

1**Studies directed toward the total synthesis of chilenine**

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The condensation of phenethylamine derivatives with ninhydrin, or its analogues, yields oxyprotoberberines. Subsequent oxidation and ring expansion can provide the aporphoadane skeleton. This study describes the preparation of model systems with increasing structural complexity, as well as the use of this methodology in the preparation of the natural product chilenine. Chilenine has demonstrated cytotoxic activity against human tumor cell lines with IC₅₀ values in the micromolar range.

3**Measuring Potassium in Muscle Tissue Through the Use of an Atomic Emission Spectrometer**

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Potassium is a cation important for a properly functioning body, especially for nerves, kidneys, and muscles. The goal of this research project is to determine the concentration of potassium in muscle tissue. It seeks to verify a relationship between the concentration of potassium in muscle tissue and previously recorded data gathered through an adaptation of the whole body counting method. Atomic emission spectrometry was utilized to analyze the samples. A method was formulated to digest the meat samples through the use of flash freezing in conjunction with grinding using a liquid nitrogen cooled mortar and pestle, followed by soaking the meat in HCl acid while shaking and then isolating the solution through centrifuging. The previously reported range of potassium readings were 1.9 g potassium for each kilogram of adipose tissue to 3.1-3.5 g/kg in muscle tissue. We obtained a range of potassium concentration from 2.76-4.66 g K⁺/kg of beef sample.

2**Total synthesis of lunamarine and analogues**

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Lunamarine is an alkaloid that was isolated from the plant *Lunasia amara* in 1943. Although it has demonstrated the ability to reduce arterial blood pressure with minimal toxicity in animal models, it has not yet been synthesized. The synthesis of lunamarine is described in this study. Highlights include the use of boron trichloride-directed acetylation and Camps cyclization to access the 4-quinolone core of the target natural product. This methodology is also used in the preparation of lunamarine analogues for biological screening.

4**Green Chemistry Synthesis of Tetrakis(methoxyphenyl)porphyrin & Tetrakis(hydroxyphenyl)porphyrin**

Wilt, Ashley; Skoner, Matthew; Liska, Erica; Zovinka, Edward P.
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One of the most common synthetic tools for chemists has been the reflux heating method. With the growth of interest in green chemistry, chemists have been searching for more efficient synthetic methods. One method we have been examining is the use of microwave techniques in both organic and inorganic synthesis. We have successfully synthesized Tetrakis(methoxyphenyl)porphyrin, H₂(DMP)P, and Tetrakis(hydroxyphenyl)porphyrin, H₂(DHP)P, by using microwave methods with less time and water waste, often without the use of solvent. By successfully replacing the lengthy and more hazardous procedure with the microwave, the synthesized H₂(DHP)P can be utilized to model the active site of the hydroxylamine oxidoreductase enzyme (HAO).

5**The Microwave Metallation of Porphyrins**

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Cobalt (II), copper (II), iron (III), nickel (II), and zinc (II) have all been successfully inserted into tetraphenylporphyrin (H₂TPP) as determined by UV-Vis. Classical procedures used for metal insertion into porphyrins use reflux methods requiring large amounts of energy, water, and time. By utilizing a CEM Discover microwave, the amount of time needed for metal insertion reactions to proceed was reduced by up to 5 hours. Furthermore, the amount of power needed for each reaction was reduced, to less than 60 watts. The development of Green Chemistry methods for metalloporphyrin synthesis will be used in modeling the active site of hydroxylamine oxidoreductase in *Nitrosomonas europaea*.

7**Green Chemistry: Developing Experiments For the Undergraduate Laboratory**

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One of the most unfortunate affects of industrialization is the environmental problems due to the chemicals released into our environment through mining and chemical synthesis of many organic and metal based compounds. In order to solve these problems many new experimental procedures are being created using less damaging chemicals, energy efficient synthetic methods, and real time analyses to help decrease our impact on the earth.

Saint Francis University was awarded an NSF-CCLI Grant #0737268 to purchase instrumentation and to develop green chemistry methodologies for the undergraduate laboratory. Due to the lack of these technologies in the past, laboratory experiments were conducted to become familiar with the equipment. Protocols and undergraduate laboratory experiments were developed for the new equipment. Throughout these experiments while using the potentiostat, microwave, and ion chromatograph the 12 steps of green chemistry were major considerations.

6**Syntheses of lactam analogues α -conotoxins.**

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Conotoxins, disulfide-rich small peptides, may provide a crucial insight into pharmaceutical development without side-effects. We have previously designed and synthesized four lactam analogues of the natural isomer of α -conotoxin SI. The [C3E,C13K]-analogue was about 70-fold more potent than the natural isomer of α -conotoxin SI. In comparison to other α -conotoxins, the affinity of α -conotoxin SI for nicotinic acetylcholine receptor types is significantly lower than α -conotoxin SIA, GI, and GII, peptides also studied in our research group. In this study we set out to explore whether changing the a disulfide bridge to a lactam bridge in these other α -conotoxins would effect their affinity for the receptor sites. The size of the intramolecular bridges and the identity and orientation of the lactam bridges are kept constant in the peptides studied.

8**An Investigation into the Internal and External Environmental Influences on the Redox Properties and Kinetics of Adsorbed Cytochrome c on Self-Assembled Monolayers**

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The thermodynamic and kinetic properties of cytochrome c on SAMs have been extensively studied. The carboxylic acid system has been utilized to establish relationships between SAM surface charge and formal potentials. Apart from the extensively studied carboxylic acid/diluent thiol systems, new thiols containing a range of previously unexamined head groups are yielding strong adsorption and electrochemical signal from cytochrome c. One monolayer in particular, the phosphonic acid terminated SAM, has demanded more than the established theories on formal potential and rate kinetics for explanation². This work focuses on the adaptation of prior theories to aid in the explanation of phenomena examined by these new monolayer systems. In an attempt to better understand the influence of charge on the electrochemistry of cytochrome c, differently charged monolayers were examined as well as an investigation into the effects of protein surface charge modification.

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Syntheses of lactam analogues of α -conotoxin SI with different intramolecular bridge sizes.

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Department of Chemistry, Saint Francis University

Conotoxins, disulfide-rich small peptides, may provide a crucial insight into pharmaceutical development without side-effects. We have previously designed and synthesized four lactam analogues of the natural isomer of α -conotoxin SI. The [C3E,C13K]-analogue was about 70-fold more potent than the natural isomer of α -conotoxin SI. Our results led us to assume that the larger disulfide loop in α -conotoxin SI plays a global structural role, while the smaller loop plays a greater role in the activity of the peptide. Based on these findings we set out to explore how changing the size of the rings in the most potent analogue would influence its affinity for the receptor sites. In these studies we have synthesized and characterized analogues where we change the size of the lactam bridge and/or of the disulfide bridge by either reducing or increasing the number of the carbon atoms in the side-chains of the amino acids.

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Interning at Ethix Systems LLC

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Ethix Systems LLC is a growing business based in Greensburg, PA, specializing in customized web-based software solutions, with an emphasis on open source technologies such as PHP and MySQL. The projects are structured around a Model-View-Controller (MVC) framework established using CodeIgniter. The key benefit of the MVC framework is team collaboration, as well as being able to partner with web designers who may implement designs without understanding the code. Coding itself is done in Eclipse using PHP, HTML, XHTML, JavaScript, AJAX, and other web based programming languages. Testing occurs via "pushing" the applications to the company Intranet and/or via utilization of WampServer on a local machine (permitting Apache, PHP, and MySQL to run on Windows). On the backend, Ethix utilizes Linux and Windows based servers and runs Subversion Control, DokuWiki, Bugzilla, and phpDocumentor to continually track changes to projects, document problems, and provide final product code documentation.

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Isolation and Characterization of Novel *Streptomyces* Bacteriophages

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Streptomyces are Gram-positive, non-pathogenic, soil-dwelling bacteria with a complicated life cycle. Bacteriophages, viruses of bacteria, are able to infect their host using either a lytic or lysogenic approach. It has been reported that there are 10^{31} phage in the environment (Hendrix, 1999), making it relatively easy to find them in soil. The variety of phages that infect *Streptomyces*, however, is not yet known. Several bacteriophages were isolated from environmental soil samples using *S. lividans*. Each phage forms a unique area of infection, or plaque. The morphology of each phage varies in size and proportion, as analyzed using electron microscopy. One isolated phage appears to be temperate, indicating that lysogenic bacteria are formed upon its infection. DNA from each isolated phage was extracted using a small-scale preparation, and has been submitted for sequencing.

12

Calculations of Thiolate pK_a using Molecular Dynamics Free Energy Perturbation

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An approach based on molecular dynamics free energy perturbation (MDFEP) with explicit water has been proposed to calculate the pK_a values of the cysteinyl thiolate in simple -Cys-xx-Cys- motifs as found in the thioredoxin and metallochaperone protein families. In the thioredoxin family the thiols, which have markedly altered pK_a s, serve a catalytic function while those in metallochaperone family ligate a single cuprous ion that the protein routes through the cell. Explicit water free energy perturbation calculations, using AMBER10, has been used to calculate the pK_a s of thiolates in -Cys-x-x-Cys- motifs. The thioredoxin family of proteins was used to establish the computational protocol. Both methods were then applied to a metallochaper system. Application of this methodology will support the experimental determination of pK_a s by providing an approximate pH range in which to develop the experiments. The computational methods are general and can be extended to other functional groups in other proteins.

13**Qualitative Analysis of Arsenic Species Using Electropray Ionization Time of Flight Mass Spectrometry in Preparation for EPA Study**

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Varying levels of toxicity between chemical species of arsenic necessitate accurate methods of arsenic speciation. In this study, three species of arsenic—arsenite [As(III)], arsenate [As(V)], and monomethylarsenate [MMA(V)]—were analyzed by electropray ionization time of flight mass spectrometry (ESI-TOF-MS). ESI overcomes the propensity of molecules to fragment during the ionization process, thus elucidating the chemical structure of each species in solution. The structural information is being used to plan a speciated isotope dilution mass spectrometry (SIDMS) method for arsenic speciation in conjunction with the EPA in an interlaboratory study. This approach offers a significant advantage over hyphenated chromatographic techniques, which simply match the retention time of arsenic species with that of known standards and provide no structural information. As(III), As(V), and MMA(V) were analyzed simultaneously in a 1:1 methanol-water solution at a concentration of 100 mg/L, and the fragmentation pattern of each species was determined.

15**Synthesis and Characterization of Fe-doped CuInS₂**

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CuInS₂ is a ternary I-III-VI₂ semiconductor currently being researched for use in solar cells.

However, indium is an expensive, rare metal. The goal of this research is to dope CuInS₂ with iron to create the series CuIn_{1-x}Fe_xS₂. Iron is cheap and abundant, and readily assumes an oxidation state of +3, the same as indium in CuInS₂. Fe-doped CuInS₂ was synthesized by a solid state reaction under vacuum, with some samples heated to 1150°C and the others heated to 650°C. CuInS₂ was doped with 5, 10 and 15 mol % Fe. The resulting products were analyzed by powder x-ray diffraction and the band gaps were measured using diffuse reflectance UV/vis/NIR spectroscopy.

14**Importance of counter ion complexation in copper catalyzed atom transfer radical addition**

Biernesser, Ashley; Pakkala, Saichand; Eckenhoff, William T.; Evanseck, Jeffrey D.; Pintauer, Tomislav Department of Chemistry and Biochemistry, Duquesne University

Atom transfer radical addition (ATRA) is a fundamental reaction used to add halogenated compounds across carbon-carbon double bonds by a radical process. Fluxional processes of nitrogen-based heterocyclic copper catalysts in ATRA such as ligand and/or counter ion dissociation are currently being investigated to better understand the mechanistic aspects of this process. These reactions are performed in the presence of radical diazo initiators which act as a reducing agent to regenerate the catalyst. High-level density functional theories have been used to explore the electronic details involving the ligand binding to the copper complex. The interaction between the halide anion and the copper center was found to be much weaker for the copper(I) complex when compared to the copper(II). We speculate that the difference in counter ion coordination affects the catalytic activity of the copper complex in ATRA. The computational and crystallographic studies will be presented.

16**Electronic Structure Calculations of Diamond-Like Semiconductors**

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Diamond-like semiconductors are normal valence compounds that resemble the structure of diamond. These compounds are of particular interest because of their unique optical and magnetic properties and their application to solar cells, nonlinear optics, and spintronics. The goal of this project is to understand the electronic structure and band gap trends in quaternary diamond-like semiconductors. To test the utility of Density Functional Theory using the Accelrys DMol3 module, the electronic structure of several known compounds was calculated. Examples include: CuInSe₂, Li₂PbGeS₄, NaLiCdS₂, and CuGaS₂. Analysis of these results determined DMol3's effectiveness in modeling known compounds. Calculations aimed at explaining the band gaps of quaternary diamond-like semiconductors of the Li₂M¹M²S₄ form (where M¹ = Cd, Zn and M² = Ge, Sn) were also performed using the DMol3 module. A tutorial was written for performing calculations in the DMol3 program.

17

Characterization of Novel Pigments in *Etheostoma caeruleum* and *E. blennioides*

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This study was conducted in order to extract, purify, and characterize the novel integument pigments produced by two species of fish in the genus *Etheostoma*. Unlike most other vertebrates, which utilize structural refraction to display blue or green color, male rainbow darters (*E. caeruleum*) and male greenside darters (*E. blennioides*) exhibit blue or green mating coloration resulting from true chromoprotein pigments. Spectral absorption profiles indicate that pigments from these two species are similar, but not identical. Pigments were extracted from intact frozen specimens and partially purified by ammonium sulfate fractionation and size-exclusion chromatography. Further purification using preparative non-denaturing Polyacrylamide Gel Electrophoresis (PAGE) followed by electroelution of the pigment was accomplished for *E. caeruleum*, but not *E. blennioides*. Analysis by SDS PAGE showed that this technique was successful in purifying the pigment completely; however, it may not be practical for subsequent applications due to the small yield.

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Synthesis and Characterization of An Oxomolybdenum Dithione Complex With Biological Relevance

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Molybdenum is a transition metal that is found in some living organisms. In this study, a dithione ligand (quinoxaline-2,3(1H,4H)-dithione, was synthesized and characterized by Fourier transform infrared spectroscopy (FT-IR), UV-vis and nuclear magnetic resonance (NMR). The ligand was then reacted with molybdenum pentachloride (MoCl_5), to obtain a molybdenum complex. This complex will act as a model in understanding the catalytic properties of the dimethyl sulfoxide enzymes, which have a catalytic site with Molybdenum, coordinated to dithione ligands together with other ligands.

18

Spectrophotometric Analysis of Cu^I Regeneration from Cu^{II} in the Presence of Free Radical Initiators

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Atom transfer radical addition (ATRA) has recently been coupled with radical reducing agents (AIBN) in order to make ATRA environmentally friendly. In the presence of reducing agents Cu^I can be continuously regenerated from Cu^{II} , minimizing accumulation of Cu^{II} deactivator species and allowing the use of ppm levels of Cu^{II} catalysts. Products of ATRA are small molecules used to create complex organic compounds and pharmaceuticals. Kinetic experiments were conducted on solutions of Cu^{II} complexes and methanol under two conditions to prevent oxidation; first solutions were purged with argon, second solutions were prepared within the glove box under argon atmosphere. Purging with argon gas was found to be ineffective, but the second method prevented oxidation. Solutions were placed in an oil bath at 60°C to allow the decomposition of AIBN. UV/vis spectroscopy was used to monitor the progress of the reaction.

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Chromium (VI) Protocol Development in Dietary Supplements to Determine Toxicity

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Dietary and diabetic pills often contain chromium as an active ingredient. Whether the species is chromium (III), an essential metal to our bodies, or has been oxidized to chromium (VI), a harmful toxin and carcinogen, is important in assessing the benefits or possible detriments from consuming the supplements. This study used Method 3060a to extract chromium (VI) from supplements to determine if the amount was significant. A variation on this method using hot water extraction to maintain a neutral pH and therefore stabilize both hexavalent and trivalent chromium was also evaluated. Method 6800, SIDMS (spiciated isotope dilution mass spectrometry), utilized spiking of the sample with isotopes and LC-ICP-MS (liquid chromatography-inductively coupled plasma-mass spectrometry) to determine concentrations of chromium (III) and chromium (VI) (with mass balance) while accounting for oxidation and reduction interconversions between species. Preliminary results showed that approximately half of the tested supplements contained the toxic chromium (VI).

21**Characterization and Synthesis of Mn doped AgInSe₂ for Use as a Dilute Magnetic Semiconductor**

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Sto-Rox High School

Dilute magnetic semiconductors differ from conventional semiconductors because they can exploit the spin of an electron as well as the band gap of the material. These materials have the potential to store and process electronic information more efficiently. In this study, AgInSe₂, a diamond like semiconductor with chalcopyrite structure, has been doped with the magnetic ion Mn, from concentrations ranging from 0 to 0.1. Several stoichiometries (Ag_{1-x}InMn_xSe₂, Ag_{1-2x}InMn_xSe₂, Ag_{1-x}In_{1-x}Mn_{2x}Se₂, and AgIn_{1-x}Mn_xSe₂) were prepared via solid state synthesis by heating the elemental reagents at 850 °C for 72 hours. Powder X-ray diffraction was used to verify phase purity. Samples were annealed to reduce secondary phase formation. Rietveld refinements were completed to further characterize the materials.

23**A Survey of Dietary Supplements Containing Cr(VI)**

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Dietary supplements and even some probiotics have been tested for Cr(VI), a toxin and carcinogen. Most of these supplements are available in common retail stores. Cr(III) is a necessary element for the processing of sugars, proteins, and fats in the human body. Cr(VI) can be detected in a supplement because either Cr(III) was oxidized and transformed into Cr(VI) during the production process, or it was there in the Cr(VI) form originally. Samples are prepared by extraction in a laboratory microwave system used for chromium extraction from the ground tablets using EPA Method 6800 ("Elemental and Speciated Isotope Dilution Mass Spectroscopy", SIDMS) as the analysis technique. SIDMS is appropriate because it uses isotopes to correct, when Cr(III) changes to Cr(VI) during the extraction process.

22**Synthesis of Dilute Magnetic Semiconductors**

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Duquesne University

Dilute magnetic semiconductors have potential applications in areas such as computers, cell phones, and other electronics. Dilute magnetic semiconductors are formed when some of the nonmagnetic ions in a semiconductor are replaced by magnetic ions. This research was conducted on AgInSe₂, a ternary I-III-VI₂ diamond like semiconductor. The material has been doped with various amounts of Mn, a magnetic ion (AgIn_{1-x}Mn_xSe₂). To synthesize the compound, high temperature solid state reactions were performed on stoichiometric mixtures of elemental reagents heated to 850 °C for 72 hours. Products were annealed for 200 hours at 820 °C to obtain a phase-pure compound. Products were characterized by powder X-ray diffraction.

24**Mechano-dependent Biosynthetic Response of Micro-integrated Cells in Elastomeric Scaffolds**¹⁴Anderson, Lauren N.; ²Stella, John A.; ²³Sacks, Michael S.¹Bioengineering & Bioinformatics Summer Institute, Dept. of Computational Biology, University of Pittsburgh²Department of Bioengineering and ³The McGowan Institute for Regenerative Medicine, University of Pittsburgh⁴Department of Bioengineering, The Pennsylvania State University

The field of tissue engineering combines the principles of biology and engineering in an effort to create biological substitutes that mimic the mechanical and structural properties of healthy native tissues. This project examines the biosynthetic effects of cyclic mechanical strain placed on a PEUU scaffold densely integrated with rat vascular smooth muscle cells. Cells isolated from rat aorta were expanded onto tissue culture plates from which specimen were prepared by concurrently electrospinning the PEUU scaffold and electrospaying the cells. The specimen was placed in a tension bioreactor that mechanically conditioned the specimen in a controlled manner. The specimen will be assessed in groups as follows: day 0 control, day 7 static, and day 7 15% and 30% strain. Soluble collagen and proteoglycan DNA production will be quantified compared to day 0 controls. It is expected that large strain will cause a statistically significant increase in the production of extracellular matrix.

25**Inheritance of mtDNA Repeats in Walleye (*Sander vitreum*)**

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The mitochondrial control region DNA of walleye (*Sander vitreum*) and other Percid fishes contain highly variable 10 VNTR repeat motifs that can be used to identify maternal lineages within a population. Individuals are heteroplasmic and have differing numbers of repeats resulting in a unique signature for most individuals. We attempt to validate the pattern of this mtDNA repeat for use in maternity studies by comparing the repeat pattern from hatchery crossed embryos and their parents. Genomic DNA was extracted from parental fin clip samples and embryos using phenol chloroform and embryo fast extraction respectively. This region was amplified through four independent Polymerase Chain Reactions (PCR) per sample using a Hex-labeled primer. Fragment analysis was conducted on an ABI-3100 Avant Genetic Analyzer and examined with GENESCAN. Composite haplotype patterns of the embryos were compared to the parents to investigate the validity of the method, mutation rates and potential for paternal leakage.

27**Synthesis and Characterization of a Fluorescent Lead Sensor, Leadglow.**

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Lead toxicity is one of the most common environmental concerns in the United States, as it can affect almost every soft tissue in the body, especially in children. The Center for Disease Control has recently set a new goal to eliminate blood lead levels in children by 2010. In order to accomplish that goal lead must be able to be detected at small amounts. The current methods for the detection of lead are highly instrumentally intensive. A fluorescent molecule, 4,4-dimethyl-4H-5-oxa-1,3dithia-6,11-diazacyclopenta[a]anthracen-2-one, patented as Leadglow, has been found to act as a selective and sensitive fluorescent lead sensor. This method of lead detection has been found to be comparable to several of the currently used methods of detection. Here we discuss the synthesis of Leadglow and its spectroscopic characterization. Its binding to other metals are also discussed.

26**Stability of Self-Assembled Monolayers at Various pH Levels**

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*Slippery Rock University

Stainless Steel (SS316L) is an important metal used in medical applications in implant devices. The surface of native oxide of the metal was modified with organic acid monolayers in an effort to prevent bacteria's cell adhesion. The greatest concern with using the surface coating is the stability of the monolayers in physiological environments. Octadecylphosphonic acid and 16-phosphonohexadecanoic acid monolayers were synthesized on SS316L and then dipped in various pH solutions. The substrates were then characterized to determine if the monolayers remained intact using infrared spectroscopy, Matrix Assisted Laser Desorption Ionization Time of Flight Mass Spectrometry (MALDI-TOF MS) and atomic force microscopy. Current results indicate that monolayers of octadecylphosphonic acid and 16-phosphonohexadecanoic acid remain intact in acidic and neutral conditions however, in basic conditions octadecylphosphonic acid monolayers gain physically bound adlayers while 16-phosphonohexadecanoic acid monolayers are lost and become disordered.

28**GC-MS Analysis of Hair Product Residues for Forensic Comparison**

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Abstract: A method was developed to extract hair-care product residues for analysis in GC-MS (Gas Chromatography/ Mass Spectrometry). Hair is a common piece of evidence found at crime scenes. This experiment tested a new method for comparing hairs that may be more accurate than traditional microscopy techniques. First the components of various products themselves, such as shampoos and conditioners, were extracted through sonication. Multiple solvents were tested, and acetone, isopropanol, and methanol proved to be the most effective. These solvents were then used to study actual hair samples.

29**Analysis of Gunshot Residue Ratios of Lead, Barium, and Antimony from Various Manufacturers Using ICP-MS**

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Duquesne University

A study was conducted to determine if the analysis of gunshot residue could be used in criminal investigations as a source of linking a suspect to a crime scene. Inductively-coupled plasma mass spectrometry, ICP-MS, was used to determine the relative amounts of lead, barium, and antimony in the gunshot residue from five different bullet manufacturers. The gunshot residue was collected from both fabric and cartridges. The ratios of the isotopes were compared within the manufacturers, as well as among the manufacturers, to determine if there was statistical significance which would allow this method to be useful in criminal investigations.

31**Synthesis and Purification of Primary Fatty Acid Amides**

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Primary fatty acid amides (PFAM's) serve as an important class of biological lipids that have been catalyzed by $N_{18}TG_2$ cells. Every amide has a specific function in the biological process, whether it is inhibiting the growth of cancer cells or regulating fluid volumes. For instance, one of the most commonly used amides is an oleamide, which serves as a neuron modulator. PFAM's were separated from bovine omentum through a process called homogenization and extraction. After the sample had been homogenized and the lipids extracted, it was prepared for solid phase extraction (SPE). The purpose of SPE was to remove unwanted compounds, leaving only amides. The remaining PFAM's were examined using gas chromatography/ mass spectroscopy (GC/MS). This technique was used to determine any impurities there may have been in the sample, along with identifying and measuring amides. In addition to GC/MS, thin layer chromatography was used to separate amides. TLC is a method that employs a silica plate on aluminum to isolate amides based on polarity. Future experimentation is required in order to perfect the measurement process.

30**Computational Analysis of nAChR $\alpha 4$ and $\beta 2$ Subunit Stability and NMR Study of Protein Anesthetic Interaction**

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Because the $\alpha 4$ and $\beta 2$ subunits of the transmembrane domain of nAChRs are naturally unstable in solution suitable for NMR experimentation and structural determination, mutation of the subunit sequences has been performed to lower subunit pI. However, as $\alpha 4$ stability is much greater than $\beta 2$ stability, further mutation of the $\beta 2$ sequence at key residues has been attempted to increase $\beta 2$ stability. Computer modeling and simulation of the $\alpha 4$ and $\beta 2$ subunits provide a basis for assessing the mutant subunit stability. NMR experiments run both with and without anesthetic were performed to provide insight as to which specific residues within the $\alpha 4$ subunit interact with anesthetic based on observed differences in chemical shifts.

32**Copper Catalyzed Atom Transfer Radical Addition (ATRA) in the Presence of Triethylborane**

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The process of adding polyhalogenated compounds to alkenes was first developed in the early 1940's with the use of free radicals. These reactions were thus improved by utilizing transition metal complexes as catalysts but typically required large concentrations to be successful (10-30 mol%). The solution to this problem has been found for copper mediated ATRA using free radical initiators (e.g. 2,2'-Azobis(2-methylpropionitrile) or AIBN). This work was extended to the use of the free radical initiator triethylborane (Et_3B). Et_3B has shown to be promising at producing efficient yields when compared to AIBN, producing TONS of 400-900 in the reaction of CCl_4 to 1-hexene. Triethylborane decomposes into radicals in the presence of oxygen, allowing this methodology to be used in ambient conditions. However, the key benefit of using Et_3B is its ability to operate as a reducing agent at low temperatures.

33**Particle Size Analysis in Tablet Dosage Form Using Near-Infrared Chemical Imaging**

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In today's pharmaceutical industry, the tablet dosage form serves as the most common delivery method due to its manufacturing and administering advantages over other dosage forms. A significant factor affecting the pharmaceutical performance of tablets is the particle size distribution (PSD) of active ingredients, which can change throughout the manufacturing process. To investigate the effect of the PSD on performance, a non-invasive analytical technique capable of measuring particle size in a tablet is the preferred approach. A method holding such analytical potential is near-infrared chemical imaging, which allows for extraction of spatial and spectral information of chemically different particles from a tablet's surface. Ultimately, the goal of this study is to determine the limit of detectable particle size in a binary mixture containing microcrystalline cellulose (PH200) and a range of polystyrene-divinylbenzene spheres with a known PSD using the MatrixNIR™ chemical imaging system (Malvern Inc, Olney, MD).

35**Understanding Protein Adhesion on Monolayer Modified SS316L**

Berrier, Anastasia; Kruszewski, Kristen; Gawalt, Ellen S.
Department of Chemistry and Biochemistry,
Duquesne University

Modifying the surface of biomedical implants with self-assembled monolayers (SAMs) has been proposed as one method of protecting the implants from bacterial and protein adhesion, which can potentially lead to higher rates of post-operative infection and rejection by the body. Long-chain phosphonic acid molecules with three different tail groups – CH₃, OH, and COOH – were used to form SAMs on stainless steel 316L. Diffuse reflectance Fourier transform spectroscopy, water contact angle measurement and matrix-assisted laser desorption ionization time-of-flight mass spectrometry were used to characterize the monolayer. Protein adhesion tests with human fibrinogen were then performed and showed increased adhesion after 24 hours on the hydrophilic surfaces and decreased adhesion on the hydrophobic surface. These results suggest that hydrophobic SAMs have a better potential for reducing non-specific protein adsorption on implants.

34**Preliminary Study in Characterizing Tissue Growth through Residual Strain**

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This research was a preliminary study done to get an idea for the basic trend of residual strain seen in pulmonary trunks. Porcine Pulmonary Trunks were used and experiments were done on both the sinotubular junction and the region near the bifurcation. Through comparisons of opening angle and circumferential stretch ratios, it was found that residual strain is significantly greater in the ring samples taken from the sinotubular junction than the ring samples from the bifurcation region. From flexural tests, it was also observed that the sinotubular sample had greater strain values than the bifurcation sample. These results will help to outline a method of study for characterizing tissue growth using residual strain and stress at various timestamps. This future study hopes to more thoroughly study native tissue behavior with creating better engineered tissue in mind.

36**Sodium phosphate effects on the helical stability of a mainly-alanine peptide**

Batey, Nichole; Ascitto, Eliana; Madura, Jeffrey
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Duquesne University

Small, positively charged peptides have been found to be able to enter a cell through its lipid bilayer. Bioengineers have been using these small peptides, along with an α -helical structure as a driving force, as a way for the peptides to enter the cell. However, if these α -helices become unstable, then there is no driving force for the peptide. Computational and experimental teams have worked to develop techniques in which to stabilize these helical structures. One way to stabilize the α -helix is through the use of ions in an aqueous solution. This study examined the effects of phosphate ions on the α -helix of a small peptide via an AMBER ff99SB modified force field. Previous computational and experimental have stated that the phosphate ion exhibited both stabilization and destabilization effects on the α -helix in an aqueous environment.

37

Impact of As(III) Exposure on Bacterial Diversity in the Murine Colon: An Ultrastructural Study

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Initial molecular studies involving Arsenic (III) exposure suggest alterations in microbial gut diversity. We hypothesize that exposure to As(III) contaminated drinking water will result in changes in colonic microbiota. Transmission electron microscopy (TEM) was used to determine community organization of the microbiota. The microbial community of the control mice exhibited definite structure with specific morphologies (e.g., a 0.5 μm diameter coccoid dominating the lining of the intestine cavity). This coccoid was absent in the experimental mice who also exhibited a general loss of biofilm organization. Light Microscopy was utilized to confirm microbial changes were consistent with treatment and not due to colonic location. The loss of some species and changes in the physiological state of the remaining gut bacteria, suggests a major shift in metabolism. Whether the changes were induced by direct exposure to As(III) or a result of the physiological changes in the mouse remains to be established.

39

Future of Antibiotics: Carboxyphosphate Binding in N⁵-CAIR Synthetase

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Drug resistant bacterial and microbial infections have grown exponentially over the past decade, primarily due to the over-use of antibiotics in every day applications. N⁵-carboxyaminoimidazole ribonucleotide (N⁵-CAIR) synthetase, an enzyme found in bacteria but not humans, allows the synthesis of effective antibiotics and potentially eliminates the resistant dilemma. Properties of carboxyphosphate, the key intermediate in the N⁵-CAIR enzymatic pathway, are being investigated using high level computational methods. Modern DFT and post-SCF methods are being used to predict the behavior of the intramolecular proton transfer and decarboxylation reactions. We hypothesize that binding pocket residues, lys-353 especially; affect the predisposition of the hydrogen toward either the phosphorus or acid side of the molecule. We have found that a pseudo-chair conformation is critical to the intramolecular proton transfer. The combination of powerful supercomputers and high levels of theory provide a fundamental analysis and aid in the development of antibiotics to fight bacterial resistance.

38

MicroRNA Extraction for Investigation of *Xenopus laevis* Limb Suppression

Fisher, Cara; Elinson, Richard P.

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Abstract: Tadpole limb development is retarded in the model organism, *Xenopus laevis*, compared to limb development in the direct-developing frog, *Eleutherodactylus coqui*. One possible mechanism of suppression is the presence of microRNAs that repress gene expression by inhibiting translation. We hypothesize that delayed limb development in *Xenopus laevis* is a result of miRNA expression in limb buds. miRNA will be extracted from *X. laevis* NF50 hindlimb bud, *E. coqui* TS4 hindlimb bud, and *E. coqui* TS4 forelimb bud for miRNA expression comparisons. A protocol for miRNA extraction from tissue has been optimized using *X. laevis* embryos. This protocol consists of three basic steps: Trizol extraction for total RNA, PEG fractionation for high- and low-molecular weight RNAs, and denaturing PAGE for selection of mature miRNAs. This protocol will be carried out on the previously mentioned tissues to isolate miRNAs and assess their involvement in *X. laevis* limb suppression.

40

Analysis of the Interaction between the X tail and NS5B Regions of the Hepatitis C Virus Genome

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Duquesne University

With over 200 million people infected, the Hepatitis C Virus (HCV), a blood borne pathogen that affects the liver, poses a major health problem worldwide. The Hepatitis C Virus has a positive strand RNA genome of approximately 9.6 kb, replicated by an error-prone RNA-dependent RNA polymerase, which confers the virus a high mutational rate. The 3'-end region of the genome is composed of a short, variable region, a poly (U/UC) tract, and a highly conserved 98-nucleotide RNA element called the X-tail. The first 55 nucleotides of the X tail are 100% conserved among all HCV strains, making this region an attractive target for anti viral therapy. In this study, we are analyzing the interactions between the HCV X tail and a conserved element within the HCV RNA coding region, interactions proved to be absolutely essential for the virus replication, by using UV-Vis spectroscopy, native gel electrophoresis, and fluorescence spectroscopy.

41

Photochemical Reduction of CO₂ to Methanol at Carbon Modified (CM)-n-TiO₂//Cu or Mo Photochemical Cell

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Photoelectrochemical reduction of CO₂ in a 0.2 M NaOH solution was carried out using carbon modified n-type titanium dioxide (CM-n-TiO₂) photoanode and Cu or Mo metal dark cathode. Methanol has been shown to produce higher yield in 0.2 M NaOH electrolyte solution. CO₂ was dissolved under pressure in a custom designed electrochemical pressure cell. While under pressure the pH of the electrolyte changed from 13.3 to 7.2. This change in pH indicated that CO₂ was dissolved in the form of carbonic acid. Analysis of the electrolyte using gas chromatography with a FID confirmed methanol production. With illumination from a 150W Xenon lamp at a light intensity of 100 mW cm⁻², a good yield of methanol is expected to be produced at a measured potential of -0.1V/SCE.

43

Prosecuting Poachers Using a DNA Marker System

Hornyak, Jennifer; Ludvico, Lisa

Department of Biological Sciences, Duquesne University

Recently in wildlife forensics, DNA has been obtained from ivory, hooves, pelts, bush meat, horns, bones, and scat. The Forensic DNA Laboratory at Duquesne University has been working to create a white-tailed deer (*Odocoileus virginianus*) DNA primer panel in collaboration with the Pennsylvania Game Commission to assist in the prosecution of poaching of white-tailed deer both out of season and within residential areas. In order to assist this agency, we have been testing STRs (short tandem repeats) from published literature on a white-tail deer taken legally during the hunting season. Eleven independent STRs have been optimized using Polymerase Chain Reaction (PCR) amplification, and we are currently attempting to multiplex these primers into two separate reaction mixes. This project will show the process of creating a viable STR multiplex panel for use in the upper level forensic DNA laboratory classes and provide a "roadmap" for creating similar panels for other species.

42

Crystal Engineering of Coordination Polymers: a Study of the Structures of Homonuclear & Heteronuclear Polymers

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Duquesne University

Cobalt(II) β-diketonate supramolecular coordination complexes are synthesized by ligand exchange processes. The structures vary as a function of the starting cobalt(II) complexes, the ligands bonded to the Co(II) species, the nitrogenous bases, and the solvent system. Ligands scramble, in a 50v/v% methanol/methylene chloride solvent system, yielding the most insoluble complex by slow evaporation. The acidity of the conjugate acid of the displaced ligand influences product formation. Additionally, the structures of the products vary with the molecular geometries of the diazoaromatic bases. Two types of supramolecular polymers are formed: coordination polymers via cobalt(II) and hydrogen bonded polymers via nitrogen-oxygen and/or oxygen-oxygen hydrogen bonds. Structural trends are observed and related to diazoaromatic base and ligand steric effects along with basicity. Wave-like polymers have been observed with backbones approximating the form of a sine wave.

44

Sodium acetate effects on the helical stability of a mainly-alanine peptide

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Peptide-based drugs have been developed to potentially treat various forms of cancer and HIV. Some α-helical peptides can access cells via crossing the cell's lipid bilayer. However, the environment could affect the peptide's α-helical stability making the crossing into the cell difficult. To overcome this problem, experimental and computational teams have developed techniques to stabilize the α-helix configuration of peptides. One such method is to select ions to stabilize the α-helix secondary structure in an aqueous environment. This work is part of the entire Hofmeister series investigation. We studied the stabilization effects of the acetate anion on a mainly alanine peptide. Replica Exchange Molecular Dynamics was also utilized in order to increase sampling of configurations of the system throughout the simulation. According to previous studies, the acetate ion is expected to stabilize the peptide less than perchlorate in an aqueous environment according to the Hofmeister series.

45**Identifying the Critical Residues of Protein Family OxyR that Cause Oxidative Stress Response in Bacteria.**Pancholi, Minjal¹²³; Nicholas, Hugh¹².¹Pittsburgh Supercomputing Center, Carnegie Mellon University²Bioinformatics and Bioengineering Summer Institute, Department of Computational Biology, University of Pittsburgh³Department of Biology, Howard University

The OxyR protein found in many bacteria works as a redox switch and activates the oxidative stress response (Zaim, 2003). OxyR is a peroxide sensor and a transcription regulator, which can sense the presence of reactive oxygen species and induce antioxidant system to protect the bacteria from hydrogen peroxide (Chen, 2008). To identify the amino acid residues, critical for this function, a subset of 125 OxyR sequences was collected. These sequences covered the entire range of variability shown by all the known protein sequences in different species. A high quality multiple sequence alignment was performed to identify the specific biochemical and physiological role carried out by the amino acid residues responsible for the oxidative stress response. The phylogenetic tree will be constructed, using the aligned sequences, to study the adaptation in different environment. The structural analysis of conserved residues will be presented in the known three dimensional structure.

47**Effect of Testosterone on Locomotory Activity in a Salamander**Feth, Caitlin; Bliley, Jacqueline; Woodley, Sarah
Department of Biological Sciences, Duquesne University

Locomotion is a basal behavior underlying many critical activities such as mate searching, feeding, and predator avoidance. Many different hormones have been shown to alter levels of locomotory activity. In a previous experiment it was found that male reproductive condition affected mobility in mountain dusky salamanders (*Desmognathus ochrophaeus*) with reproductive males being more active than non-reproductive males. It was hypothesized that this difference in activity was due to elevated testosterone levels in reproductive males. To test this hypothesis, *D. ochrophaeus* salamanders were castrated. Controls were males that received surgery but their testes were not removed. Their activity was then videotaped on substrates moistened with chemosensory cues including prey cues, female-derived cues, male-derived cues, predator-derived cues, and water controls. Results will be discussed.

46**Acute Stress Response as an Adaptive Mechanism in Salamanders**Bliley, Jacqueline; Feth, Caitlin; Woodley, Sarah
Department of Biological Sciences, Duquesne University

Vertebrates express a suite of physiological and behavioral responses to stressors. The stress response is thought to be beneficial in the short term, but becomes detrimental when expressed long-term. This response is believed to promote survival behaviors while also suppressing non-essential functions such as mating. Therefore, an acute stress response would suppress mating and decrease locomotory activity as a form of adaptation. In experiment one; activity was analyzed immediately following an acute stress response for 4 hours. A dramatic decrease in activity was seen in stressed salamanders as compared to their non-stressed counterparts for up to 3 hours. In experiment two, *D. ochrophaeus* salamanders were subjected to capture stress and their response was recorded for a period of 5 hours. No difference was found in activity or mating levels between captured and non-captured salamanders. The acute stress response appears to be a beneficial adaptive mechanism.

48**Cloning of *Eleutherodactylus coqui* DEADSouth Gene**Krohn, Kourtney; Elinson, Richard P.
Department of Biological Sciences, Duquesne University

Xenopus laevis is a frog that has been used widely for scientific research. A related frog, *Eleutherodactylus coqui*, has been used as a comparison for developmental and evolutionary research. Far less is known about the coqui and its evolutionarily distinct features as a direct developing frog. *DEADSouth* is a gene responsible for *Xenopus* germ cell fate. To compare germ cell development in *E. coqui*, I am attempting to clone a full length cDNA of *DEADSouth* in *coqui* based on a 212 bp fragment cloned by Cara Fisher. A PCR based screening method of a coqui ovarian library as well as isolation of *EcDEADSouth* from the library through PCR using combinations of exact and plasmid primers is underway. Sequencing of the amplicon through transformation into the T-easy vector as well as direct sequencing of the PCR product will be attempted.

49**Chemicals Targeting an HIV-1 Nef/Host Cell Kinase Complex as Novel Anti-Retroviral Compounds**

Adepegba, Damilola; Day, Billy

Department of Natural Sciences, University of Maryland Eastern Shore

Departments of Pharmaceutical Sciences and of Chemistry, University of Pittsburgh

HIV-1 possesses accessory proteins that are essential participants in the progression of AIDS. Nef has been identified to be an essential protein and therefore has become a target. Nef forms a complex with its host cell binding partner, the Src family kinase Hck. Nef activates Hck through a mechanism that involves displacement of the SH3 domain from a negative regulatory interaction with the catalytic domain. Nef, is known to influence signaling molecules, such as protein kinases. These characteristics of Nef enhance viral replication as well as survival of infected cells. High-throughput screening identified two classes of inhibitors of HIV activity and Nef:Hck interaction. One class was diphenylfuopyrimidines, the other 2-arylsulfonamido-3-arylaminequinoxalines. Remarkably, these agents block Nef-dependent HIV replication and show no cytotoxicity. The present studies were on the design and synthesis of a new member of the latter class of compounds, perhaps a new approach to the development of anti-HIV agents.

51**Weighted Ensemble Simulation of Alternating Access in Sodium Symporter vSGLT**

Scarborough, Amy; Grabe, Michael

Department of Biological Sciences, University of Pittsburgh

Many transport proteins use the energy in sodium gradients to drive the uptake of small molecules. These proteins clear neurotransmitters from the synaptic cleft and remove sugar from the gut. It is thought they operate via an alternating access mechanism in which substrate is bound in an outward-facing conformation followed by a transition to an inward state that delivers the cargo to the cell. X-ray structures of both states exist, but the long time required to see such slow events makes studying this transition using traditional molecular simulations prohibitive. We employed the weighted ensemble method, which focuses computational efforts on rare events, to study changes in the sugar symporter vSGLT. With this method we have observed hundreds of transitions. Analysis of these trajectories reveals insights into the mechanism of alternating access, which we believe will impact our understanding of the operation of these proteins and their roles in human disease.

50**Understanding the role of 15 kilodalton Selenoprotein's promoter region in cancer development**Poliner, Eric; Sneddon, W. Bruce; Rosiek, Kellie
Department of Biological Sciences, Duquesne University

The Selenoprotein of 15 kilodaltons (Sep15) is a protein hypothesized to assist in folding proteins and is suppressed in some breast cancers. The promoter of Sep15 has several regions of high homology across several species, which likely contain key regulatory elements. Interaction between these regulatory regions and breast cancer's altered transcription factors may be the reason why Sep15 is suppressed. Sep15's promoter was isolated using custom primers and PCR and was inserted into a luciferase vector. The vector will be placed in control breast cells and breast cancer cells. Using a luciferase assay it will be possible to quantify expression levels of luciferase, which will be a measure of Sep15's promoter's activity. We hypothesize that luciferase activity will be absent in breast cancer cells due to transcription factors required to interact with Sep15's promoter being absent. These results would indicate that defects in transcription factors cause the suppression of Sep15.

52**Towards a Hybrid Drug Delivery System by Combining Particles and Membranes**

George, Amanda; Zheng, Ying; Buckner, Ira; Gawalt, Ellen S.; Meng, Wilson S.

Graduate School of Pharmaceutical Sciences, Duquesne University

The main objective of this project is to understand the interactions between polymeric particles and peptide membranes. It was hypothesized that drug-loaded particles fabricated from a polyester (PLGA) and a lipid (DOGS) containing a metal ion (nickel) can be mounted onto membranes displaying six consecutive histidine residues. The particles were observed to capture a His-tagged peptide in a concentration dependent manner (as measured by changes in the zeta potential). The interaction was found to be reversible by the addition of imidazole (1 mM). When injected into saline solutions the particles were embedded in the membranes and remained associated for up to one week. The association appears to occur through specific (histidine-nickel coordination) and non-specific (charge pairing and hydrogen bonds) interactions. It is envisioned that such hybrid systems (particle-mounted membranes) may be developed into drug delivery devices by fine-tuning the physiochemical and mechanical properties.

53**Compartmental Models in the Spread of Influenza A H1N1 Virus**

Rusu, Victor; Ta'Asan, Shlomo
Department of Mathematical Sciences, Carnegie Mellon University
Indiana University

The influenza A H1N1 virus, responsible for the current outbreak of swine flu, is considered particularly dangerous since the swapping of entire RNA segments between viruses and an absence of RNA proofreading enzymes lead to large genetic diversity in the virus population. For many infectious diseases, compartmental models have been good mathematical models. They organize individuals with varying susceptibility or infectivity into different classes, and use ordinary differential equations to model the relationships between these classes. From these models, one can obtain a system of ordinary differential equations which describes the severity of the epidemic. However, there seems to be difficulties in fitting the existing models to the swine flu data. This study focuses on the disagreement between these theoretical models and the number of infected individuals in the fifty states as well as countries around the world in an attempt to provide insight into improving existing models.

55**Synthesizing of Primary Fatty Amides and Their Extraction from Bovine Omentum.**

Marcano, Maurice; Johnson, Mitchell; Dent, Gary; Johnson; Ryan
Department of Chemistry and Biochemistry,
Duquesne University

Primary fatty acid amides are a class of bio-organic molecules called lipids, which actively carry out a number of intrinsic roles in mammals, where they assist in regulatory functions similar in nature to that of hormones. An example of one of these regulatory functions can be seen in the PFAM oleamide which was discovered in the cerebrospinal fluid of sleep deprived cats. The first aim of this research is to develop through synthesis and purification a set of amide standards, which can be used as a comparison to measure and quantify PFAM's in mammalian tissue. The second aim is to extract PFAM's from omentum (mammalian tissue and stomach of cows) to purify them through solid phase extraction and to measure them in comparison with the previously mentioned standards using GC/MS. Research on oleamide has far reaching implications for not only the scientific community but the wider community at large, considering that a better understanding of PFAM's and their hormone like functions could only serve to benefit better healthcare.

54**Visualization and Simulation in the High School Curriculum**

Winek, Rebecca; Olejar, Kristin; Sidun, Christopher; Madura, Jeffrey
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Duquesne University

The importance of the role of structure to the function of molecules has been well documented. Three workbooks, aimed primarily at upper high school and undergraduate students, have been written to introduce students to the possible three-dimensional structures of molecules through the use of the Molecular Operating Environment (MOE) software. These workbooks will help the user to visualize various molecular conformations, protein-ligand complexes and the docking of different ligand structures in a macromolecule receptor. A series of easy to use exercises utilizing MOE are found in each of the books with step-by-step instructions and in depth descriptions of the various processes. In addition, students will gain an understanding of the relationship between form and function and their importance in the development of pharmaceuticals.

56**Conformational Analysis using MOE software**

Olejar, Kristin; Madura, Jeffrey D.
Center for Computational Sciences and Department of Chemistry and Biochemistry, Duquesne University

Conformational analysis is a method used to explore the spatial arrangements of atoms in a molecule. Conformational analysis is commonly used to understand drug interactions and the binding of molecules. The conformational analysis of molecules through computer software allows students to visualize these types of interactions. A workbook is being constructed that is directed toward high school and undergraduate students and serves as a guide for some simple exercises in the Molecular Operating Environment (MOE) software. The exercises demonstrate how to perform a conformational analysis on molecules with various numbers of rotatable bonds. The workbook provides an understanding of what a conformational analysis is and gives users a simple set of directions for successfully completing a task on MOE.

57

Trace Metal Fingerprinting in Ground Water using Elemental RatioingPillar, Elizabeth¹; Martone, Naudia²; Kingston, H.M.²¹Department of Chemistry and Biochemistry, Mercyhurst College²Department of Chemistry and Biochemistry, Duquesne University

Coal fly-ash, a bi-product of coal combustion, is well-known for its high metal content. Due to its physical properties, fly-ash frequently leaches metals such as arsenic, chromium, and lead among others into water when it becomes wet. Metals that are in ground water can be attributed to either natural or anthropogenic sources via elemental ratioing or elemental fingerprinting. Anthropogenic fingerprinting is accomplished using an element that has limited anthropogenic sources and is stable throughout the environment, like scandium, and then it is utilized to create a crustal enrichment factor. This factor and other ratios can be used to facilitate comparisons between different elements and helps compose an elemental fingerprint for the area being studied, which allows for metals in the environment to have their sources determined. These concepts are being applied to Little Blue in Beaver, PA and its watershed to test for contamination in the ground water supplies.

59

Luminosity Standardization of New High Redshift Type IIP Supernovae

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The expansion of the universe holds information regarding its age and evolution. One technique for measuring the expansion rate involves finding a family of bright objects that possess similar luminosities. Work by Nugent et al. (2006) and Poznanski et al. (2008) has attempted to present a simple, reproducible method of standardizing nearby Type IIP Supernovae luminosities. We apply this method to three more distant Type IIP SNe from the ESSENCE survey. We derive a Hubble diagram where our data from SN m011 agrees marginally with the conclusions reached by P08. Next we will place SNe m014 and m041 onto the Hubble diagram. We expect them to agree with P08's conclusions also. If they don't agree, the discrepancy may be attributed to the difference in quality between our data and that of P08, and that the methods of P08 may not be adequate for more distant objects.

58

Drug Quantification: Simultaneous analysis of *gamma*-hydroxybutyric acid and *gamma*-butyrolactone by SIDMS using ESI-TOFMS, NanoESI-TOFMS, and MALDI-TOFMS.

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Today's forensic scientists are facing two major problems: recent scrutiny of methods of analysis and a rapidly growing backlog of samples. This project's goal is to produce a legally defensible method for analyzing *gamma*-hydroxybutyric acid (GHB) and *gamma*-butyrolactone (GBL) simultaneously using speciated isotope dilution mass spectrometry (SIDMS). By using SIDMS with the Time of Flight Mass Spectrometer (TOF-MS) the derivatization step in most currently used methods can be eliminated, thereby making the analysis quicker. GHB and GBL will be analyzed by Electrospray Ionization (ESI)-TOF-MS, NanoESI-TOF-MS, and Matrix-assisted laser desorption/ionization (MALDI)-TOF-MS. The molecules will be analyzed in both positive and negative mode by the ESI-TOF-MS and MALDI-TOF-MS, but only in the positive mode by NanoESI-TOF-MS. Deuterium labeled GHB and GBL were obtained and will be used to carryout the SIDMS analysis. Urine is the first matrix that will be used with this method.

60

Gravitational radiation from an electro-weak phase transition in the early universe

Stickel, Justin

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As a scientific community we are still interested in the early universe as a probe for high energy physics. Our objective is to establish that gravity waves can be used for such a probe. We will be solving for the transverse traceless portion of the stress energy tensor by contracting it with the projection tensor. This will give us the gravitational radiation produced by inhomogeneous structure formed in an electro-weak phase transition that is first order. We will use a numerical technique to integrate over the various "bubbles" in order to produce a frequency dependent spectrum. Our analysis will compare our numerically produced spectrum with other spectrums made for this transition by other researchers and predict necessary detectability required for future Laser interferometers searching for gravity waves. Our specific goal is to look at the high frequency tail and solve a discrepancy that arose in its numerical solution.

61**Reprocessing DEEP II Galaxy Redshift Survey Spectra**

Vincent, Chelsea

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University of Pittsburgh

Using data from the DEEP II Galaxy Redshift survey, which collected the spectra of some 53,000 objects at a distance corresponding to when the universe was approximately half its age now, astronomers can map out the distribution, determine the properties, and analyze the evolution of galaxies that are distant in both space and time. A set of computer programs implemented in the IDL programming language then processes the spectra, extracting the relevant galactic photons and subtracting the unwanted photons emitted from earth's atmosphere. An unfortunate three percent failure rate of the automated processing means that roughly 1,800 spectra, equivalent to approximately three nights on the Keck telescope, are extracted or sky subtracted incorrectly. I have been manually re-extracting and re-subtracting each of the 1,800 spectra to prevent this large amount of data and valuable Keck time, which averages a cost of one dollar per second, from being lost.

63**Modified Calcium Aluminate Surfaces for use as a Tissue Scaffold.**

Romeo, Jared D.; Palchesko, Rachelle N.; Gawalt, Ellen S.

Department of Chemistry and Biochemistry,
Duquesne University

Providing an optimal tissue scaffold is critical in the regrowth of tissue and bone at a major injury site. In this study, calcium aluminate surfaces were investigated as a potential bone tissue scaffold. Further, calcium aluminate was modified with melatonin (N-acetyl-5-methoxytryptamine) in an effort to enhance the surface tissue interface. Cell viability on these surfaces was measured to determine if melatonin increases cell viability and/or adhesion. Melatonin was attached to the calcium aluminate surfaces via a two-step process and attachment was confirmed using Diffuse Reflectance Infrared Fourier Transform (DRIFT) spectroscopy. Both unmodified and melatonin-treated calcium aluminate samples were autoclaved prior to cell adhesions to ensure sample sterility. Melatonin attachment following autoclave was separately confirmed using DRIFT spectroscopy. Fibroblast viability on modified and control calcium aluminate surfaces was quantitatively measured at growth points of one, four, and seven days using fluorescence microscopy.

62**Probing the Inhibitor Binding Site of Neurotransmitter Symporters Using FEP Calculations**

Miller, Chad; Madura, Jeffry

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Department of Chemistry & Biochemistry, Duquesne University

Dopaminergic pathways comprise a significant portion of the motor control and reward systems of the brain. The dopamine active transporter (DAT) concentrates dopamine in the presynaptic terminal by cotransporting ions down their concentration gradients. DAT is the target of several inhibitors, including the tricyclic antidepressants (TCAs) desipramine, clomipramine, and imipramine. Crystal structures of the homologous bacterial transporter, LeuT, have been solved with these inhibitors bound. The inhibitors were parameterized in the CHARMM force field by performing free energy perturbation (FEP) calculations of LeuT—TCA binding and comparing the results to experimental values. Using a mouse DAT homology model, further FEP calculations will be performed to simulate the mutation of residues important for TCA binding. These will be compared to experimental mutagenesis studies to better elucidate the characteristics of the mDAT inhibition site. A greater understanding of mammalian DAT inhibition may support research into DAT physiology and drug design.

64**Synthesis and Characterization of Lithium-Containing Quaternary Diamond-Like Semiconductors**

Karey, Emma; Leverett, Beth; Lekse, Jonathan W.; MacNeil, Joe; Aitken, Jennifer A.

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Diamond-like semiconductors (DLS) are crystalline compounds whose ions are tetrahedrally coordinated and adopt the closest packed cubic or hexagonal structure of diamonds. DLS of the formula $I_2-II-IV-VI_4$ are of particular interest because of their compositional flexibility and potential applications in non-linear optics and spintronics. The synthesis of $Li_2-Fe-IV-S_4$ crystals was explored, with IV representing either Sn or Ge. Two methods of synthesis were utilized: high temperature solid-state and polychalcogenide flux. Synthetic parameters, including dwell temperature and time, cooling conditions, and ratios of starting reagent materials, were modified to synthesize phase-pure compounds. Products were characterized by powder X-ray diffraction, UV-Vis/NIR spectroscopy, scanning electron microscopy, energy dispersive spectroscopy, and when applicable, single crystal X-ray diffraction.

65**Synthesis of Bicyclic Nitriles**

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Duquesne University
State University of New York*

Zinc can be readily inserted into various alkyl-iodotosylates that can be subsequently trans-metallated with $\text{CuCN}\cdot 2\text{LiCl}$ to the corresponding Knochel cuprate. This cuprate can then undergo conjugate addition to α,β unsaturated ketonitriles. The resultant can undergo an intramolecular dimethyl sulfoxide oxidation-cyclization forming functionalized bicyclic nitriles. This reaction is thought to proceed first by a Kornblum oxidation followed by a Mukaiyama aldol cyclization.

67**Data Intelligence, Adaptability and Accessibility for RAE: An interactive web-based biomedical informatics system for pediatric orthopedic patients**

Sherbondy, Martin; Martincic, Cynthia; Raab, Mandy; Sangimino, Mark

1 Bioinformatics Program and CIS Department, Saint Vincent College
2 Department of Orthopaedic Surgery, Allegheny General Hospital

The primary aspiration of RAE is facilitation of organized yet dynamic interaction between Orthopaedic physicians and their adolescent patients. Utilizing a MySQL database and PHP scripting RAE interprets input data and gathers a collection of relevant images and text for each presentation. My contribution to this project included the addition of primitive data intelligence, dynamic image handling, and enhanced maintainability and accessibility. RAE now exhibits primitive data intelligence by searching for alternatives if the ideal images do not exist. The Document Object Model was used to increase maintainability by separating the content, structure, and style of presentations. Accessibility was achieved by dynamically interpreting and resizing images to efficiently utilize screen space. In addition, the RAE database and web servers have been installed on a flash drive to achieve portability for the client.

66**Differential Expression of TRPV1 in Rats**

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The Transient Receptor Potential (TRP) protein superfamily consists of twenty-eight known mammalian TRP channels. A small number of these are thought to be involved in pain pathways and are responsible for the transduction of various noxious stimuli. These stimuli include thermal, chemical, and/or mechanical stimulation. The TRP protein of interest to this research project is transient receptor potential vanilloid 1 (TRPV1). TRPV1 is a member of the vanilloid subfamily and is activated by pain, noxious heat, and capsaicin. Like all other TRP channels, TRPV1 is an integral membrane protein consisting of six transmembrane domains and an ankyrin repeat domain at the N-terminal region. The goal of this project is to visualize TRPV1 protein and mRNA distribution in rat dorsal root ganglia tissue and determine if expression is increased when chronic pain is induced through the use of a chronic constriction injury protocol.

68**G quadruplex mediated interactions between the fragile X mental retardation protein and the elongation factor 1A mRNA**

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Fragile X Syndrome is the most prevalent inherited mental retardation, being caused by the loss of fragile X mental retardation protein (FMRP) expression. FMRP binds to specific messenger RNAs and regulates their transcription. Although not all FMRP mRNA targets are known, an mRNA of particular interest encodes for elongation factor 1A (EF1A). FMRP has been shown to bind this RNA, but it's unclear if these interactions are mediated by the presence of a G-quadruplex in EF1A mRNA. Prior studies indicate that FMRP binding to at least a sub-set of mRNA targets involves the recognition of their G-quadruplex structure by the protein RGG box domain. Moreover, super-stoichiometric FMRP RGG box unwinds the G-quadruplex structure of these RNAs. This study used circular dichroism spectroscopy and NMR spectroscopy to elucidate if EF1A mRNA forms a G-quadruplex structure and determine if the FMRP RGG box retains the ability to unwind this structure.

69

Information interfacing for RAE: An interactive web-based biomedical informatics system for pediatric orthopedic patients

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The objective of the RAE project is to facilitate educational discussions between pediatric orthopaedic surgeons and their patients concerning how patients will successfully manage their condition. My portion of this project included converting static HTML pages into dynamic HTML forms, making HTML pages and forms printer-friendly, developing buttons, and editing page content. A key feature of the presentation is to relay condition specific information to the patient through HTML forms in place of static HTML pages. These forms require interaction between the doctor and the patient and allow input of information using checkboxes, radio buttons, and text boxes. The pages are configured to print using cascading style sheets for the patient to take home. Attractive buttons offer smooth transitions between pages and different discussion topics. Page content is structured to communicate specifically to the adolescent patient or the parents.

71

Tetrahedral Cu(I) Binding of Cysteiny Sulfurs in ProteinsDeVasto, Robert^{1,2}; Evanseck, Jeffrey D.²; Harrison, Melinda¹¹Department of Science, Cabrini College²Center for Computational Sciences; Department of Chemistry and Biochemistry, Duquesne University

Density functional theory (DFT) and second-order Møller-Plesset theory (MP2) have been used to predict energies, structures, and vibrational frequencies of copper I bound to four cysteiny sulfurs in a tetrahedral arrangement. Basis sets up to 6-311+G(3df,3dp) were used with B3LYP, M05-2X and MP2. Comparison with linear and trigonal planar configurations are made to understand the different bonding motifs of copper binding proteins and to discover any possible relation to fuction. Higher-order symmetry point groups up to D_{2d} cannot be interpreted due to multiple imaginary frequencies after vibrational analysis. The research impacts the structure of Cu(I) binding proteins and specific diseases which deal with Cu(I) metabolism including Menkes disease, copper deficiency resulting in coarse or limited hair, growth failure and the deterioration of the nervous system, and Wilson's disease, a genetic disorder, in which copper accumulates in tissues leading to neurological and psychiatric symptoms and liver disease.

70

Developing a Methodology for a Bending Test Device and Verification with Tissue and Non-tissue samples

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A bending test is needed in order to properly determine the mechanical properties of various tissues in the body which deform by bending while in vivo. This device works by tracking the change in curvature a known applied load produces in a sample. However, for such a device to work, the exact methodology for its use must be determined before any reliable measurements for tissue can be ascertained. Variables, such as the initial curvature in a sample, the calibration of the bending bar, and placement of the tracking dots, affect the final conclusions. The verification of the accuracy of the results was done by testing a tissue scaffold as well as several tissue samples. The effective modulus of elasticity (E) for each sample aligned with published data, indicating a reliable device.

72

Identifying Regions of Genome Linked to Cancer

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Data from a tiling array indicated 357 regions of the human genome are potentially linked to breast cancer. Comparative analysis was performed on these regions using the UCSC Genome Browser to tentatively investigate and identify regions best conserved across different species of animals. We found regions that are well conserved in mammals and regions that are well conserved across vertebrates, suggesting that these regions might be relevant to human biology. We hope to further find that some of these regions partially match cancer related genes. Our analysis should provide a focused set of novel gene regions to facilitate the experimental validation of previously missed genes in breast cancer studies.

73

Detecting Respiratory Arsenate Reductase, Aldehyde Ferredoxin Oxidoreductase, and Nitroreductase Activity in *Alkaliphilus oremlandii* strain OhLAs

Badhan, Rezwan; Watkins, Courtney; Chovanec, Peter; Basu, Partha; Stolz, John

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Roxarsone (3-nitro-4-hydroxybenzenearsonic acid) is an organoarsenical used as a feed additive in the poultry industry. Most passes through the chicken unchanged and winds up in the chicken litter. *Alkaliphilus oremlandii* strain OhLAs, a fermentative clostridium, was found to metabolize roxarsone to 3-amino-4-hydroxybenzenearsonic acid and inorganic arsenic (As(V)). Genomic analysis failed to identify established aromatic degradative pathways. However, genomic and proteomic data indicate that strain OhLAs has respiratory arsenate reductase (Arr), aldehyde ferredoxin oxidoreductase (Aor), and nitroreductase (Ntr). The purpose of this project was to demonstrate the functionality of Arr, Aor, and Ntr in strain OhLAs. Cultures were grown with roxarsone (electron acceptor) and lactate (electron donor), thiosulfate (electron acceptor) and roxarsone (electron donor), or lactate alone (fermentative control). Colorimetric enzyme assays were done in the complete absence of oxygen, using methyl viologen and arsenate (Arr), benzyl viologen and crotonaldehyde (Aor), and NADPH and nitrophenol or roxarsone (Ntr).

75

Parameterization of Small Molecules that Interact with the Dopamine Active Transporter

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Many molecules bind to the dopamine active transporter (DAT), like antidepressants and narcotics. Some of these molecules, like tricyclic antidepressants, can bind to DAT and block the reuptake of dopamine. How and why specific molecules bind to and inhibit DAT is of high pharmacological interest. To study the binding of substrates to DAT, force-field parameters are needed for the tricyclic antidepressants: clomipramine, imipramine, and desimipramine. Lennard-Jones parameters were taken from the OPLS-AA force-field and partial charges were obtained from Molecular Operating Environment (MOE) charge calculations. These charges and parameters were then tested by calculating pKa's for the molecules and comparing them to experimental data. The results of these calculations and current force-field parameters for the tricyclic antidepressants will be presented.

74

Identification of Novel Aromatase Inhibitors Using Pharmacophore ModelingMuftuoglu, Yagmur; Mustata, Gabriela
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University of Pittsburgh

Pharmacophore modeling has become established as one of the most successful computational tools in modern drug design. This work describes how ligand- and structure-based pharmacophore modeling can be used to identify novel anti-breast cancer drugs. Human aromatase (CYP19), a cytochrome P450 enzyme present in breast tissue, catalyzes the biosynthesis of estrogens from androgens. It is an important pharmacological target in anti-cancer therapy because intratumoral aromatase produces estrogen necessary for tumor growth in breast cancer tissues. Suppression of estrogen biosynthesis via aromatase inhibition represents an effective treatment for hormone-sensitive breast cancer, and several classes of aromatase inhibitors have been developed. However, important side effects associated with prolonged clinical use call for new CYP19 inhibitors. However, important side effects associated with prolonged clinical use call for new CYP19 inhibitors. The recent elucidation of the crystal structure of aromatase provides an excellent opportunity for designing the next generation of inhibitors. We will demonstrate the power of structure- and ligand-based pharmacophore modeling in identifying novel anti-breast cancer drugs.

76

Mechanism of Delay in Olfactory Granule Cells

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The ability to encode olfactory information in the brain is dependent on distinct, reliable patterns of neuronal firing. An individual inhibitory granule cell of the olfactory bulb displays an extremely reliable, consistent delay in firing. Such consistent delay in inhibitory interneurons is believed to give rise to reliable patterns of mitral cell firing, which allows the brain to encode olfactory information. However, not much is known about the mechanism for delay in the olfactory granule cells. Several potential contributing factors were explored using the simulation software XPP. The effects of NMDA, A-type potassium current, and CAN currents on the delay of firing were studied. The reliability of such delay after introducing noise was also investigated.

77

Identification and Analysis of a Novel TRPM8 Splice Variant Using a Rat Neuropathic Pain Model

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Neuropathic pain is a type of chronic pain that afflicts nearly four million in the United States alone. Our studies and others' suggest that transient receptor potential (TRP) splice variants may contribute to pain hypersensitivity associated with neuropathic pain conditions. TRP genes code for calcium channels that act as an interface between the environment and nervous system. Through alternative splicing, functionally distinct protein variants are produced from a single TRP gene. Alternative splicing is a major source of protein variation in humans, and splice variants have been linked to various diseases. This study utilized a rat neuropathic pain model to mimic a human chronic pain condition. By performing quantitative polymerase chain reaction (qPCR) and 5' rapid amplification of cDNA ends (5' RACE), we have demonstrated the presence of a novel TRPM8 splice variant in rat. This discovery may help to elucidate the role of TRP splice variants in neuropathic pain.

79

The Effects of Selenium, Sep15, and PTHrP on the Invasive Properties of Breast Cancer Cells

Ondrizek, Christine; Sneddon, Bruce W.

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Previous research has indicated that Selenium and protein Sep15 act as tumor suppressors in breast cancer. We hypothesize that suppressor activity occurs partly by modulating the effects of Parathyroid Hormone-Related Protein (PTHrP), which stimulates breast cancer invasion. The hypothesis for this experiment was that breast cancer cells treated with Selenium, Sep15, and PTHrP would be less invasive than untreated controls. We assessed cell invasion using the soft agar assay. Cells transfected with Sep15 and treated with/without Selenium and PTHrP were plated on soft agar plates and incubated for 2-3 weeks. Looking under the microscope, the Sep15 and Selenium treated plates had more breast cancer growth than the untreated control. These results didn't support the hypothesis because Sep15 and Selenium treatments were thought to decrease breast cancer cell proliferation. These data may have been complicated by the presence of yeast contamination, which may have confounded results and made data interpretation difficult.

78

Separation and Detection of Fluorescently Tagged Amines

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Fatty acid amides have been linked to various disorders such as schizophrenia and bipolar disorder. Amides are often converted to their conjugate amines in order to facilitate separation and detection methods. In this work, primary saturated amines (C10-C18) are fluorescently tagged with 3-(2-furoyl)-quinoline-2-carboxaldehyde (FQ) at micromolar concentrations, and then serially diluted over a concentration range spanning seven orders of magnitude. These are then separated by Reverse Phase High Performance Liquid Chromatography (HPLC) and detected by fluorescence. The goal is to determine whether sub-picomolar detection is possible. Results so far show that it is possible to detect the 1pM amine because of signs of the possibility of linear peak areas. Future work includes decreasing the concentration at which the tagging reaction is performed and continuing to lower the detection limit using microfluidics and laser-induced fluorescence.

80

Structure-Function Relationships in the Terpene Synthase FamilyYoung, Ashley¹; Hugh, Nicolas²; Wymore, Troy²¹North Carolina A&T State University²Pittsburgh Supercomputing Center

The attainment of new catalytic functions from an existing protein scaffold is a major force guiding evolutionary change but one that is perhaps only beginning to be understood. Through a landmark study of terpene synthases, in which one with a specific activity was engineered to obtain a different specific activity through mutational swaps of nine residues as well as *characterization of 418 proteins* with different combinations of these nine residues, a catalytic landscape underlying the evolution of sesquiterpene chemical diversity was revealed (O'Maille et al, *Nature Chemical Biology*, 2008, 4:617-623). Notably, only two of the nine residues are localized on the active site surface with the remainder scattered throughout the second sphere. In this presentation, we will highlight the results from sequence-based bioinformatics that reveal where these nine residues are located with respect to conserved residues and motifs as well as assigning functional attributes for the motifs in this enzyme family.

81**Performing reactions in microdroplets**

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Microfluidic devices are gaining popularity due to shorter reaction times, the ability to acquire large amounts of data in a short period of time, and the fact that the devices are relatively fast and easy to make. This project focuses on the use of segmented flow microchips to perform reactions at ultratrace levels in nanoliter-sized droplets produced on the microchip. Mixing in the droplets was tested by a proton transfer reaction using fluorescein-5-isothiocyanate (FITC) and HCl. Once the mixing has been profiled, these segmented flow chips will be used for fluorescently derivatizing saturated fatty amines with 3-(2-furoyl)quinoline-2-carboxyaldehyde (FQ) to determine the FQ-amine kinetics as a function of chain length and concentration. This reaction has been studied using Reverse-Phase High-Performance Liquid Chromatography coupled to in-line fluorescence detection. Ultimately, the concentrations of the analyte and reagents will be lowered to determine if it is possible to fluorescently derivatize amines at sub-nanomolar concentrations.

83**Sodium iodide effects on the helical stability of a mainly alanine peptide**

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Peptide-based drugs have the potential to treat many diseases. Some α -helical peptides have the ability to enter cells by crossing the lipid bilayer. However, the environment could affect the peptide's α -helical stability and hinder its entrance into the cell. To overcome this difficulty both experimental and computational teams have developed various techniques to stabilize the α -helix configuration of peptides. One method is to select ions to stabilize the α -helix secondary structure in an aqueous environment. This work studied the stabilization effects of the iodide anion on a mainly alanine peptide as a portion of the entire Hofmeister series investigation. Additionally, Replica Exchange Molecular Dynamics was employed to increase the sampling of configurations of the system throughout simulation. According to previous studies, the iodide ion is expected to stabilize the peptide less than perchlorate in an aqueous environment according to the Hofmeister series.

82**Constructing Red TRAF6 Using Standard Molecular Cloning Techniques**

Perleman, Malka; Su, An-Jey; Auron, Philip
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The immune and skeletal systems share many molecules in their signaling repertoire. Particularly, TNF receptor-associated factor 6 (TRAF6) plays an important role in osteoclast differentiation, initiated through its interaction with the cytoplasmic domain of RANK receptor in a process that requires the downstream activation of Tec family kinases. Knockout of either RANK, TRAF6 or Tec results in osteopetrosis and anemia. In order to visualize the interaction among these three molecules, standard molecular cloning techniques were used to construct an expression vector coding for a TRAF6 engineered to generate a red fluorescent color within living cells. When co transfected along with a vector coding for green fluorescent Tec kinase, it is then possible to observe the relative localization of these two tagged molecules following cell treatment with RANK ligand. This addresses the question of whether these two critical molecules associate as part of the osteoclast activation process.

84**The role of ectoderm/mesenchyme interactions on limb bud development**

Beer, Dominik; Elinson, Richard P.
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Most amphibians develop from tadpoles to frogs through metamorphosis. *Eleutherodactylus coqui* does not follow this path but is instead a direct developer. One of the most notable differences observed in *coqui* development compared to tadpole development is the early formation of limb buds. We hypothesize that the large limb development in *coqui* is due to interactions between the ectoderm and mesenchyme. A series of cross species ectoderm transplantations were carried out to see if embryonic ectoderm from a tadpole species could support rapid limb growth. Successful xenotransplantations were executed by replacing *coqui* limb ectoderm with *Rana* flank ectoderm and early stage *Xenopus* ectoderm. The foreign ectoderm successfully integrated with the *coqui* limb mesoderm but did not grow with the embryo and subsequently fell off the host limb. The transplantation techniques are being improved empirically and more comprehensive surgeries are planned.

85**Further Decreasing the Environmental Impact of Copper Catalyzed Atom Transfer Radical Addition**

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The development of catalyst regeneration techniques in atom transfer radical addition (ATRA) has allowed for a substantial lowering in the amount of transition metal required to catalyze the addition of polyhalogenated compounds across unsaturated carbon-carbon bonds. Previous studies utilized radical initiators to regenerate the catalyst. Although such reducing agents were very efficient with less reactive alkenes, significant problems were encountered with alkenes that readily polymerize under free radical conditions. Ascorbic acid was used as a non-radical reducing agent for ATRA reactions and successfully enabled catalyst regeneration in the presence of limited amounts of oxygen in considerably smaller quantities than the previously utilized radical initiators. Furthermore, self-assembled monolayers (SAMs) of thiols on gold substrates provided a novel catalytic support system for this reaction. Both techniques introduce and utilize more economical and environmentally-friendly chemistry while maintaining focus on product selectivity and yield.

87**Conceptual Density Functional Theory: Periodic Trends in Brønsted-Lowry Acidity**

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Energy of deprotonation has been traditionally used to judge the strength of Brønsted-Lowry acidity. To better understand the factors that control Brønsted-Lowry acidity, conceptual density functional theory and second-order Moller-Plesset theory have been used to analyze periodic trends across the second and third periods, as well as down groups 5-9, in terms of electronegativity, size, electrophilicity and hardness. Across the second period, it is found that electronegativity and electrophilicity strongly correlate with the energy of deprotonation, as typically taught in introductory classes. However, size and hardness also correlate with the energy of deprotonation across the second period, which is usually assumed to be negligible. Electronegativity plays a significant role as compared to size across the third period. It is also found that electronegativity plays a larger role than previously thought down groups. The research shows a weakness in previous rules and periodic trends in the prediction of Brønsted-Lowry acidity.

86**Small Molecule Inhibitors of Breast Cancer Cell Proliferation**

Burkholder, Sydney; Monlish, Darlene; Cavanaugh, Jane E.
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Each year approximately 500,000 women succumb to breast cancer making it the second leading cause of cancer-related death among women. Extracellular signal-regulated kinase 5 (ERK5) is an intracellular signaling protein that has been shown to increase breast cancer cell growth. This study is designed to further investigate the role of ERK5 in breast cancer cell proliferation using novel specific inhibitors of ERK5 activation. This study investigated how benzimidazole compounds can act as inhibitors of ERK5 signaling in mouse (MMC) and human (BT-474) breast cancer cells. Cells were treated with the putative inhibitors of ERK5 and then subject to Western blot analysis to investigate ERK5 expression and activation. These studies will advance our knowledge of the role of ERK5 in breast cancer progression and may lead to the development of novel therapies for breast cancer.

88**Citalopram can bind in two different pockets in the Serotonin Transporter**

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Duquesne University

Citalopram is an antidepressant drug used to treat major depression associated with mood disorders. It is an SSRI (selective serotonin reuptake inhibitor) which is a class of compounds used as antidepressants in the treatment of depression. The serotonin transporter is a monoamine transporter protein that transports serotonin from synaptic spaces into presynaptic neurons. It is hypothesized that Citalopram binds in a secondary binding pocket of the serotonin transporter. In order to prove this hypothesis, a set of force-field parameters were developed for Citalopram and molecular dynamics on the serotonin transporter in the presence of Citalopram were performed. Results from our simulations will be presented.

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Electronic Structure of CM-TiO₂

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The popularity of the semiconductor TiO₂ as a photocatalyst; aiding in the photoinduced decomposition of water and other photodegradation applications has steadily increased within recent times. The low cost and high photostability of TiO₂ renders it an optimum compound for photocatalytic applications however its relatively wide band gap poses to be a disadvantage. By means of periodic three dimensional Density Functional Theory (DFT) calculations, optimized surface structures of pure TiO₂ were created and analyzed along with the respective electronic structure and density of states. These surface structures were then modified with the incorporation of carbon into the structure which resulted in a narrowing of the band gap of the photocatalyst by introducing localized states at the top of the valence band; consequently increasing the photocatalytic activity of TiO₂.

91

Cocaine Interaction with Dopamine Transporter Proteins

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Millions of people are affected by cocaine addiction and overdose, yet knowledge of the mechanism by which cocaine functions is limited. It is known that cocaine binds to the plasmal dopamine transporter protein (DAT) and inhibits dopamine reuptake from the synaptic cleft. It is hypothesized that cocaine binds to DAT in a binding pocket near valine residue 152. To test this hypothesis we have developed topology and parameter files for cocaine were developed according to CHARMM force-field specifications. The force-field was tested using NAMD 2.7. Cocaine was docked to DAT at the hypothesized binding site using MOE 2008. The complex was minimized in vacuum for 5 picoseconds using NAMD. The force-field parameters along with initial molecular simulation results will be presented.

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Ammonia Borane as a Hydrogen Fuel- Green Catalyst Support

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Ammonia borane (AB) is a leading candidate for hydrogen storage in commercial vehicle hydrogen fuel cells. As a hydrogen storage media AB meets the Department of Energy gravimetric/volumetric requirements upon metal and acid catalysis. H₂(g) production from acid catalysis has been verified by this work. The reported Pt-Al₂O₃ metal has been tested, and in efforts to make a more environmentally friendly system, a cellulose stabilized Pt catalyst was created to generate H₂. Large scale computations reveal new details on an acid catalyzed mechanism not previously considered. The reaction follows an S_N2-like path, which explains experimental data. The combined computational and experimental methods are used in efforts to test the viability of AB as an H₂ storage media with green components.

92

Theoretical Studies of Halogen Bonded Systems

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Halogen bonding is an attractive force between a halogen atom and an atom containing a lone pair, where the halogen acts as a Lewis acid. Halogen bonding is often compared with hydrogen bonding because of similarities in strength and directionality. Simple halogen bonded systems of ammonia with Cl₂, Br₂, BrCl, and ICl were modeled to determine what level of computational theory is appropriate for these systems. Using the DFT method M052X, the geometries and energies of the complexes started to converge around the aug-cc-pVTZ basis set. The strength of the halogen bond increased as predicted with increasing size of the halogen, as did the extent of charge transfer from the ammonia to the halogen molecule.