1

An Intermolecular Conjugate Addition Approach to the Synthesis of Lunamarine

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The alkaloid lunamarine, first isolated from *Lunasia amara* in 1943, has been shown to decrease arterial blood pressure in cats and to have very low toxicity in mice. Lunamarine has not been synthesized in the 64 years since its isolation. This study is directed at the total synthesis of lunamarine via linchpin coupling of the 4-quinolone and benzodioxole moieties.

2

An Intramolecular Conjugate Addition Approach to the Synthesis of Lunamarine

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The alkaloid lunamarine, first isolated from *Lunasia amara* in 1943, has been shown to decrease arterial blood pressure in cats and to have very low toxicity in mice. Lunamarine has not been synthesized in the 64 years since its isolation. This study is directed at the total synthesis of lunamarine with the key step being a boron-trichloride-directed Friedel-Crafts acylation of *m*-anisidine with a cinnamoyl chloride derivative.

3

An Intramolecular Conjugate Addition Approach to the Synthesis of Lunamarine Congeners

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The alkaloid lunamarine, first isolated from *Lunasia amara* in 1943, has been shown to decrease arterial blood pressure in cats and to have very low toxicity in mice. Lunamarine has not been synthesized in the 64 years since its isolation, and no attempt has been made to optimize its activity. This study is directed at the total synthesis of lunamarine analogues with the key step being a boron-trichloride-directed Friedel-Crafts acylation of *m*-anisidine with a cinnamoyl chloride derivative.

4

A Study of the Heck Reaction, a Key Step in the Synthesis of Lunamarine Congeners

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The alkaloid lunamarine, first isolated from *Lunasia amara* in 1943, has been shown to decrease arterial blood pressure in cats and to have very low toxicity in mice. Lunamarine has not been synthesized in the 64 years since its isolation. Our goal is to prepare this compound via total synthesis, employing the Heck reaction as a key step. This study describes the optimization of the Heck reaction for the preparation of the target compound, as well as for analogue synthesis.

5

Mössbauer Spectroscopy Study of the $xZrO_2$-(1-x)α-Fe_20_3 Nanoparticles System (x=0.1 and x=0.5)

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The $xZrO_2$-(1-x)α-Fe_20_3 nanoparticles system was synthesized for x=0.1 and x=0.5 molarities using the ball milling technique for durations ranging from 0 to 12 hours. Mössbauer spectroscopy was then performed on samples of each of the respective molarities. For the x=0.1 sample a second sextet appeared after 2 hours while the 4 and 8 hour milled samples showed a third sextet. A fourth sextet was observed in the 12 hour milled sample. This is indicative of the appearance of zirconium atoms in the system as nearest neighbors. For the x=0.5 samples, a doublet appeared along with a second sextet in all milling times except for 0 hours. The doublet increased in intensity with the ball milling time. The appearance of a doublet shows that as zirconium atoms become more prevalent, iron atoms begin to replace zirconium atoms in the zirconia structure. This system is believed to have application in gas sensing.

6

Use of Asymmetric Disulfides for Analysis of Cytochrome *c*

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Cytochrome *c* is an important protein in the mitochondria of our cells as a part of the electron transfer chain. This presentation demonstrates how asymmetric disulfides can be used in order to study the kinetics of cytochrome *c* adsorbed to a self-assembled monolayers (SAM).. In order to do this, the asymmetric disulfide was synthesized from a brominated chain and a thiolated chain. The two chains chosen matched thiols that are commonly used for cytochrome *c* research. The results indicate that a film had formed on the gold electrode based on capitance and by cyclic voltammetry that cytochrome c was adsorbed on the electrode surface.. The capacitance of a gold electrode with no SAM was ~13.2 and with the disulfide it was 4.2.

7

Investigation of Cytochrome *c* Electron Transfer Kinetics and Formal Potential with Varying Composition of Self-Assembled Monolayers

Schrock, Kimberly A.; Kirby, David J.; and Clark, Rose A., Department of Chemistry, Saint Francis University

Cytochrome *c* is a solution protein found in the mitochondria, where cytochrome *c* transfers electrons between two inner membrane redox partners, cytochrome *c* reductase and cytochrome *c* oxidase. The interactions between the two proteins are facilitated by the two surfaces having opposite charges. A self-assembled monolayer (SAM) can be used to mimic the protein/protein interaction. The SAMs were made with varying percent solution of the carboxylic acid to compare changes in the rate constants and formal charge for cyt *c*. By changing the percent of the carboxylic acid, a relationship between the electron transfer rate and the length of the diluent thiol is observed. The formal potential is used to verify the kinetic data. Variations of the percent solution will be explained.

8

Probing the Self-Assembled Monolayer Structure and the Electrodes Influence on Cytochrome c Electrochemistry

Kirby, David J.; Schrock, Kimberly A.; Clark, Rose A.; Department of Chemistry, Saint Francis University

Self-Assembled Monolayers have been used to study electron transfer kinetics and many other surface properties. In this experiment, the surface of the SAM is probed to further understand the coverage of 16-mercaptohexadecanoic acid and 11-mercapto-1-undecanol in the monolayers. Electrochemistry, X-ray Photoelectron Spectroscopy, and Grazing Angle Infrared were all techniques used to examine the surface. Peak area of XPS carbon spectra will be used to compare the percent of component in solution with the percent of component on the monolayer. Electrochemistry allowed for examination of changing surface charge where changes in formal potential of cytochrome *c* (cyt *c*) is used to demonstrate the monolayer change. Rate constants of electron transfer between cyt *c* and the SAM will also be used to show the changing monolayer composition with changing solution percentages. Study of these SAMs show them to be useful as biological system mimics and for biological sensor equipment.

9

Green Oxidation of Organic Compounds Using Metalloporphyrins

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The functionalization of organic compounds has been a very important research topic in recent years. Because of their many uses, the functionalized organic compounds are widely used in the petrochemical industry. However functionalization of organic compounds is not always completed in an environmentally sound method. The topic of Green Chemistry has increased in importance in recent years in the chemistry community to address better ways to obtain desired products. Traditionally organic substrates had been oxidized using compounds such as iodosylbenzene which produced harmful byproducts. This project seeks to further integrate green chemistry into the field of inorganic chemistry education by using hydrogen peroxide as a 'green' oxidant with iron (III) metalloporphyrins as the catalyst.

10

Biophysical Analysis of Hepatitis C Viral RNA Dimerization

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Worldwide, approximately 170 million people are chronically infected with Hepatitis C, caused by the hepatitis C virus (HCV). The infection has been linked to liver failure, cirrhosis and hepatocellular carcinoma. The virus itself consists of a 9.5 kb single-stranded RNA of positive polarity. This is comprised of a 5' untranslated region (5'-UTR), a single open reading frame (ORF), and a 3' untranslated region (3'-UTR). A well conserved sequence of 98 nucleotides in the 3'-UTR—referred to as the X-tail—has previously been shown to be both essential for viral RNA replication and to dimerize in the presence of HCV's core protein. Within this region lies a short palindrome, termed the dimer linkage sequence (DLS), that has been specifically implicated in this dimerization process. In this study, we use biophysical techniques to characterize the dimerization of the DLS via a proposed kissing complex intermediate.

11

Testing of Species-Specific Primers for Infectious Organisms Hosted in Cat Populations

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Felines are host to numerous bacteria and other types of organisms. This study investigates the difference between organisms found in the feral cat verses domesticated cat populations. Seventeen different bacteria species have been identified to be part of the cat flora. We are developing species-specific primers for each bacteria to determine its prevalence in different cat populations. If the primers amplify their specific stretch of DNA through PCR, producing a predicable and reproducible band, it can be concluded that that specific organism's DNA is present. The primers designed to amplify DNA of organisms isolated in cat stool samples are being multiplexed to further the efficiency of diagnosis. Primers to recognize the retroviruses, Feline Immunodeficiency Virus (FIV) and Feline Leukemia Virus (FeLV) are still in preliminary stages due to the fact the RNA is not as highly conserved as DNA.

12

Derivitization and Analysis of Benzoylecgonine on US Currency

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Benzoylecgonine is a metabolite produced from the hydrolysis of cocaine. Due to its polar nature, the compound is not highly retained when analyzed with gas-chromatography-mass spectrometry (GC-MS). Through derivitization using pentaflouropropanol (PFP) and pentaflouropropanol anhydride (PFPA), it is possible to detect this compound using GC-MS. Quantification is possible through the use of a deuterated internal standard (D3- benzoylecgonine). In this experiment, Cocaine and its metabolite were extracted from US paper currency, derivitized, and analyzed using the GC-MS. Paper currency was utilized as the matrix due to the highly prevalent nature of minute quantities of cocaine. The cocaine was detectable without derivitization, but it was necessary to derivitize the extract to allow visualization and quantification of benzoylecgonine. This technique can also be applied to other matrices such as urine and blood.

13

The Formation of Octacosanoic Acid Monolayers on Stainless Steel

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Modification of the surface of stainless steel by forming self-assembled monolayers may make biomaterials more biocompatible by preventing the adhesion of cells to these biomaterials. Carboxylic and phosphonic acid monolayers were formed on the surface of stainless steel through a solution deposition technique, and the presence of these monolayers was confirmed using diffuse reflectance infrared fourier transform spectroscopy (DRIFT), matrix assisted laser desorption ionization mass spectroscopy (MALDI), and atomic force microscopy (AFM). Modified substrates were exposed to 3T3 fibroblast cells and analyzed using fluorescent microscopy. It was found that octacosanoic acid easily formed an ordered monolayer that proved an effective inhibitor of cell adhesion to the surface of stainless steel. The role of octacosanoic acid as an inhibitor of cell adhesion will increase its application to stainless steel and other metals in the manufacture of future biomaterials.

14

Determining the Source of Polymeric Fibers Using Microwave Extraction (ME) and GC/MS

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Polymer fibers exist in many forms and are synthesized from many synthetic materials
Fibers can be found almost anywhere and thus are a part of our everyday life. These fibers also play a very crucial role in the field of Forensic Science since they can connect possible suspects to a crime scene. Within these fibers exists many polymeric additives which have a variety of functions and sources. To determine whether fibers could be distinguished based on color, polymer type and additives, experiments were conducted. This project was a continuation of a previous research and is geared towards specifically determining the source of fibers based on their results using microwave extraction (ME) and gas chromatography/mass spectrometry (GC/MS). Another method of extraction investigated during this research was heating and sonication. This experiment involved ten carpets that varied in color and the material in which they were synthesized.

15

Near-infrared Dye Staining of Cyanoacrylate-fumed Fingerprints

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Latent fingerprints are extremely valuable forensic evidence, so it is advantageous to create new fingerprint development methods that further increase the contrast between the fingerprint and the surface upon which it had been deposited. One such method is the use of a near-infrared dye, such as IR 786, that undergoes laser-induced fluorescence (LIF). As few surfaces fluoresce in this region (> 800 nm), the cyanoacrylate-fumed fingerprint can be developed by IR 786 with great contrast between the fingerprint and its background surface. The IR 786 technique has been used to successfully develop fingerprints under conditions similar to those experienced in the field. Such conditions are simulated by aging the fingerprints by exposure to either UV light or ozone. Fingerprints were also developed on a variety of surface types often found at crime scenes—plastics, aluminum, and adhesive tapes. The level of detail seen in the recovered fingerprints is enough for identification purposes.

16

Derivatization and Fluorescent Tagging of Primary Fatty Acid Amides for Trace Detection Using HPLC and Laser Induced Fluorescence

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Primary fatty acid amides (PFAMs) play an important role in mammalian intercellular communication, but the exact role is relatively unknown. High performance liquid chromatography (HPLC) and laser induced fluorescence (LIF) are useful techniques for this application due to their high sensitivities. Amides are relatively inert towards common tagging groups, therefore PFAM analysis with LIF is largely unknown. A method that we are using to enable the detection of these PFAMs is to convert the amides to amines using phenyliodine-bis-trifluoroacetate (PIFA) via a Hoffmann rearrangement, and to then tag the amines using 3-(2-furoyl)-quinoline-2-carbaldehyde (FQCA). This tagging method has shown to be successful using HPLC with 10 mM standards of pure amines (C10 through C18) and is currently being tested on the converted pure amide samples. Once the converted amides are successfully detected, we will move to LIF to further the sensitivity of detection.

17

Design and Synthesis of Anti-cancer Agents Based on Tubulysin

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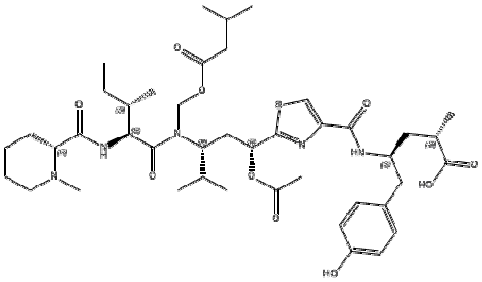

Tubulysins are a family of natural products (tubulysin D is shown) originally isolated from several myxobacteria and exhibiting potent cytotoxicity. Although tubulysin exhibits good *in vitro* activity against cancer cell lines, rapid *in vivo* metabolism limits its practical utility as a drug. Tubulysin exhibits some structural similarity to and binding site specificity with the dolastatins. Molecular modeling of the acylhemiaminal side chain of tubulysin followed by comparison with dolastatin 10 and 15 presented four tubulysin analogs as reasonable for synthesis and likely to be more stable *in vivo*. Progress in the modeling, synthesis, and testing of these compounds are presented.

18

Biophysical Study of the Fragile X Mental Retardation Protein Interactions with Human Semaphorin RNA

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Fragile X syndrome, the most common form of inherited mental retardation is an X-linked recessive trait caused by the expansion of a trinucleotide CGG repeat in the fragile X mental retardation 1 (*FMR1)* gene. The fragile X mental retardation protein (FMRP) has been proposed to bind to messenger RNAs forming G-quartet structures. Semaphorin 3F (S3F) RNA, encoding for a protein involved in the guidance of growth cones during neuronal extension, has been proposed to interact with FMRP, via the recognition of its G quartet structure. We demonstrate in this study, by using fluorescence, UV, circular dichroism and NMR spectroscopy that human semaphorin 3F RNA forms an intramolecular parallel G-quartet structure to which the FMRP RGG Box binds with high affinity and specificity.

19

Crystal Engineering of Coordination Polymers: a Study of the Structures of Homonuclear and Heteronuclear Polymers and the Metal Arrangements in Bimetallic Polymers

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Polymer chains of Co(II) and Ni(II) acetylacetonates and 1,3-diphenyl-1,3-propanedionate, with the ligand nitrogenous bases such as quinoxaline and 4,7-phenanthroline are being developed and characterized. $M(acac)_2$ complexes (where M = Ni or Co) are reacted with 1,3-diphenyl-1,3-propandione and a nitrogenous base. The crystal structures of these polymer complexes were determined by using single crystal x-ray diffraction. Structures are also verified by reflectance and infrared spectral data and elemental analysis. Chains containing both Co(II) and Ni(II) acetylacetonates, 1,3-diphenyl-1,3-propanedionate, and ligand nitrogenous bases are also being synthesized. This is done by reacting both $Co(acac)_2$ and $Ni(acac)_2$ with1,3-diphenyl-1,3-propanedione and a bridging nitrogenous ligand. In order to determine the metal arrangements, the metal properties and geometric principles must be used.

20

Role of Proline in the Formation of Biologically Active Regioisomers of α-conotoxins

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Evaluation of the role of disulfide bridges plays an important part in understanding the concept of protein folding. We are investigating how slight changes – the presence *vs.* the absence of the cyclic amino acid proline in a certain position of the peptide-chain – in the sequence of small peptides influence their folding properties. The present studies focus on the folding of a group of small peptides found in *Conus* snails, a-conotoxins SI, SIA (found in *Conus Striatus*), GI, and GII (*Conus Geographus*) under two different oxidizing conditions. Each peptide has two disulfide bridges leading to three possible regioisomers, only one of which is found in nature. Our results indicate that peptides containing the cyclic amino acid proline had very high selectivity for the natural isomer, suggesting that this amino acid enforces a structural rigidity on the peptides.

21

Attachment of Polystyrene to Modified Nitinol and Nickel Substrates

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The attachment of a polymer coating to a metal surface is an ongoing area of scientific research due to its applications in both corrosion prevention and biomedicine. The polymer effectively provides a protective barrier between the bare surface of the metal and its surrounding environment. The purpose of this study was to investigate several procedures for the attachment of polystyrene to the surfaces of both nitinol and nickel to determine which procedure provided the most stable polymer adhesion. Four different procedures were studied: attachment of the polymer directly to the bare surface of the metal, attachment of the polymer to a linker on the surface, and polymerization of the polymer on two different activated self-assembled monolayers on the surface. Diffuse reflectance infrared spectroscopy (DRIFT), contact angle, and MALDI-TOF MS were used to characterize the bare metal surface and modified substrates.

22

Aggressiveness of Parental Male Bluegill, Lepomis Macrochirus, with and Without the Presence of Eggs in Nests

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The bluegill, Lepomis macrochirus, is known for its behavioral characteristics among Pennsylvanian fish. Bluegills naturally begin spawning when the temperature of their freshwater ecosystem reaches 68˚ F. The objective of the research experiment was to determine if there was a difference in aggressiveness of parental male bluegill with and without the presence of eggs in their nests. The aggressiveness of the parental males was determined by trying to lure a targeted fish out of his nest by using a fishing pole and worms at predetermined increments while underwater. The data showed that there was no difference between the bluegills that did not have eggs in their nests compared to the bluegills that did have eggs in their nests. However, once temperature was considered, there was a difference in the males aggressiveness when it was 68˚+ F compared to when it ranged 55˚ to 66˚ F.

23

Comparison of Over-the-Counter Medications Using Powder X-Ray Diffraction

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Powder X-Ray Diffraction is a method of analysis which has many applications in forensic science. It is used to identify and quantify the crystalline components of samples, and due to its non-destructive nature it is especially useful, as the quality of evidence is not compromised. Analysis of over-the-counter drugs was conducted in order to compare the components of expired medications to their non-expired counterparts and also to compare generic drugs to their brand name equivalents. Quantification of the components within the drugs was also undertaken; using the ratio of the caffeine and acetaminophen peak areas from the sample scans to construct a calibration curve. It is hoped that by conducting this calibration the components of over-the-counter medications can be quantified and more insight can be provided into their distinguishing characteristics. This would allow for a more accurate identification of unknown drug mixtures.

24

Analysis of Phosphatidylinositol Turnover in *S. cerevisiae* and *C. albicans*

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Both *Saccharomyces cerevisiae* and *Candida albicans* contain phospholipases of the B-type, which act upon phospholipids to generate glycerophosphodiesters. We analyzed the production of glycerophoinositol (GroPIns), produced through phospholipase B action on phosphatidylinositol, in both wild type and mutant stains of *S. cerevisiae* and *C. albicans.* Pulse-chase analysis of strains labeled with [^{3}H]- inositol indicates that while *S. cerevisiae* produces external GroPIns, *C. albicans* does not. *S. cerevisiae* strains bearing mutations in genes involved in the RAS/cAMP signaling pathway were also analyzed.

25

Improving Health Literacy and Science Knowledge with Art

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Health Literacy is defined as an individual's capacity to obtain, process, and understand basic health related information. It is staggering that around 90 million Americans, basically half of the adult population have an extremely poor understanding of health related information. To improve Health Literacy across the United States, Science Education Partnership Award, at Duquesne University is striving to create a series of educational media which will assist both the young and elderly in increasing their knowledge of basic health related information. The focus of the work conducted over the course of this summer has been on children grades three to five. A website and a workbook have been created to supplement several videos which have already been produced. We plan to test these materials by conducting surveys on both students and educators as to whether or not they are effective teaching resources.

26

Studies of the Energies in the Electronic Orbitals of the conformers of trans- $[Co^{II}(acac)_2(py)_2]$ in a Crystalline and Matric Environment

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Co(II) and Ni(II) readily bond to two acac- groups ($C_3H_7O_2$). These compounds can then be attached to pyrimidine or triazine ligands to form a polymeric chain. The compounds can also be attached to pyridine ligands to form monomers. These monomers can be crystallized and inserted into a matrix yielding a crystalline lattice. Computational Chemistry can be used to do diverse calculations on small molecules. $Co(acac)_2(py)_2$ in the crystal state and $Co(acac)_2(py)_2$ imbedded in the matrix have been previously synthesized. The energy of theses two conformers and of their electronic orbitals has been calculated using Gaussian programs. The energy of these orbitals help us assign the electronic transition in the two conformers.

27

The Nitroreductase from Clostridium(italic)sp.strain OhILAs

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The organoarsenical 3-nitro-4-hydroxybenzene arsonic acid (roxarsone) has seen wide use in the poultry industry to prevent coccidiosis and promote increased weight gain and coloration in chickens. Recent evidence has suggested that microbes associated with poultry litter are capable of transforming roxarsone into 3-amino-4-hydroxybenzene arsonic acid and inorganic arsenic (Stolz *et al*., 2007, Environ. Sci. Technol. 41:818-823). It has been proposed that *Clostridium* sp. strain OhILAs actually uses roxarsone as the terminal electron acceptor in a novel type of anaerobic respiration and that the process may involve a nitroreductase. Candidate nitroreductases have been identified in the annotated genome of *Clostridium* sp. strain OhILAs. Here, we have tested the *in vitro* assay for nitroreductase activity (Rafii and Cerniglia, 1993, Appl. Environ. Microbiol. 59:1731-1734) and show that the assay can also detect 3-amino-4-hydroxybenzene arsonic acid. The potential for NADPH, NADH, FAD, or hydrogen to serve as the electron donor is currently being tested.

28

Lipstick Analysis Using HPLC Detection

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High- Performance Liquid Chromatography (HPLC) is an established method for separating chemical compounds quickly and efficiently. HPLC with Fluorescent and Ultraviolet detection can be used to analyze lipsticks. Lipstick contains many components such as Silicone, Carbon, Oxygen, Bromine, dyes, oils, and waxes. In this poster a gradient method using acetonitrile, and water is developed for separating the components of 4 lipstick samples using HPLC.

29

Docking Simulation Workbook

Christopher Sidun and Jeffry D. Madura; Center for Computational Sciences; Department of Chemistry and Biochemistry; Duquesne University

Docking is a computational method used to find favorable molecular conformations of different ligand structures that complex a macromolecule receptor (in this case, a protein) present in the Molecular Operating Environment (MOE) window. The workbook, aimed primarily at high school students, is an introduction to the docking simulation located in the MOE software. Using the MOE software, and several carbonic anhydrase protein-ligand complexes, an easy to understand set of exercises was created that demonstrate the operation of the docking simulation. Tutorials on how to use configure the available options in the docking simulation along with detailed descriptions of MOE's docking methodology were included. In conclusion, this workshop will give high school students the opportunity, knowledge, and drive to pursue a science related field, in which the use of this technology, specifically to find new drugs is used.

30

Preparation of Intermetallic Compounds via Solid-State Microwave Synthesis

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Microwave irradiation is a unique process that can be applied to many different areas of chemistry. A large volume of work had been performed in areas such as analytical sample preparation and organic synthesis. A much smaller body of research has concerned inorganic synthesis, both in solution and in the solid-state. Solid-state microwave synthesis has been used to prepare diverse materials including carbides, complex oxides, and metal vanadates, among others. However, reports of intermetallic compounds prepared via this method are rare. The goals of this project are to determine which intermetallic compounds can be prepared using solid-state microwave synthesis and to identify important variables for these reactions. Microwave synthesis of intermetallics in the Cu-In, Ag-In, Au-In, Bi-Ni, and Ni-Sn systems were conducted and the products were characterized using powder X-ray diffraction, scanning electron microscopy, and energy dispersive spectroscopy. The results of these experiments will be presented.

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.

32

The Synthesis of a New Class of Lead Sensor Fluorophores

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Lead toxicity is the most common environmental disease in the United States. Complications can affect virtually every soft tissue in the body. We are interested in developing a new class of fluorescent molecules that can be used as lead sensors. This molecule has a thiol-based binding site, and thus differs from other fluorophores with more hard donors such as oxygen or nitrogen. Lead is a soft metal and therefore favors sulfur-rich binding sites. Therefore, the proposed molecule can serve as a highly sensitive fluorescent lead sensor in aqueous samples. In this presentation we discuss the details of the synthetic strategy and characterization of the synthesized molecules.

33

Project SEED Program at Duquesne University

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Project SEED is a program sponsored by the American Chemical Society that places economically disadvantaged high school students in a laboratory setting for eight weeks. Funding for this summer program was awarded by the American Chemical Society and local donors PPG Industries, R.J. Lee Group, The Spectroscopy Society of Pittsburgh, Acusis, Westinghouse, Walmart, The Society for Analytical Chemists of Pittsburgh, and Ms. Tabitha Riggio. Applications were solicited from area high schools and students were chosen based upon grade point average, teacher recommendations, and a personal statement. These students were paired up with a Duquesne University faculty mentor and a graduate student supervisor. Each student conducted their own research project, interacted with other summer research students, and participated in many enriching activities. A description of how to start a Project SEED program and the types of opportunities one can provide to an exceptional student will be described in this poster.

34

Total and Speciated Mercury Analysis in Hair Samples from an Individual Exposed to Thimerosal

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Hair samples from an individual exposed to thimerosal, an ethylmercury-containing compound, were analyzed for total mercury using EPA method 7473 and for mercury species using EPA method 6800 (SIDMS). The first facial hair sample was collected during the first week after the injection, and the first head hair sample was collected in the second month after the injection. The total mercury value for the first facial hair sample was 1.44 ± 0.03 ppm, and that for the first head hair sample was 1.29 ± 0.48 ppm. SIDMS analysis indicated that most of the mercury in the hair was in the form of methylmercury. No ethylmercury was detected in either sample. Total mercury concentrations declined over time in facial hair samples but remained relatively constant in head hair samples. These results suggest that ethylmercury is converted to methylmercury in the body, but more research is needed to confirm this conversion.

35

Identifying DR-3 and DR-4 Alleles in HLA Gene in Type I Diabetes Mellitus Patients

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Type 1 diabetes (T1D) is an autoimmune disease with genetic and environmental predisposing factors. Important predisposing genes include Human Leukocyte antigen (HLA) alleles HLA-DR3 and HLA-DR4. The purpose of the experiment was to determine the HLA-DR genotype of two families with T1D. In the families tested, both children possessed T1D, but the parents did not. This experiment involved extracting DNA from peripheral blood cells. HLA DR genes were amplified using PCR. The amplified DNA was analyzed by gel electropheresis to insure that DNA was present or amplified. The PCR DNA was blotted onto Hybond-N+ membranes. The DNA was probed with labeled oligonucleotides that would indicate if the DNA carried the specific alleles that have proved to be a genetic precursor to T1D.

36

TRAF6 Activation of NF-κB Within the Inflammatory Response System

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Vertebrate innate immunity provides the first line of defense against pathogens generating an immediate inflammatory response regulated by Toll-Interleukin-1 Receptors (TIR) which, in turn, activate an essential molecule designated as TRAF6. Throughout my research, I focused on the activities of TRAF6 and how it eventually stimulates NF-κB, a transcription factor that induces the expression of numerous target genes. I used different TRAF6 expression vector constructs transfected in 293R cells and stimulated with IL-1β in order to quantify inflammatory responses. I also performed a titration of the IL1B stimulant to determine the minimal amount of IL1B required for cell response. Another goal was to determine the expression levels of IL1R and TLR4 receptors in a variety of cell lines, followed by IL-1B or LPS stimulation and detection of NF-κB reporter activity. Finally, I tested whether NF-κB is involved in the transcription regulation of the IL-1B gene.

37

Iso-butyl Substituted Aza-bis(oxazoline)-Copper Complexes: Enantioselective Catalysts for Homogeneous and Heterogeneous Cyclopropanation Reactions

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With increases in the demand for new pharmaceutical agents, enantioselective chemical reactions have become more important. One way in which enantioselectivity may be obtained is through the use of chiral catalysts. In particular, aza-bis(oxazolines) have proved to be effective ligands in the copper catalyzed cyclopropanation of styrene and EDA, although enantioselectivity varies with the C-2 substituent of the ligand. In this study, homogeneous and heterogeneous catalysis methods utilizing iso-butyl substituted aza-bis(oxazoline) were examined. The homogeneous cyclopropanation of styrene was carried out in solution, whereas the heterogeneous reaction required the immobilization of the ligand on a gold-coated slide. This was achieved by binding the ligand to a self-assembled monolayer via the Mitsunobu reaction. NMR was used to determine the cis/trans ratio of the product, thereby displaying the stereoselectivity of these two methods. Prep TLC was then utilized to isolate the enantiomers. This type of heterogeneous catalysis may lead to the development of reusable catalytic chips, benefiting both industry and academia.

38

Dr. Allevable and Regenerobot Explore Tissue Engineering

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Hands-on learning creates long-lasting knowledge. Data supporting this approach led me to create a fun, engaging, activity-based workbook for the Dr. Allevable and Regenerobot movies (sepa.duq.edu). I wanted to design activities that make science come alive in classrooms; an exciting departure from text-based lessons traditionally taught. After creating the Bone and Spinal Cord Modules, I tested the workbook's effectiveness and usability with my colleague, Molly Bugaile. We surveyed two populations of users: teachers and students. Teachers received surveys about professional backgrounds and instructional preferences before evaluating the workbook. Upon reviewing the materials, they completed another survey about design, activities, and usability. Students were surveyed twice at the Sewickley Valley YMCA Camp about prior scientific interest and opinions toward completed activities. I found that pairing hands-on learning with animated movies provides unique educational opportunities.

39

Expression and Purification of Two Fragile X Mental Retardation Protein Isoforms

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Fragile X syndrome is the most common form of inherited mental retardation, being caused by the loss of the expression of fragile X metal retardation protein (FMRP). FMRP is proposed to regulate the localization and translation of specific mRNAs. It has been shown that FMRP undergoes posttranslational modifications such as methylation of specific arginine residues and serine phosphorylation. In this study, recombinant methods are being used to try to express and purify two short isoforms of FMRP, which contain the proposed methylation and phosphorylation sites and RNA binding domain in RGG box by using Rosetta2 (DE3) pLacI *Escherichia Coli*. Once the proteins are purified characterization of their binding properties to specific RNA targets will be conducted. Subsequently, the effects of posttranslational modifications on their respective RNA binding properties of the FMRP RGG Box will be analyzed.

40

Simulation of Catecholamine Release through Patch Clamp Amperometry using MCell and DReAMM

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A popular method of voltage detection across a cell membrane involves patch clamp amperometry. With the assistance of Blender, a 3D visualization may be constructed to model the patch clamp, with the carbon fibre electrode (CFE), connecting to the cell membrane, with corresponding cations. MCell, reads MDL (Model Description Language) files to interpret and create the simulation of objects. The DreaMM program displays a 3D visualization of how ions are detected on the CFE and how different variables may affect the release rate of ions through the channel. Neurotransmitters such as catecholamines are released through the fusion pore by a process of exocytosis. Efflux of catecholamines hitting the carbon fibre electrode after they have been released from the vesicle produce an amperometric current. The position of the CFE within the patch clamp, as well as vesicle and pore size is varied to determine the rate of efflux across the pore.

41

Transcriptional Regulatory Elements and Transcription Factors That Control Kaposi's Sarcoma Human Virus Genes.

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Kaposi's sarcoma human virus (KSHV) is a tumor developing agent that belongs to the human herpes virus 8 family. Functional studies of KSHV indicate that its genes interfere with established tumor suppressor pathways, modify the host cellular environment, and thus contribute to the pathogenesis of KSHV-associated disorders. We are currently endeavoring to identify the transcriptional sites and factors that are involved in regulating the KSHV genome. In reaching this goal we have characterized the upstream regions of all the protein coding genes. These upstream sequences will be loaded into a web program that will identify transcription factors by comparing them against the database of known transcription factors. With the identification of these transcription factors we hope to better understand the regulation and infection of the Kaposi virus.

42

Study of the RNA Binding Properties of the Truncated Isoform 3 of the Fragile X Mental Retardation Protein.

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Fragile X Syndrome, the most common inherited form of mental retardation, is caused by the expansion of the CGG repeat prior to the *FMR1* gene. As a result, the fragile X mental retardation protein (FMRP) is no longer expressed. FMRP is an RNA binding protein which has been proposed to be involved in the binding and translation regulation of neuronal mRNAs containing a G-quartet structure. The FMRP domain responsible for G-quartet RNA binding is its arginine-glycine-glycine (RGG) box. There are several FMRP isoforms, and in this study we have been working on the truncated FMRP (Isoform 3) that contains the RGG box domain. Current efforts are towards expression of the isoform in Rosetta2 (DE3) pLacI *Escherichia coli* cells and purification using immobilized Nickel (II) affinity chromatography. Once the protein is purified its binding to G-quartet forming MAP1B RNA will be characterized by 2-D NMR spectroscopy.

43

Biophysical Study of an RNA Quadruplex Structure Formed by a Mixed Purine Sequence

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G-quadruplexes, which are formed by both DNA and RNA with specific sequences, are proposed to be important in a variety of biological processes. Such structures, formed by stacking rings of four guanine residues, are stabilized by Hoogsteen H-bonds, and by the presence of K+ ions. It has been suggested that not only stretches of Gs can form quadruplexes, but also mixed purine sequences, in which adenines are flanked by guanine residues. In addition, mixed purine sequences have been proposed to form a variety of higher structures based off the core G-quadruplex, including hexads and A-quartets. In this study, biophysical techniques that include NMR spectroscopy (1D-^{1}H NMR, ^{1}H-^{1}H NOESY and deuterium exchange methods), UV spectroscopy and CD spectroscopy were employed to characterize the intermolecular quadruplex structure formed by the sequence r(UGGAGGU).

44

Solid-State Kinetic Study of the Maillard Reaction using Acetaminophen and Lactose Tablets as a Model System

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The purpose of this work was to study the Maillard reaction in the solid-state. The Maillard reaction, as relevant to pharmaceutical compounds, is the reaction between reducing sugars and amines, common constituents in drug products. A preliminary study to define experimental parameters indicated Maillard browning was evident after 1:1 weight ratios of acetaminophen and lactose tablets were heated at 95^{o}C for 72 hours. A kinetic study of the reaction was then done at 95^{o}C over a five day period using samples of 40%, 45%, 50%, 55%, and 60% (by weight) acetaminophen tablets with lactose. Near-infrared spectroscopy was used to analyze reaction progress and was advantageous over other analytical techniques because it is non-destructive, allowing repetitive data collection on an individual sample.

45

Analysis of Organics in Soils

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Procedures were studied to extract and analyze organic content from soil which eventually may be used, in conjunction with other methods, to definitively characterize locations that a particular soil may have originated from. Several extraction techniques – microwave extraction, heating, sonication, and heating followed by sonication – as well as several different extracting solvents – (1:1) acetone:hexane, methylene chloride, acetone, methanol, and acetonitrile – were studied and the extractions were analyzed using gas chromatography coupled with mass spectrometry (GC-MS). Preliminary findings indicate that acetone:hexane and methylene chloride are the best choices of solvents. Heating followed by sonicating proved to be an effective extraction method. Instrumental difficulties were faced when using the microwave – this will need to be looked into as the research continues. More research needs to be done to refine these procedures for finding distinguishing characteristics.

46

Harderian Gland And Pheromone Detection In *Plethodon shermani*

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The Harderian gland is found in many vertebrates and is located near the orbit . Although described in 1694 by Johann Jacob Harder, the exact function of the Harderian gland remains unclear. We tested whether the harderian gland is involved in detection of pheromones in the terrestrial salamander, *Plethodon shermani*. The salamander is a good model for this experiment because the vomeronasal organ (VNO), a sensory neuroepithelium specialized to detect pheromones, is sexually dimorphic in volume. We found a strong positive correlation between VNO volume and harderian gland volume. Next, we either removed the harderian gland or left it intact. We found no differences in chemo-investigative behavior between the treatment groups. A future study will test for differences in vomeronasal sensory neuron responsiveness to pheromones.

47

Communicating Science Through Language and Images

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Precise language and support images are valuable tools in teaching and explaining. I have explored using both tools to educate students about health-related science over the Internet in the context of the project "Regenerative Medicine Partnership in Education" (www.sepa.duq.edu). The project's main educational tool was video but has expanded to include online learning modules. To create modules to pair with the videos I used the iterative process of researching, writing, and revising. Research tools included scientific texts and informal online sources. While researching, I created visual materials, such as slideshows and video clips with subtitles, to help explain biological processes. Through the writing process I found that rhetorical strategies such as word choice, sentence structure, and organization greatly altered the meaning and clarity of the text. In the future survey responses will guide further changes.

48

Developing a Temperature Control System for Atomic Force Microscopy of Lipid Systems

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Supported Lipid Bilayers can be used as biosensors and as model membranes. To explore the phase behavior of the bilayers prepared in different ways, variable temperature AFM experiments are going to be performed. For this purpose, a variable temperature control chamber was created by combining a Minco temperature control unit with a Minco heating pad. The requirements were that the temperature be stable over the temperature range of 25ºC to 50ºC. After changing parameters on the temperature controller, the temperature was stable within 0.1ºC for temperatures from 30ºC to 45ºC. After adding more insulation, the temperature was found to be stable from 30ºC to 50ºC. The temperature could also be changed in 1ºC steps in one minute. This implies that the chamber is suitable for the variable temperature experiments in the AFM. The next step is to run the experiments and view the phase change in the Supported Lipid Bilayers.

49

Effect of Unsaturated Long Chain Lipids on Bicelle Systems

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Bicelles are a planar, liquid-crystalline lipid system that serve as an excellent model lipid bilayer for structural studies of membrane proteins. Typically, bicelles are a binary mixture of dimyristoyl-phosphatidylcholine (DMPC) and dihexanoyl-phosphatidylcholine (DHPC)and form a bilayer in which membrane proteins retain their function.However, these two fully saturated synthetic lipids are a poor model for cellular membranes, which include up to 50% unsaturated lipids. In order to make these lipid mixtures more biologically relevant,palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) was introduced into DMPC/DHPC binary lipid mixtures in varying ratios, with a consistent q molar ratio of long chain lipids to short chain lipids of 3. 31P nuclear magnetic resonance (NMR) was used to characterize the degree of alignment, the homogeneity, and the phase behavior of the unsaturated bicelle samples.

50

Alkali Chalcogenide Flux Synthesis and Characterization of Quaternary Diamond-Like Semiconductors, I_2-II-IV-VI_4

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Diamond-like semiconductors are normal valence compounds that adopt the cubic or hexagonal diamond structures. Diamond-like semiconductors of the formula I_2-II-IV-VI_4 are of interest because they have potential uses in nonlinear optics, light emitting diodes and spin-based electronics. Among diamond-like semiconductors, quaternary materials have been less studied. Due to the compositional flexibility of these quaternary compounds, various chemical substitutions can be made, where I_2 = Li, II = Zn, Cd, Mn, IV = Sn, and VI_4 = S, allowing the fine tuning of the products' physical properties. The goal of our research is to grow single crystals of these materials by alkali chalcogenide fluxes. The products of these solid state reactions will be characterized with differential thermal analysis (DTA), powder X-ray diffraction (PXRD), UV-Vis/NIR spectroscopy, and, when applicable, single crystal X-ray diffraction.

51

Isothermal Titration Calorimetry Analysis

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When a protein-ligand complex forms, energy in the form of heat is released. The amount of heat released as a function of ligand added can be measured using isothermal titration calorimetry (ITC). The ITC data can be used to obtain parameters such as n, number of binding sites, ΔH, enthalpy, K, equilibrium constant and ΔS, entropy. Analysis of the ITC data involves integrating the heat per unit time vs time and then performing a non-linear least square fit. A series of Matlab scripts have been written to perform the analysis and determine n, K, ΔH and ΔS.

52

Building Additional Tools for *in vivo* Transposon Mutagenesis of a Filamentous Sporulating Bacterium

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Streptomyces coelicolor is a gram positive filamentous soil bacterium. In *E. coli,* which divides by binary fission, null mutations in cell division genes are lethal. In contrast, S*. coelicolor* has a very complex lifecycle and its cell division genes are dispensable for growth and viability. In order to identify new cell division genes, a transposon mutagenesis system was developed in our laboratory. This system uses a plasmid containing a mini-*neo*-transposon derived from Tn*5*, and is a suicide vector. At present, transposon mutagenesis occurs only when DNA is introduced using transformation. My research project currently focuses on manipulating this plasmid to function when introduced via conjugation. Conjugation of the transposon mutagenesis plasmid would be a faster and easier method than transformation. In addition, I created a derivative of the mini-transposon containing an apramycin-resistance marker. These additional tools can be used to identify new cell division genes in *S. coelicolor.*

53

QSAR of Microtubule Stabilizing Dictyostatins

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Microtubule stabilization is a validated mechanism for cancer chemotherapy. Dictyostatin, an analog of the failed drug discodermolide, binds to the β-tubulin subunit of microtubules, inhibiting cell growth by blockage at the G2/M phase of the cell cycle. Dictyostatin and analogs were synthesized and their antiproliferative activities against ovarian cancer cells were measured. These data, along with that from some discodermolides, were used to determine a quantitative structure-activity relationship (QSAR). Molecular models of the dictyostatins were built from NMR coordinates of discodermolide and their global minimum energy conformations determined. Models were superimposed to provide maximum structural overlap and a collection of electronic, thermodynamic and steric descriptors were calculated for each model. A special multiple linear regression analysis, the genetic function approximation, was then used to find the descriptors that best explained the differences in activity. A population of statistically-compelling QSAR equations was found and may be useful in future analog design.

54

Evaluation of Different Biological Data and Computational Classification Methods for Use in Protein Interaction Prediction in Signaling Pathways in Arabidopsis Thaliana

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A recent study conducted by this research group concluded that using the correct combination of classifiers and features, supervised machine learning could be used to make predictions regarding protein interactions based on direct and indirect biological datasets for yeast cells. We sought to repeat these results for *Arabidopsis thaliana*, a model organism for flowering plants, and defined "protein interactions" in three overlapping subdivided categories: (1) physical interaction, (2) co-complex relationship, and (3) pathway co-membership. To investigate systematically the utility of different data sources and the way the data is encoded as features for predicting each of these types of protein interactions, we assembled a large set of biological features and varied their encoding for use in each of the three prediction tasks. It is predicted that the importance of different features depends on the specific prediction task and the way they are encoded.

55

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

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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.

56

Model of NOS/TGF-Beta1/Plasmodia System in Humans and Mosquitoes

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Malaria, one of the world's Top 10 deadliest diseases, has been shown to be regulated by two key chemicals: nitric oxide and TGF-Beta1 protein. Nitric oxide kills plasmodia and activates TGF-Beta1 protein in both humans and mosquitoes. TGF-Beta1, however, inhibits the production of NOS in humans, but induces the production of NOS in mosquitoes. This implies a NOS/TGF-Beta1 positive feedback loop in the mosquito, but in humans, the growth of Nitric Oxide is limited by TGF-Beta1, so Nitric Oxide may not be able to kill as many malaria parasites. This project will attempt to model the transmittance of malaria, TGF-Beta1, and Nitric Oxide between mosquitoes and humans. After the system has been successfully modeled with proper differential equations and accurate constants, our aim will be to determine the proper range of Nitric Oxide and TGF-Beta1 levels needed (in humans and mosquitoes) to suppress the malaria situation at an optimum level.
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57

Communicating Complex Concepts through Complex Visuals

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The technological advancements made in computer graphics create the opportunity for effective teaching with visual aids that may be more effective than traditional text books. Computer simulation offers the general public a window of knowledge about scientific mechanisms that would otherwise be difficult to explain. The Regenerative Medicine Partnership in Education (www.sepa.duq.edu), produces multiple educational platforms including movies, web resources and teaching tools. I have produced an accurate representation of the beating human heart. I have also produced a representation of the functioning human lymphatic system and its evolution. The use of complex visual technology that portrays in accurate detail the scientific process will help educate the general public and school children about otherwise complex scientific content. In the future, rigorous testing with target audiences will demonstrate the success of this paradigm.

58

Dr. Allevable and Regenerobot's Exploration Adventure

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The project goal was to develop educational programs focusing on regenerative medicine and health care of the future (www.sepa.duq.edu). Animated movies and supporting web pages discuss tissue engineering in bone and heart. To be useful for elementary education, grade appropriate teacher resource guides and student workbooks were needed. Together with education major Brianne Miller, we created teacher and student materials which support the movies or can be used as stand-alone workbooks. We reviewed numerous sources before developing our curriculum – such as science textbooks, the project's tissue engineering movies, as well as other SEPA projects and web resources. The educational goals of the workbooks were put into the context of the Pennsylvania and National Teaching Standards for each of the target grades. Evaluation that assesses teacher usability and student learning is in progress.

59

Genetic Sex Determination of Amur Tiger

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The phenotypic male Amur tiger born at the Pittsburgh Zoo in late 2006 displayed various sex organ deformities. Suspicions about the tiger being an intersexed male having an XXY chromosomal profile was solved using cytological and genetic techniques. Numerous experiments were performed on the tiger's blood sample in order to determine the true genetic sex. A drop-test used to identify barr bodies was inconclusive. The next experiments featured several marker systems in conjuction with the polymerase chain reaction (PCR) method. This allowed specific regions on the X and Y chromosomes to be amplified. The presence of bands in the SRY region confirmed the presence of a Y chromosome. By amplifying the zinc-finger and amelogenin regions of the sex chromosomes and using the genetic analyzer to genotype the tiger it was possible to determine the Amur tiger is a genotypic male having only one copy of the X and Y chromosomes.

60

Validating Species Identification Using Cytochrome B and 12S rRNA Mitochondrial DNA Primers

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Mitochondrial DNA (mtDNA) has been utilized in forensic applications to determine relationships and identity. Recently, sequence segments have been designated as "barcodes" for species identification. The cytochrome B and 12S rRNA regions of the DNA are used as genetic markers to differentiate between species. There is speculation, however, about the accuracy of species identification based on these regions. This study used literature-based vertebrate primers of the cytochrome B and 12S regions to test the accuracy of species identification. A double blind experimental design was employed on twenty vertebrate tissue samples. Methodology included extracting the DNA and amplifying the extracted DNA via polymerase chain reaction (PCR). Additionally, separation was achieved via agarose gel electrophoresis and ultimately the product was sequenced. The subsequent sequence was "BLASTED" into the NIH database for species identification. "BLAST" results were then compared to the known identity coded by one of the PIs.

61

Improving Students' Understanding of Concepts Related to Conductors and Insulators

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We examine the difficulties that introductory physics students have with concepts concerning conductors and insulators and evaluate the effectiveness of research-based tutorials on this topic. Results of a multiple-choice test given to undergraduate as well as graduate students reveal the high level of difficulty of the subject. We compare the results of pretests and posttests taken by students who have been taught by lecture and by students who have received their instruction with the use of the tutorials. We find that the designed tutorials significantly improved understanding while lecturing alone was not effective.

62

Categories and Hierarchical Knowledge in Physics Education

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The goal of this project is to discover the methods by which people learn and understand physics concepts. Tests were given to first year undergraduate and graduate students as well as faculty members. The problems were not to be solved, but instead each was to be placed into categories based on the principles of physics that would be needed to solve the problem. Using theories of hierarchical knowledge it is expected that those that do well in this categorization exercise will have a higher level of understanding of these laws, and in the students' cases, some correlation with students' grades is expected. Not only must the tests be checked for having good categories, but the placement of each problem in these categories must be compared as well. By doing this research, we hope to show whether or not categorization techniques could be used as an instructional tool in physics courses.

63

Hydronuclear Radiofrequency Coil for the Imaging of Breast Tissue at High Magnetic Fields

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A surface coil was constructed and bent into a "butterfly" configuration. An adjustable 40 pF tuning capacitor was connected in series with the inductor. Two adjustable 15 pF matching capacitors were connected in series with the inductor. These were used to match and tune the specified resonance frequency. This butterfly design was then tested at 1.5 Tesla to see if a homogenous magnetic field was produced. Using these results, a hydronuclear coil was constructed for the imaging of breast tissue. The "butterfly" two loop design was used for the outer coil. The coil placed inside the butterfly design was a volume coil. These coils were matched and tuned to resonate at the frequency for 3 T. These two coils are advantageous when put together because breast tissue is mainly carbon and proton based.

64

Creating Image Analysis Software for Photonics

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In analyzing the light emitted from captured excitons in a polariton superfluid, there is a lack in the variety of specialized imaging software available to observe and process the captured spectrum. Working closely with graduate students in the photonics group, I've combined all of the useful programs and procedures needed into a quick and intuitive interface they'll use for analyzing spectra captured from CCD cameras. This was done in hopes of streamlining the currently convoluted and tedious process of efficiently obtaining useful cross sections and new image data.

65

Quasar Spectroscopy: The Evolution of Zinc and Chromium in the Universe

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Quasars are the most distant and luminous objects in the universe and so they can be used as background light bulbs for studying intervening galaxies. During previous summers, spectra from the Sloan Digital Sky Survey database have been studied for strong absorption lines like singly ionized Magnesium and Iron, i.e., MgII and FeII. Examination of the strongest of these systems has revealed the presence of associated weak lines of Zinc (ZnII) and Chromium (CrII) which can be used to estimate the metallicity and dust content of the galaxies that host them. Using the principles of Hubble's Law and the redshift of the object being viewed, the strengths of ZnII and CrII can be used to produce an evolutionary timeline of metallicity. In addition, the correlation between the strength of the absorption lines measured and the formerly studied elements will be analyzed.

66

The Newtonian View of Cosmology: An Alternate Approach to Our Standard Model

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The Newtonian view of Cosmology provides an alternate view to the standard model of the universe. Using only Newtonian gravity, the same equations governing the contents and scale factor of the universe are derived as from general relativity. Moreover, the two approaches are consistent to first and second order perturbation. Currently, physical implications of the terms in the equations are being investigated. Specifically, the relativistic model predicts that the total energy of the universe is not conserved due to the expansion of particle wavelengths as a result of redshift. Therefore, it is being considered how the Newtonian model incorporates this energy loss. The goal of this project is to provide a new framework to describe the contemporary model of the universe. This may be potentially useful as a teaching device as well as when exploring current mysteries such as the nature of dark energy.

67

Spin Coherence in Quantum Dots

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The nano-scale sized semiconductor structures known as quantum dots show great promise for the advancement of electronic technology in our society. They can be used for such applications as low-threshold laser diodes, quantum computing, and smaller logic devices for classical computing. In this project, the resistive properties of electrical contacts on GaAs quantum dots were investigated. A method was developed to measure the resistance of the contacts, for the purpose of determining their adherence to Ohm's Law. Ideally, the contacts should be obey Ohm's Law in order to effectively trap electrons and holes in the dots. Once trapped in the wells formed by the dots, the electron's spin hopefully can be used as a method of realizing a qubit. The lifetimes of the spins, measured using Time Resolved Faraday Rotation (TRFR), are relatively long in GaAs quantum dots, making them even more promising for quantum computing.

68

High-Velocity Ejecta From Broad Absorption Line QSOs

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Quasi-Stellar Objects (QSOs) are the Universe's most luminous objects, powered by supermassive black holes at the centers of galaxies. About 10% of QSO spectra exhibit absorption troughs extending up to 30,000 km s^-1 from the QSO itself. These Broad Absorption Lines (BALs) arise either in clouds accelerated by radiation pressure or in winds blown off a surrounding torus of cooler gas by the intense luminosity of the central disk. We present results from a search for extremely high velocity (>30,000 km s^-1) CIV absorbers in BAL QSOs. We selected QSOs with redshift z > 1.5, for which the QSO CIV line is shifted into the visible spectrum. Only QSOs with positive Balnicity Index as measured by Trump et al. (2006) were considered. Our final sample comprises ~1600 BAL QSOs containing 221 measured CIV absorption systems. We compare their occurrence in velocity space to those found in a sample of 15150 non-BAL QSOs.

69

Mapping the Sunyaev-Zeldovich Distortions of the Cosmic Microwave Background for Regions Surrounding a Black Hole

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The distortions caused by the Sunyaev-Zeldovich effect in the cosmic microwave background radiation are a powerful way to locate galaxy clusters and black holes as well as to observe how they affect their environment. However, detailed maps of the cosmic microwave background radiation for regions around galaxy clusters are not yet available due to the fact that current telescopes have noise levels that are of the same magnitude or larger than the distortions. Using data from an altered version of the GADGET-2 cosmological simulator and programs that were written in C, an artificial map is being constructed of what the Sunyaev-Zeldovich distortion of the cosmic microwave background radiation should look like for a hot bubble of gas surrounding a black hole.

70

Characterizing the Behavior of Silicon Photomultipliers

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The Silicon Photomultiplier (SiPM) represents a recent advance in light detection electronics. With a low cost and energy requirement on a small, robust body, it stands to take the place of the standard Photomultiplier Tube (PMT) in applications from scintillation counting in Positron Emission Tomography (PET) to measurements of Cherenkov radiation. Two SiPM units of each of two models produced by Hamamatsu have been received and characterized. The attainable levels of gain have been related to the bias voltage placed across the array of photodiodes at the heart of the SiPM – yielding an effective capacitance value – at various ambient temperatures. Noise production in the absence of a light source has also been measured as a function of bias voltage and temperature, providing a guideline for the conditions at which a SiPM would be useful in a given experimental set-up. The research provides a comparison of SiPMs and PMTs.

71

Temperature-Dependent Piezoelectric Response of $SrTiO_3$ Thin Films on Si: Possible Applications in Quantum Computing Architectures

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Recent experiments in our laboratory indicate that $SrTiO_3$ thin films undergo a ferroelectric phase transition at T_c~315 K. Using AFM lithography to write polarization patterns in the thin films, we have determined that it is possible to write stable domains for $T<T_c$, while those domains quickly disappear for $T>T_c$. These results have significant implications for use in quantum computers. The temperature dependent ferroelectric properties place an upper limit on the maximum operating temperature for devices such as quantum computers.

72

The Effect of Rotation on the Surface Temperature of a Star

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We get a wealth of information about a star from its spectrum which includes the surface temperature, the abundances of elements and their ions and the mass of the star. Therefore it is important to understand how the rotation of a star will change its spectrum. All stars rotate, and in the case of a slowly rotating star there are methods to easily calculate the effects that this rotation has on the star's spectrum. However, things become complicated in the rapidly rotating case because phenomena that were insignificant in the slowly rotating case become very important. It is the goal of this project to design a web application that will show how rotation changes the shape, surface temperature distribution and the spectrum of a star. The result will be a web application that visualizes the how rotation affects a star, and is accessible to the general public.

73

Determining Pressure Differences in a Venturi Tube

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My research this summer deals with Venturi tubes and how they work. A Venturi tube is a device commonly used to measure pressure differences. I am using a Venturi tube that is typically used as a demonstration in introductory physics courses. I have found that at certain areas in the tube, the pressure values do not agree well with theoretical predictions. This is possibly due to turbulent air flow in the tube. Accordingly, I have been studying the effects of the location of pressure ports and length of the tube to design a Venturi tube that agrees well with theoretical values.

74

Nitrile Anion Dimers in Lithium Tetrahydrofuran Solvent

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Nitrile anions and the complexes that they form are potentially useful for asymmetric synthesis. Organic chemists have utilized this property of the complexes for years, but have not studied the aggregates formed by the nitrile anion. Nitrile anions in the presence of lithium and THF are known to form dimers. These dimers have been observed by NMR; however, their structure has not been resolved. Electronic structure methods have been used to evaluate four nitrile anion dimers and used to compute carbon-13 chemical shifts. The computed chemical shifts will be compared to the experimental data to determine which dimer is most prevalent in solution.

75

Highly Efficient Copper (I/II) Mediated Atom Transfer Radical Addition in the Presence of AIBN

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Atom transfer radical addition (ATRA) is a synthetic methodology used to add halogenated compounds to carbon-carbon double bonds through a radical process. The drawback of this reaction is the large catalyst loading required to achieve the desired product. The solution to this has been found using a new process termed initiators for continuous activator regeneration (ICAR) atom transfer radical polymerization (ATRP). This process utilizes copper (II) complexes that are continually reduced to copper (I) complexes in the presence of radical initiators, allowing for lower catalyst loadings and making ATRA more viable. Work has focused on ICAR ATRP using $[Cu^{II}(TPMA)Br][Br]$ catalyst complexes with 2,2'-azobis(2-methylpropionitrile) (AIBN) as the radical initiator, as its slow decomposition rate allows for a continuous source of radicals. Various brominated compounds, including bromoform, were added to simple olefins such as 1-hexene. Turnover numbers (TONs) of 10,000 were achieved. Further work will make use of other catalyst complexes.

76

Exploring an Alternative Method to Compute Protein Electrostatics

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Protein electrostatics is the driving force behind molecular dynamics. The main equation governing these electrostatic forces is the Poisson Boltzmann equation for the potential. This project explores a novel approach to solving this equation. Instead of the standard finite difference or finite element methods we explore the use of the Boundary Element Method. The key to this approach is the implementation of the ACA algorithm to compress the matrix generated by the Boundary Element Method in hopes of generating an accurate result in a timely fashion. Another main component to the Boundary Element Method is the creation of a functional representation of the protein surface. Rather than using naïve spherical or cylindrical approach, we attempt to use a more precise spherical harmonics representation of the surface. The overall goal is an algorithm that can compute the potential in both a more accurate and a more timely fashion.

77

Folding Path of a Trp-cage Mini-protein

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Breaking the folding code of biomolecules is one of the major problems facing science today. Further insight into this problem was gained by using molecular dynamics to simulate the folding of a 20 residue mini-protein, known as TC5b, which despite its size, has a compact tertiary structure. More than fifty, one nanosecond, gas phase molecular dynamics simulations of TC5b were performed using the CHARMM force field. Principal component analysis (PCA) was used to visualize the similarity of structures along the folding path from the unfolded to folded state as compared to NMR. In addition, specific structures along one trajectory were hydrated to evaluate solvation forces. The role of water in the early stages of folding is of interest. A separate MD simulation was performed in explicit solvent to look more realistically at solvent forces on folding and to serve as a basis of comparison for the solvated gas phase simulations.

78

Time Delay in Structural Shifts: Modeling Multiple States

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The reaction rates of most biological processes are linked to the concentrations of reactants. Models of the simplest systems (many with biological importance) consider two states: “on” and “off” or “open” and “closed”. However, state mediation takes place via any number of intermediary states that correspond to structural shifts, allosteric interactions, induced fitting, etc. Although intermediate observation is difficult experimentally, our introduction of time-delay and intermediate states can more accurately model entire systems where only equilibria were before considered. Specifically, intermediate steps prevent the subtle assumption of simpler models that structural conformations shift immediately, and provide instead predictions correlating with the experimentally observed and intuitive. By carefully choosing intermediate rate coefficients, we can describe an “on/off” system with equilibria identical to the simpler model, but with different mediating landscapes and time scales. Because structural shifts always involve an intermediate state or states, we see this approach as providing needed variability.

79

Defining the Role of G-proteins in Inorganic and Organic Arsenic Metabolism using MT1-CHO Cells as a Model

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3-nitro-4-hydroxy-benzene arsonic acid (roxarsone) is a common feed additive given to prevent coccidiosis in broiler chickens with the added benefits of increasing growth and pigmentation. Biotransformation of roxarsone results in increased environmental exposure of both the parent compounds and its metabolites. Studies from our laboratories indicate that roxarsone may promote the formation of blood vessels via Gi proteins. Our central hypothesis is that these arsenicals modulate G-protein activity through the receptor coupled to the G-protein or by direct binding to the G-protein itself. MT1-CHO cells have shown great promise for probing the effect of agents acting through G-proteins becaue these cells undergo morphological changes that are easily measured. These cellular extensions are driven by the inactive state of Gi proteins to polymerize themicrotubules. In this presentation we will discuss the effect of arsenicals on these melatonin-induced morphological changes to further identify those mechanisms underlying arsenical action in vivo.

80

Flow Cytometry Data Analysis and Management

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Flow cytometry is the analysis of biological materials by detection of the light-absorbing properties of cells or subcellular fractions passing in a narrow stream through a laser beam. Data collected through flow cytometry can be used to identify potential drug targets, detect molecular content of cells, and detect gene expression patterns. Despite its practical significance, flow cytometry suffers some setbacks in terms of handling the data output. Increasing data throughput, error-prone analysis methods and non-standardized formats are some of the major issues. The purpose of this study is to investigate ongoing efforts to standardize flow data. We mainly focus on a prevailing standard flow data structure and prism-based data analysis approach, which allow the exchange and reuse of data. We will also explore the flexibility of these approaches in regards to addressing underlying biological issues.

81

Synthesis and Characterization of Dithione Ligands and Their Metal Complexes.

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Dithiolenes are redox non-innocent ligands that can bind to a variety of metal ions. Their metal complexes are of interest due to the unusual properties they exhibit as well as models for metalloenzyme active centers. In most cases, metal binding of the reduced dithiolene has been explored. In our laboratory, the metal binding of the oxidized form of this ligand, the dithione form, is being investigated. To this end, two dithione ligands, N,N-isopropylpiperazinium-2,3 dithione and N,N-dimethylpiperazinium-2,3 dithione, have been synthesized. Both ligands have been characterized by 1H NMR and IR spectroscopy. Also, Ni complexes of these ligands have been synthesized and their properties have been investigated using IR spectroscopy, UV-visible, and mass spectrometry.

82

Hypoxia and Microbial Stimulation Via Toll-Like Receptor-2 (Tlr-2) Interact to Amplify a Pro-Angiogenic Phenotype in Human Lung Fibroblasts.

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Hypoxia stimulates angiogenesis, which is likely regulated via the concerted action of multiple angiogenic (CXCL8, VEGF) and angiostatic (IP-10) factors. Since several of these also act as chemokines during infection and inflammation we sought to evaluate how hypoxia and microbial stimuli interact to regulate these factors. We exposed human lung fibroblasts (HLF) to hypoxia mimetics, desferoxamine (DFX) and cobalt(II)chloride ($CoCl_2$,) with and without the TLR-2 agonist, macrophage-activating lipopeptide-2 (MALP-2) and measured the release of angiogenic factors in conditioned media by ELISA. DFX or $CoCl_2$ alone stimulated the release of VEGF from HLF and were unaffected by the addition of MALP-2. While DFX or $CoCl_2$ alone failed to stimulate CXCL8, both dramatically enhanced release in response to MALP-2. Both hypoxia mimetics antagonized the MALP-2-induced release of the angiostatic chemokine IP-10. These data suggest that hypoxic and microbial stimuli may interact to promote a pro-angiogenic environment within the lung.

83

The Use of Salivary Cortisol as a Means to Assess Plasma Levels

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Elevated cortisol levels are a common indicator of stress. Plasma cortisol is the prevailing method in determining these levels. In many species, such as dogs and humans, salivary cortisol has been confirmed as a valid alternative to plasma cortisol which is much more invasive to retrieve. Cats have thus far been neglected in these studies, but a technique that measures cortisol levels without stressing the animal would be highly beneficial for further stress-related studies. In this study, saliva and blood was gathered from feral cats under anesthesia awaiting spay/neuter surgery. A spongy swab gathered saliva and was placed in a filter inside an eppendorf tube which was spun to expel the saliva. Blood was drawn at the same time and stored in EDTA tubes with an anticoagulant. An enzyme-linked immunosorbent assay (ELISA) was performed on all samples and preliminary results suggest a correlation between plasma and salivary cortisol levels.

84

Synthesis and Chemistry of Phenylacrylonitrile

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Nitriles are important components of over 30 commercial pharmaceutical drugs. The nitrile exerts two main functions; polarizing the electron density at an adjacent center and facilitating molecular recognition. A particularly attractive route to install the nitrile group is by a conjugate addition. In this type of reaction, the α,β unsaturated compound reacts via nucleophilic substitution and the nucleophile adds to the β carbon. The compound is stabilized by conjugation and hydrogen bonding provided by the nitrile substituent. The key to this research is to establish methodology for additions to these substituted alkenenitriles. These compounds are favored because of their reactivity and stability. In developing this reaction, phenylacrylonitrile is an attractive substrate because the phenyl ring and the acrylonitrile polarize the alkene center facilitating the conjugate addition. The synthesis of phenylacrylonitrile by the formation of HI to terminal phenylacetylene will be presented in addition to some exploratory conjugate addition reactions.

85

Glucose Sensing in Yeast: Site-directed and Randomized Mutagenesis of the Snf1 Protein Kinase Regulatory Subunit Snf4

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Many regulatory mechanisms have evolved to ensure proper cellular responses to environmental change. The *Saccharomyces cerevisiae* protein kinase Snf1 is required for cellular response to change of carbon source in the absence of glucose. Snf1 is the yeast homologue of the human enzyme AMP-activated protein kinase (AMPK), a major therapeutic target for Type II Diabetes. In humans, AMPK is activated when its ligand, AMP, binds to its regulatory subunit. Homologous residues involved in ligand binding were identified in the yeast Snf1 regulatory subunit Snf4. These residues were changed by site-directed mutagenesis and the functional consequences assessed. Preliminary results suggest that the homologous AMP binding residues are not important for Snf4 function. Therefore our results suggest that Snf4 may not bind AMP and the regulation of yeast Snf1 complex may be fundamentally different from the regulation of its mammalian homologues.

86

Solution Microwave Synthesis and Characterization of the Ternary Diamond-like Semiconductors $AgInS_2$ and $AgInSe_2$

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The goal of this research is to prepare $AgInS_2$ and $AgInSe_2$ using the relatively new method of solution microwave synthesis with triethylene glycol as a solvent. These compounds are ternary diamond-like semiconductors which have potentially useful magnetic and optical properties. Compared to the conventional high-temperature solid state method carried out in a furnace, solution microwave synthesis is significantly more time and cost efficient, and more environmentally friendly. In order to produce pure $AgInS_2$ and $AgInSe_2$, the variation of synthetic parameters, including irradiation time and power level, were explored. The resulting products were characterized via powder X-ray diffraction, UV/Vis/NIR diffuse reflectance spectroscopy, scanning electron microscopy, and energy dispersive spectroscopy. Additionally, the microwave-prepared products were compared to the traditionally-prepared samples.

87

Synthesis and Study of Diamond-Like Semiconductor Chalcogenides

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Diamond-like semiconductors may possess interesting optical properties such as second harmonic generation. They may also exhibit magnetic properties that could allow these compounds to be used in technologies such as spin-based electronics. Thus far, the majority of research involving diamond-like semiconductors has focused on binary and ternary systems. However, there are many quaternary compounds that are predicted to form, but have not yet been synthesized or fully studied. One class of quaternary diamond-like semiconductors has the general formula $Ag_2M^1M^2Q_4$ (where M^1 = Mn, Zn, or Cd, M^2= Ge or Sn, and Q = S or Se). Recently, we have prepared several of these compounds using high-temperature solid-state synthesis in a furnace. Specifically, the compound Ag_2CdGeS_4 has been synthesized at 800°C for four days. All reaction products have been characterized using powder X-ray diffraction, UV/Visible/NIR diffuse reflectance spectroscopy, differential thermal analysis, scanning electron microscopy, and energy dispersive spectroscopy.

88

Solving Einstein's Equations for a Dynamic Schwarzschild Black Hole

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The problem of solving Einstein's equations is primarily a computational one, with numerical stability being the major obstacle. Einstein's equations are a set of ten coupled non-linear partial-differential equations which produce a metric dictating how distance is measured at a given time and point in space. Using finite difference methods these equations are solved to determine how a Schwarzschild black hole grows. This problem is of significance since the behavior of the solutions is not well understood for dynamic situations. Because numerical solutions present themselves as large lists of numbers, further analysis and visualization is imperative. Towards these ends visualizations known as embeddings have been made to illustrate the accretion of a black hole as it consumes surrounding matter. These visualizations show the metric for two-dimensional 'slices' of space-time as curved surfaces in three-dimensional space. Finally, recent efforts have been made to improve numerical stability via the CLAWPACK integration package.

89

T_3-induced Precocious Metamorphosis Initiates Limb Muscle Growth in *Xenopus laevis*

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Thyroid hormone (T_3) controls many of the normal metamorphic changes within *Xenopus laevis*, including muscle growth beginning in limb buds at stage NF53. A ten-day bioassay was performed on embryos varying from stages NF47 to NF50 with T_3 in the rearing water to see if thyroid hormone is responsible for initiating limb muscles or merely promoting their growth. We demonstrate that T_3 initiates limb muscle formation because immunocytochemistry with primary antibody 12-101 indicates the presence of muscle in all limbs when T_3 treatment began at NF50. The bioassay also demonstrates morphological changes that depend upon the stage that T_3 treatment begins. T_3-induced precocious metamorphosis beginning at NF47 causes significant lower jaw protrusion while treatment beginning at NF49 and NF50 causes significant fore-limb and hind-limb growth with slight jaw protrusion. These differences imply changes in development that cause cells to respond differently to the thyroid treatment.

90

Model Selection for Copper (I) Catalyzed Cyclopropanation

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Density functional theory has been used to investigate the stereoselectivity of the aza-bis(oxazoline) copper(I) catalyzed cyclopropanation reaction of carbene acetate and propene. The activation barriers for *cis* versus *trans* approach of the olefin calculated at the B3LYP/6-31G(d) level of theory in vacuum and in the absence of a counterion showed a higher activation barrier for the *cis* approach of the olefin, in agreement with experimental data. However, these calculations were unable to predict the effects of various C_2 substituents on the stereoselectivity. The failure of this model to predict the energetics of this reaction is notable, as it has been employed in a number of studies on copper catalyzed cyclopropanation. Calculations using the B3LYP and MPW1K functionals with a larger number of basis functions are currently being performed, along with calculations using second order Møller-Plesset theory. The incorporation of solvent and counterion into the model is also under investigation.

91

Analyzing Pericytes and Endothelial Cells Response and Interaction to Growth Factors and Chemokines

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Angiogenesis plays an important role in development and homeostasis. When unchecked it can lead to pathological conditions. Pericyte are found to cover the abluminal surface of microvessels and have been shown to play a role in the formation and stabilization of vessels. These cells are not well characterized and their function is not well defined. Thus, this study examines the role pericytes play in modulating vascular stability. A migration assay was employed to analyze. the ability of growth factors (VEGF, PDGF-B, and EGF) and chemokines (IP-10, 1P-9, and PF-4) to regulate pericyte motility. Secondy, a matrigel assay was used to observe the affects of pericytes on endothelial cells during vasculogenesis. Here we analyzed the ability of pericytes to enhance tube formation and inhibit tube dissociation in the presence of various angiostatic factors. Understandinig pericytes-endothelial interaction will provide significant insight on the role pericytes play in modulating vascular stability and endothelial cells function.

92

Characterization and Sequence Analysis of Phage Demeter using *Mycobacterium smegmatis* as a Host Organism.

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Tuberculosis has become an increasing threat to the global population, and with the increase in antibiotic resistant strains of the organism the need for new therapy has become more urgent. One possible solution to the rising epidemic is the use of phage therapy, which involves treating the disease with a virus that infects bacteria. As a result, an interest has developed in bacteriophages and their medicinal potential. There are approximately 10^{31} bacteriophages in the world and as such the focus of this research has been on the characterization of one of those bacteriophages. The bacteriophage Demeter was isolated in the spring of 2006 and is currently undergoing genomic sequencing. Using *Mycobacterium smegmatis* (a model organism for the study of *Mycobacterium tuberculosis*) as a host, further understanding of the role Demeter plays in the microbial world can be reached.

93

Surface-modified Poly(D, L-lactic-co-glycolic acid) Nanoparticles as Carriers of siRNA for Delivery into Mammalian Cells

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The purpose of this research was to modify nanoparticles vector for delivery of siRNA into mammalian cells. The nanoparticles, poly(D, L-lactic-*co*-glycolic acid) (PLGA), are biodegradable polymers with a molecular weight ranging from 16,500-22,000 Daltons. We will produce effective methods of chemical modification of PLGA nanoparticles targeted at improving siRNA loading and delivery. The surface of the nanoparticle has been functionalized to allow the binding of the ornithine/histadine-based cationic peptide (O10H6). This then may create a nanoparticle with improved stability for docking of the siRNA. The particle modification was studied by infrared spectroscopy.

94

Analysis of Steroid Sulfatase Inhibitors in Human Bone and Breast Cancer Cell Lines

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Steroid sulfatase removes the sulfate group from sulfo-conjugated steroids. Various tissues may use this enzyme to convert inactive steroids, especially estrogens, to active forms. Local production of estrogens by steroid sulfatase may be beneficial for maintaining bone cell growth but may be harmful for breast tissue by stimulating hormone-dependent cancers. The purpose of this study was to examine the effects of two steroid sulfatase inhibitors, DU-14 and EMATE, on this enzyme in bone (MG-63) and breast cancer (MDA-MB-231) cell lines. Effects of the inhibitors were analyzed through whole-cell and microsomal steroid conversion assays, using radiolabeled precursors. Both inhibitors were able to block steroid sulfatase activity of both cell lines. Steroid sulfatase was also analyzed in the two cell lines by Western blotting using an antibody for steroid sulfatase. The ultimate goal of these experiments is to find inhibitors that block breast cancer sulfatase but not bone sulfatase.

95

Evaluation of Anti-tumor CD8 + T Cell Responses with IFN-γ ELISPOT Assays.

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The enzyme-linked immunospot (ELISPOT) assay is a sensitive technique that detects and quantifies T lymphocytes forming cytokine spots after antigen recognition. In particular the IFN- ELISPOT assays measures the frequency of T cells that produce IFN-γ specifically in the presence of an epitope presented in the context of the relevant HLA molecule. Here, we have used the HLA-A2-restricted clone 4/43 derived from peripheral blood lymphocyte (PBL) of one melanoma patient to assess its capability to specifically recognize the HLA-A2-restricted epitope Melan-A/MART-1 27-35. We have also tested the capability of clone 4/43 to recognize HLA-$A2^+$/MART-1^+ melanoma cells (i.e. the normally processed and presented epitope). We have further used CD8+ T cells isolated from PBLs of HLA-$A2^+$ melanoma patients to measure the frequency of circulating antigen-specific CD8+ T cells recognizing antigen-presenting cells (T2.DR4 cells) pulsed with Melan-A/MART-1 27-35. Spot numbers and spot sizes were determined with computer-assisted video image analysis.

96

Computational Study of the Counterion and Solvent Effect on Stereoselectivity in S_N2 Reactions of Cyclic Nitrile Anions

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Nitrile functional groups see extensive use in organic synthesis due to their electron withdrawing power, low steric interactions, and ability to stabilize cations, anions, and radicals. The stereochemistry of a product involving a nitrile anion is influenced by the presence of specific cations and the use of specific solvent. To determine the role of counterions and solvent on the S_N2 reaction of chloromethane with asymmetric cyclic nitrile anions (1-cyano-2-methylcyclohexane anion and 1-cyano-2-methylcyclopentane anion) we performed electronic structure calculations using HF/6-31+G* and MP2/6-31+G* model chemistries. Reactants, transition states, and products were optimized to map the energy pathways of these reactions. We explored how counterion and solvent affect activation energies and stereoselectivity of these systems by studying them in the gas phase, then with a Li^+ counterion, and finally with both Li^+ counterion and three explicit tetrahydrofuran (THF) solvent molecules.

97

A Model Based Analysis of Steady-State versus Dynamic Aspects of the Relationship between Calcium and Force

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Although the calcium-force relationship is dynamic (i.e., calcium-induced force generation is not instantaneous) during physiological contractions of cardiac muscle, this relationship is often studied only under steady-state conditions. We used a mathematical model that links intracellular free calcium and force to investigate how dynamic and steady-state aspects are affected by perturbations of three cellular processes: calcium binding kinetics, crossbridge kinetics, and cooperativity. Model parameters corresponding to the three processes were systematically varied. Indices describing steady-state and dynamic aspects were quantified using the model-based solutions. Results indicate that changes in all three processes affected both steady-state and dynamic aspects; however, the relative sensitivity of changes in the dynamic aspects were significantly greater (2.3-21.4 fold increase, $P = 0.011$). Thus, the dynamic aspects of calcium-force relationship are physiologically important in cardiac contraction and the model-based analysis may help guide future experimental work in this area.

98

The Identification and Quantification of Botanically Significant Volatile Organic Compounds

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Abstract: Volatile organic compounds (VOCs) play a vital role in the lifecycles of plants. Their role in attracting pollinators and aiding in the interaction between plants, insects, and surrounding environment has aroused interest. Non-invasive VOC analysis offers the most accurate portrayal of plant metabolic processes. Utilizing a Flowing Afterglow mass spectrometer, VOCs released from plants can be identified and quantified via chemical reaction mass spectroscopy (CRMS). The ability to analyze VOC emissions from plants depends upon the assessment of the following questions: (1) Can CRMS methods detect and differentiate the presence of multiple VOCs? (2) What is the lowest level of detection? (3) How can current techniques be improved to optimize analysis? (4) Which reagent ion can improve in the detection of VOCs? The data collected from these experiments will assist in the optimization of detection methods of VOCs for future analysis of plant emissions.

99

Debate of Pyramidal versus Planar Acetonitrile Anion

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The issue of acetonitrile anion pyramidalization with and without the lithium counterion was investigated at different levels of theory using Gaussian 03. Acetonitrile anion (Cs and C2v symmetry) and the anion with the lithium counterion (Cs and C2v symmetry) was optimized using Hartree-Fock (HF), Becke three-parameter exchange functional and the non local correlation functional of Lee, Yang and Parr (B3LYP), and second-order Moller-Plesset (MP2) theory with the 3-21G, 6-31G(d), 6-31+G(d), and 6-311++G(3df,2p) basis sets. The pyramidal and planar structures of the acetonitrile anion are found not to be Lewis resonance structures with each other. In fact, the planar structure is found to be the transition structure for the inversion of the pyramidal anion.

100

Rotation of Oscillating Waves in Electroencephalograms

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The neurons of the brain communicate by electrical signals known as action potentials. For signals to propagate, separate parts of large neural networks must fire in different patterns. This results in waves that oscillate over the surface of the brain. Electroencephalograms can capture these electrical oscillations, and rotations of these oscillations are often observed. Modeling the movement of these oscillating waves would be useful in better understanding information processing. The best model for this network is one in which there are n oscillating points on a sphere. For a simpler model, XPPAut was first used to model the dodecahedron, a solid which places 20 points equidistant on a sphere's surface, with each point coupled to its neighbors. Oscillators tend to synchronous movement, where each oscillator in the network ultimately mimics every other oscillator. Our model determines when the oscillators move synchronously and when they move non-synchronously on a sphere's surface.

101

Protein Stability of a 21 Residue Alanine Based Peptide

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The central dogma of biochemistry today is to understand how proteins go from a chain of amino acids to a 3-dimensional folded structure. It is well known that the stability of proteins is strongly affected by ion interactions, hence the conformations that a protein may adopt depend on the environment. A short polyalanin 21 residue peptide, immersed in different environments, has been studied, through molecular dynamics, to understand the role ions play in peptide stability. This knowledge will be useful in understanding the folding problem for much larger proteins. Computer simulations were ran using the same peptide in Na_2SO_4, $NaCH_3COO$, and Na_3PO_4 salt solutions. AMBER9 was used to perform the molecular simulations and the goal was to identify which salts would stabilize and which would destabilize the protein and why.

103

Biocompatibility Evaluation of the Levitronix PediVAS in Ovines

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More than 1,000 children annually could benefit from ventricular assist device (VAD) support. However, there are currently no FDA approved VADs for infants in the United States. The Levitronix PediVAS is a magnetically-levitated rotary blood pump currently under development that could provide cardiac support for these patients. This device is currently undergoing pre-clinical studies in ovines to assess cardiovascular performance and biocompatibility. Platelet activation was measured by quantifying p-selectin positive platelets and platelet microaggregates using flow cytometry during the course of the implant. Platelet activation markers increased following surgery and remained elevated for the entire study. This suggests that the pump is causing ongoing platelet activation. Necropsy results did not indicate the presence of kidney infarcts; however, ring thrombus was noted at the pump/cannula junction. The Levitronix PediVAS provided cardiac support for 30 days in an ovine without end-organ infarcts, suggesting that it may possess acceptable biocompatibility.

102

Integrated Laboratory: Proteomics Peptide Mass Fingerprinting (PMF) Using Mass Spectrometry Measurements and Identification Through Bioinformatics

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A challenging lab assignment for undergraduates has been produced, familiarizing students with a widely used protein/peptide identification technique in the field of proteomics, peptide mass fingerprinting (PMF), and introducing them to Agilent’s Time-of-Flight Mass Spectrometer, configured with an electrospray ionization source and a matrix assisted laser desorption ionization source. Three known protein standards had been selected: Bovine Serum Albumin, Cytochrome C, and Lysozyme, one of which would be used by students to learn to perform their own standard protein digestions with Trypsin or Lys-C. This digest, in addition to commercially available “digested peptide mixtures” would be run through the TOF-MS, and subsequently analyzed, identified, and compared based on peptide fragmentation patterns. The students would then be provided with one of several unknown proteins: Ubiquitin, Transferrin, Myoglobin, or Insulin. They would now be able to perform their own digestions, run their digestion on the instrument, and analyze and identify their results.

104

Using Probabilistic Methods and Ordinary/Stochastic Differential Equations to Simulate Biological Processes

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Agent-based models are used for simulating cellular and subcellular processes because they are straightforward to visualize and use and easily extensible. BioLogic is an agent-based simulator of cells, which adapts to the high variability of experimental data by simple logical variables such as high, low, or none. Extensions were added to the simulator to be able to simulate reactions using 1) probabilistic models, when the number of agents is small 2) stochastic differental equations, when the number of agents is moderate and 3) ordinary differential equations when the number of agents is large. Ideally, the algorithm shold use a combination of the three methods for maximal eficiency. In the probabilistic model we calculate probablities for reactions baed on rate constants and the law of mass action. Both the stochastic differential equations as well as the ordinary differential equations models use Euler's method to approximate the solution. The software uses as input descriptive XML files to represent the hierarchy of structures within the simulation environment and regular text files to define the reaction rates.

105

Approaches in Heart Valve Tissue Engineering

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As the application of biomechanical stimuli to developing tissue has shown to be beneficial in terms of overall tissue properties, custom-built devices, termed bioreactors are designed so that they can provide appropriate mechanical conditioning to the engineered tissue. In heart valve tissue engineering applications, a bioreactor was successfully designed and used by Engelmayr et al [1]. This bioreactor subjected engineered tissue samples to flexure, flow and stretch modes of mechanical stimui [2]. In this project, we focus on this bioreactor design and proceed with relevant cell/tissue culture followed by engineered valvular tissue development. As a clinically viable cell source, we made use of ovine bone marrow mesenchymal stem cells. These cells were used to seed strips of nonwoven 50:50 blend poly(glycolic acid) (PGA) and poly(l-lactic acid) (PLLA) scaffolds. Seeded scaffolds that underwent mechanical conditioning were compared to static controls. Relevant assays to measure cell extracellular matrix production and density were performed. These results are their interpretation are discussed.

106

Designing a Computational System to Predict Protein-protein Interactions in *Arabidopsis Thaliana*

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Proteins are unique amongst organic compounds in supporting every reaction occurring in biological systems. It is important to identify the structures and understand the dynamics and functions of proteins. Further, it becomes essential to understand the mechanism by which a set of proteins communicate and collaborate toward a common cellular function. There are several genomic and proteomic databases that maintain valuable information for model organisms. These databases can be used to ease and optimize the task of predicting protein-protein interactions. Moreover, various computational methods are utilized to identify interactions. Recent studies conducted by Yanjun Qi, Ziv Bar-Josepth, and Judith Klein-Seetharaman indicate that the Random Forest (RF) classifier performed the best in terms of accurately predicting interactions in yeast. The results from previous studies and online-databases such as The Arabidopsis Information Resource (TAIR) and Biomolecular Interaction Network Database (BIND) will be employed to construct a proteome of the model organism *Arabidopsis Thaliana*.

107

Winter Flounder Antifreeze Protein: Examining its Water Distribution in Bulk Water to Compare with Previous Studies of the Protein Adjacent to Ice

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Antifreeze proteins (AFPs) are a unique class of proteins that inhibit ice growth without changing the melting point of ice. The specific properties that are responsible for this novel ability to inhibit ice growth are unknown. One hypothesis is that the water distribution around the AFP in bulk water is similar to the protein adjacent to ice. A molecular dynamics (MD) simulation of an AFP in explicit water box has been carried out using AMBER9. To test the above hypothesis we have analyzed the MD simulation by calculating the water distribution data and the hydrogen bonding profile.

108

Determination of the Effects of Parathyroid Hormone Related Protein on Cell Cycle Regulators to Enhance β-Cell Proliferation

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Diabetes is a disease that results from the body's inability to produce insulin due to insufficient functional pancreatic β-cell mass, or the inability to use insulin properly, or both. Parathyroid hormone related protein (PTHrP) is known to enhance functional β-cell mass in mice by increasing β-cell proliferation. It is also known that PTHrP mediates its proliferative effect on the β-cell through activation of the atypical Protein Kinase C (PKC) signaling pathway. However, nothing is known regarding the regulation of cell cycle molecules by PTHrP in the β-cell. Based on the effects of PTHrP on cell cycle regulation in other cell types, we hypothesize that PTHrP increases β-cell proliferation through inhibiting cell cycle inhibitors. Therefore, this study examines the effects of PTHrP on the expression of members of the Cip/Kip and INK families of cyclin-dependent kinase inhibitors.

109

The Induction of Mixing in Microcapsules Using Internal Structures

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We aim to simulate induced mixing within microcapsules through the use of internal structures. We use a combination of Lattice-Boltzmann and Lattice-Spring models to simulate both the microcapsules and the fluid that they move in. The capsules are simulated as non-rigid objects rolling along a flat surface, and initially filled with two separate fluids, which are subject only to convection and not to diffusion. Through the use of internal struts of varying numbers and lengths, we find a way to induce fast or complete mixing. Applications for this include using microcapsules for delayed release of medicines and uses as microreactors.

110

The Effects of Surface and Shell Patterning on Microcapsule Movement

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We aim to understand the movement of capsules which are either nonhomogenous or rolling on a patterned surface. These capsules are simulated using both Lattice-Boltzmann and Lattice-Spring models in both two and three dimensions, and are primarily affected by different capsule rigidities or different surface adhesions. This promotes smooth movement in certain situations, while promoting a more staggered movement with other initial conditions. Applications of this research include the use of microcapsules in either biological or artificial vasculature systems.

111

Using Patterned Surfaces to Direct Microcapsules in Microchannels

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Using computational modeling, we simulate the motion of compliant microcapsules on patterned surfaces. The microcapsules, which consist of an elastic shell and an encapsulated fluid, model biological cells or polymeric particles. We focus on a surface that is decorated with a Y-shaped pattern and we vary the relative adhesiveness of the stem and the two branches of the Y. The capsules are driven to move over this substrate by an imposed fluid flow. Upon reaching the junction point, we find that certain capsules preferentially move onto one branch, while other capsules move onto the other. Thus, through their inherent interactions with the patterned domains, the microcapsules are driven to "make decisions" about their path along the surface. Such surface patterning provides a facile means of routing particular capsules to specified locations in microfluidic devices and can form a fundamental component in creating fluidic circuits where microcapsules carry out simple logic operations.

112

Iron Porphyrins as Model Compounds for Hydroxylamine Oxidoreductase (HAO)

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Hydroxylamine oxidoreductase enzyme (HAO) of *Nitrosomonas europaea*, a soil bacterium, oxidizes hydroxylamine to nitrite through a two electron transfer reaction. The active site of this enzyme is believed to contain a specific metalloporphyrin, heme P460, that possibly contains an ortho-substitued tyrosine. The two electron transfer of heme P460 is not yet understood because previously studied hemes are only capable of singular electron transfer. In order to model the natural heme P460 system, a systematic study of ortho-substituted metalloporphyrins has been undertaken. The research presented focuses on the reaction of chloro-iron(III)dimethoxyphenylporphyrin ClFe(DMP)P with hydroxylamine. The hypothesis is that the methyl group of ClFe(DMP)P that forms the ether substituent serves as a protecting group for the oxygen, causing a reaction similar to that of chloro-iron(III)tetraphenylporphyrin ClFeTPP, resulting in the formation of (NO)FeTPP and (NO)Fe(DMP)P.