrations that correlate with protein desolvation were observed in the presence of strongly hydrated SO_4^{2-} anions. The vibrations that correlate with protein solvation were observed in the presence of weakly hydrated Cl^- and ClO_4^- anions. An increase in the IR frequency of amide I (or I') correlated with increasing concentrations of trifluoroethanol (TFE) and sucrose. This result suggests an increase in desolvation of the amide backbone with an increase in the concentration of co-solvents. Additionally, increasing concentrations of TFE resulted in an increase in RecA aggregation. These results show that salts and co-solvents alter the solvation water surrounding proteins and influences overall structure and aggregation. This research was supported by NSF grants NSF-RUI CHE-0814716 and NSF-REU CHE-1062629.

SMD SIMULATIONS OF THE M-BAND TITIN-OBSCURIN INTERACTION. Tracy A. Caldwell, Isaiah C. Sumner & Nathan T. Wright, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg, VA 22807. Titin and obscurin, two giant muscle proteins, bind to each other in an antiparallel Ig-Ig fashion at the M-band. This interaction must be able to withstand the mechanical strain that the M-band typically experiences and remain intact. The mechanical force on these domains is likely exerted along one of two axes: a longitudinal axis, resulting in a 'shearing' force, or a lateral axis, resulting in a 'peeling' force. Hre we present molecular dynamics data suggesting that these forces result in distinct unraveling pathways of the titin-obscurin complex and that peeling the domains apart requires less work and force.

MECHANISM OF UFM1 CONJUGATION: STUDIES OF UFC1. Emily A. Todd, Nathan, Wright & Christopher E. Berndsen, Dept. of Chemistry & Biochemistry, James Madison University, Harrisonburg, VA 22807. Ufm-ylation is the process by which the ubiquitin-fold modifier (Ufm1) is transferred to a substrate lysine. This process is crucial for morphology changes in many parasites and is linked to regulation of ER stress and breast cancer. There are two known enzymes in the pathway, Uba5, the Ufm1 activating enzyme and Ufc1 the conjugating enzyme. The Ufm-ylation pathway is similar to the ubiquitin conjugation pathway however many of the structural

characteristics of ubiquitin conjugating enzymes are not apparent in Ufc1. Previous studies on the E2 enzyme Ubc13 showed that the HPN motif and an active site loop are critical for activity. However, none of these conserved characteristics are present in Ufc1. To elucidate the function of Ufc1 structural and functional differences we present NMR and molecular modeling studies of Ufc1. Future studies include understanding the structural characteristics of Ufc1 in substrate and Uba5 binding and the biochemical mechanism of Ufc1 conjugation.

THE IMPORTANCE OF THE DISULFIDE BONDS WITHIN BST-2 FOR STRUCTURE AND VIRAL TETHERING. Kelly E. Du Pont, Aidan M. McKenzie, Oleksandr Kokhan, Isaiah C. Sumner & Christopher E. Berndsen, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg, VA 22807. Human BST-2/tetherin is a host factor that inhibits release of enveloped viruses, including HIV-1, HIV-2, and SIV, from the cell surface by tethering viruses to the host cell membrane. BST-2 consists of an N-terminal cytoplasmic domain, a transmembrane domain, an alpha helical ectodomain, and a C-terminal membrane anchor. In cells, BST-2 forms disulfide-linked dimers between the ectodomains of each monomer forming a coiled-coil. The N-terminal half of the ectodomain contains three cysteine residues which can participate in disulfide bond formation and are critical for viral tethering. The role of the disulfides in viral tethering is unknown, but proposed to be for maintenance of the dimer. We explored the role of the disulfides in maintaining BST-2 structure in order to propose the molecular basis for the requirement for disulfides in viral tethering. We found that the disulfide bonds strengthen the coiled-coil structure of BST-2 but do not appear to affect the dimeric state of the protein. To further explore the role of the disulfides, we chose to take a novel approach and simulated viral tethering and observe changes in BST-2 structure. These simulations of viral tethering revealed that the disulfides alter the unfolding pathway of BST-2 and that the disulfide-linked dimer of BST-2 is more resistant to virus induced stretching. These data provide new insights into viral tethering by the innate immune system and have generated novel models of viral tethering a previously inaccessible biological phenomenon.

STRUCTURAL ELUCIDATION OF THE IG58, IG59, AND IG58/59 DOMAINS OF OBSCURIN. Rachel A. Policke, Tracy Caldwell, Logan Meyer & Nathan T. Wright, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg, VA 22807. Obscurin (800-900 kDa) is a giant muscle protein vital to muscle cell maintenance and organization. It is the only known linker between the contractile apparatus and the sarcoplasmic reticulum of myocytes and may also bind to cytoskeletal, signaling, or membrane-associated proteins. One such interaction is the binding of obscurin domains Ig58/59 to titin domains ZIg9/10. This binding, which requires all four domains to be present, is hypothesized to stabilize the sarcomeric cytoskeleton. Mutations in this region of obscurin lead to malformed muscle architecture and may lead to hypertrophic cardiomyopathy (HCM). In order to better

understand the molecular underpinnings of this disease, we used X-ray crystallography and NMR to solve high-resolution structures of the Ig58 and 59 domains of obscurin individually as well as in tandem.

IDENTIFICATION AND CHARACTERIZATION OF *THERMOTOGA MARITIMA* Hfq PROTEIN BINDING PARTNERS. Thushani Nilaweera, Lissa Anderson, Jennifer Patterson, Donald Hunt & Cameron Mura, Department of Chemistry, University of Virginia, Charlottesville, VA 22904 USA. The host factor for bacteriophage Qβ (Hfq) is the bacterial branch of Sm family proteins which are involved in RNA metabolism. In bacteria, Hfq acts a global post-transcriptional regulator, affecting the stability and translation of messenger RNA (mRNA) by facilitating the annealing between small regulatory RNAs (sRNA) and their target mRNAs. Hfq has also been linked to proteins involved in general cellular RNA metabolism (RNA synthesis and degradation). An Hfq homolog is present in *Thermotoga maritima* (*Tma*), an early-branching anaerobic thermophile. In previous work, a novel class of nanoRNAs (~5-6 nts) was found to co-purify with recombinant *Tma* Hfq expressed in *Escherichia coli*. NanoRNAs are regulated by oligoribonuclease (Orn), and a putative homolog of this enzyme can be detected in *Tma* based on sequence similarity. We have successfully cloned, expressed and purified the recombinant *Tma* Orn in *E.coli*. We are investigating the putative function of *Tma* Orn and potential interactions between *Tma* Hfq and nanoRNA degradation pathways. Additionally, we are attempting to isolate endogenous *Tma* Hfq protein binding partners using Co-immunoprecipitation (CoIP) and using liquid chromatography tandem mass spectrometry (LC-MS/MS) analysis. By providing a map of *Tma* Hfq *in vivo* interactions, this work will lay a foundation for understanding the roles of Hfq as a global ribo-regulator.

BIOLOGICAL QUEUEING: A FRAMEWORK FOR PROTEIN SYNTHESIS AND DEGREDATION NETWORKS. Nicholas Butzin, Philip Hochendoner, Curtis Ogle & W.H. Mather, Dept. of Physics, Virginia Tech, Blacksburg VA, 24061. It is known that all biological cells must cope with limited resources, but less appreciated is the impact of finite *processing* resources behind a myriad of tasks, including not only metabolism but also protein production, degradation, and modification. I will discuss the experimental and theoretical development of a biological queueing theory, which fundamentally assumes limited processing resources. In particular, recent results demonstrate that shared degradation machinery can form a strong effective mutual activation between protein species, which forces a rewriting of regulation diagrams currently assumed for many gene networks. Complementing this work, limited translational resources can lead to "riboqueueing," establishing mutually repressive interactions between gene activities. I conclude with very recent developments concerning competition within polysomes.

Posters

IDENTIFICATION OF NOVEL ALLOSTERIC MODULATOR BINDING SITES IN NMDA RECEPTORS: A MOLECULAR MODELING STUDY. Lucas T. Kane[1] & Blaise M. Costa[1,2] [1]Edward Via Virginia College of Osteopathic Medicine & [2]Department of Biochemistry, Virginia Tech, Blacksburg VA, 24061. The dysfunction of N-methyl-D-Aspartate receptors (NMDARs), a subtype of glutamate receptors, is correlated with schizophrenia, stroke, and many other neuropathological disorders. However, not all NMDAR subtypes equally contribute towards these disorders. Since NMDARs composed of different GluN2 subunits (GluN2A-D) confer varied physiological properties and have different distributions in the brain, pharmacological agents that target NMDARs with specific GluN2 subunits have significant potential for therapeutic applications. In our previous research, we have identified a family of novel allosteric modulators that differentially potentiate and/or inhibit NMDARs of differing GluN2 subunit composition. To further elucidate their molecular mechanisms, in the present study, we have identified four potential binding sites for novel allosteric modulators by performing molecular modeling, docking, and *in silico* mutations. The molecular determinants of the modulator binding sites (MBS), analysis of particular MBS electrostatics, and the specific loss or gain of binding after mutations have revealed modulators that have strong potential affinities for specific MBS on given subunits and the role of key amino acids in either promoting or obstructing modulator binding. These findings will help design higher affinity GluN2 subunit-selective pharmaceuticals, which are currently unavailable to treat psychiatric and neurological disorders.

INVESTIGATING THE ENZYMATIC ACETYL TRANSFER REACTION PATHWAY. B. Hamilton Young & Christopher. E. Berndsen, Dept. of Chemistry & Biochemistry, James Madison University, Harrisonburg, VA 22807. Protein acetylation, which involves the transfer of an acetyl group to the side chain of a lysine residue, serves many vital cellular purposes. Defects in enzymatic acetylation have been linked to diseases such as cancer, insomnia, and anemia. Despite decades of research into the biological function of protein acetylation, the enzymatic mechanism of acetyl transfer is unknown. We aim to determine the mechanism of catalysis for acetyl transfer using the yeast protein acetyltransferase GCN5. Using a fluorescent activity assay, we have found a normal deuterium solvent isotope effect for this reaction, suggesting that proton transfer occurs during the acetyl transfer reaction. This information is crucial for understanding the enzyme mechanism. Upon investigation of an inhibitor-bound GCN5 X-ray crystallography structure, the presence of multiple steric and geometric anomalies were observed. Molecular dynamics was used to investigate the validity of these published structures. Future experiments will determine the number of protons being transferred, measure the kinetic isotope effects on the GCN5 acetyl transfer reaction, and investigate the mechanism of acetyl transfer using molecular dynamics. We aim to compare data obtained on the GCN5 reaction

mechanism to that of the ubiquitin transfer reaction catalyzed by the enzyme Ubc13, which performs the same basic reaction using a vastly different structure. This comparison will allow for determination of whether the mechanism of acetyl transfer is conserved between the two enzymes.

AN ARGININE CLAW IN PHOSPHORYLATED DESMOPLAKIN SUGGESTS A MECHANISM FOR CONTROL OF INTERMEDIATE FILAMENT BINDING. Charles E McAnany & Cameron Mura, Department of Chemistry, University of Virginia, Charlottesville, VA, 22904. Cellular adhesion is governed by desmosomes, large transmembrane complexes that tether the intermediate filaments of separate cells. It has recently been shown that the serine-rich C-terminus of desmoplakin governs binding to intermediate filaments. Several phosphorylation sites on the C-terminal region have been shown to regulate the strength of the binding. Here, we show that the phosphorylation of S2849 leads to the formation of an arginine claw that is not present in the non-phosphorylated protein. We show that the methylation of R2834 causes the protein to adopt a structure suited to processive phosphorylation. This suggests that the conformation of desmoplakin acts as a switch to control the action of GSK3, a kinase noted for its low substrate specificity. We further show that the site of these modifications is not free in solution, but contacts other parts of desmoplakin, suggesting a binding competition mechanism for the regulation of intermediate filament adhesion.

COMPARISON OF KINETIC PROPERTIES OF AROMATIC DESULFINASES. Ianna Hutchinson-Lundy, Austin Crithary, Jonathan Schmitz & Linette M. Watkins, Department of Chemistry & Biochemistry, James Madison University, 901 Carrier Dr. Harrisonburg, VA 22807. Dibenzothiophene (DBT) and its derivatives comprised up to 60% of the organosulfur contamination of crude oil. The enzyme 2-(2'-hydroxyphenyl) benzenesulfinate desulfinase (DszB) catalyzes the carbon-sulfur bond cleavage in the final, and rate-limiting step in the biodesulfurization of DBT. The DszB enzymes from *Nocardia asteroides* A3H1 and *Rhodococcus erythropolis* IGTS8 were overexpressed in *E. coli*, purified and characterized kinetically. The stability of the enzyme was measured under various storage conditions and increased stability was observed upon immobilization of the enzyme to CNBr-activated Sepharose beads.

EFFECT OF IMMOBILIZATION ON THE STABILITY AND SPECIFICITY OF CHOLINE OXIDASE. Jonathan Schmitz & Linette M. Watkins, Department of Chemistry & Biochemistry, James Madison University, 901 Carrier Dr. Harrisonburg, VA 22807. Choline oxidase catalyzes the conversion of choline into glycine betaine and hydrogen peroxide. Choline oxidase has two roles in industry and medicine, as a sensor of choline, and in the synthesis of glycine betaine. For optimal utility in industrial synthesis pathways choline oxidase must have a broad specificity while maintaining activity over a range of pH and temperature. The specificity, pH optimum, temperature optimum and temperature stability of choline oxidase from three different

sources was determined. In order to address low stability at elevated temperatures, choline oxidase was immobilized on CNBr-activated Sepharose beads. Immobilized choline oxidase showed enhanced stability over broader range of temperature and pH. The turbidity of the immobilized enzyme prevents the use of continuous spectrophotometric assays to test the specificity and alternative methods for testing specificity are under investigation.

INFRARED STUDIES OF SALT-INDUCED EFFECTS OF AMINO ACIDS. Elizabeth P. Mortimer, Elijah T. Johnson, Taylor P. Light & Gina MacDonald, Department of Chemistry & Biochemistry, James Madison University, Harrisonburg VA 22801. Infrared spectroscopy was used to study glycine at different pH and salt conditions. The addition of various Hofmeister salts was studied to determine how these ions influence glycine infrared spectra. Changes in pH affect the protonated or deprotonated state of the amino and carboxyl groups suggesting altered vibrational spectra. The presence of a kosmotropic salt should desolvate the amino acid while the chaotropic salts should solvate the amino acid. These studies aimed to determine if infrared spectroscopy could identify if the presence of salts alters glycine absorptions. The spectrum of glycine was obtained at pH's of 1.5, 7, and 12.5 in phosphate buffer in deuterium oxide. Glycine spectra were also obtained at pH 7.0 in sodium chloride, sodium perchlorate, and sodium sulfate. Glycine infrared spectra show clear pH and salt induced shifts in infrared vibrations. Comparison of the various infrared spectra will be discussed. This research was supported by NSF grants NSF-RUI CHE-0814716 and NSF-REU CHE-1062629.

ASSESSING THE RNA-BINDING SITES OF HFQ VIA COMPUTATIONAL DOCKING. Matthew A. Cline & Cameron Mura, Department of Chemistry, University of Virginia; Charlottesville, VA 22904 USA. The Sm superfamily of proteins bind RNA and are found in all domains of life. The RNA binding characteristics have yet to be fully characterized, particularly for the Sm-like archaeal proteins (SmAPs). In principle, molecular docking may be used to determine RNA binding sites; while in practice, docking force fields have been parameterized for use with small organic compounds rather than for RNA. Therefore, we must first examine the suitablity of our docking approach (using AutoDock 4 and AutoDock Vina) for the prediction of RNA binding sites. We began explorations in the bacterial branch of the Sm superfamily, Hfq, where the binding has been experimentally characterized. Hfq is known to chaperone RNA-RNA interactions, thus regulating translation of mRNA. To validate the use of docking for the prediction of RNA binding sites on Hfq, NTPs were docked to *Pseudomonas aeruginosa* Hfq and compared to known crystal structures of *Pseudomonas aeruginosa* Hfq bound to NTPs. Preliminary results suggest that AutoDock 4 does not predict accurate RNA binding pockets of Hfq reliably, while AutoDock Vina is capable of predicting binding pockets.

INTERPLAY AMONG E3 UBIQUITIN LIGASES REGULATES TIMELY DEGRADATION OF THE CIRCADIAN FACTOR PERIOD 2. JingJing Liu & Carla V. Finkielstein, Integrated Cellular Responses Laboratory, Department of Biological Sciences, Virginia Tech. Circadian rhythms are mechanisms that measure time on a scale of about 24 h and that adjusts our body to external environmental signals. Core circadian clock genes are defined as genes whose protein products are necessary components for the generation and regulation of circadian rhythms. Oscillatory rhythms are generated as result of the activation of positive and negative transcriptional feedback loops in which post-translational modifications, shuttling, and degradation are common themes. Ubiquitin E3 ligases-mediated protein degradation is critical to sustain physiological rhythms. Here we show beside the F-box β-TrCP1/2 targeting PER1 and PER2 for degradation via ubiquitination, the mouse double-minute 2 homolog (Mdm2) RING finger E3 ligase binds to PER2 and promotes PER2 polyubiquitination occurring both *in vitro* and in cells. Overexpression Mdm2 or down-regulation Mdm2 by siRNA, results in decreasing or increasing PER2 stability reciprocally. Furthermore, we found Mdm2-dependent post-translational modification of PER2 directly influences the amplitude of the circadian oscillatory response in synchronized cells and that both, ?-TrCP and Mdm2 target PER2 at different circadian times. Overall, our findings support a model in which, the rate of nuclear degradation of PER2 leads to slow accumulation of the protein in the nucleus and, later in the day, to a temporal switch in which ?-TrCP takes control over PER2 degradation. Thus, the interplaying between these two E3 ligases is indispensible for sustaining robust circadian oscillation.