

2008 Summer Research Symposium

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Looking at an Oscillating Wire in a Soap Film Flow

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A stationary wire in a two-dimensional flowing soap film creates a wake of vortices with its own natural shedding frequency. By oscillating the wire transverse to the mean flow of the soap film using an alternating current and a magnetic field around the wire, the vortex shedding can be altered depending on the frequency and amplitude of the driven oscillations. A study by D. J. Olinger and K. R. Sreenivasan has demonstrated that the transition from regular to chaotic vortex shedding can be induced and accounted for by a sine-circle map. By implementing experiment in a two-dimensional soap film, we attempt to link the spatial patterns of vortices with their temporal fluctuations.

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First Order Corrections of pKa Values for Crystallization Optimization Trials

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Crystallization of a macromolecule involves careful manipulation of environmental parameters to form a crystal lattice with a high degree of internal order. Utilizing a combination of parameters surrounding a successful crystallization, crystallographers systematically vary one or two parameters across a grid screen via programming of a crystallization robot. Application of a grid screen can pose errors in accuracy and precision. To avoid such errors, use of the four corners method is preferred. Recent experiments using the buffer BTP have produced results exhibiting minimal accuracy. Concentration and pH were varied across a grid screen; however, measured pH values digressed from target values beyond the permitted ± 0.05 units. This issue can be attributed to the use of an acid dissociation constant for a solution subject to nonideal behavior. To eliminate this discrepancy, an application of the Henderson Hasselbalch equation and Taylor Series will be used to correct the error in the pKa.

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Kinetics of Growth and Chromium Reduction in *Geobacter metallireducens* and *Sulfurospirillum barnesii* Grown on Nitrate and Chromium

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Chromium is used in a wide variety of industrial processes. Chromium (III) is required in trace amounts for sugar metabolism. Chromium (VI) however is very toxic and mutagenic. This study investigated the ability of two metal-reducing bacteria, *Geobacter metallireducens* and *Sulfurospirillum barnesii*, to grow on nitrate while reducing chromium (VI) to chromium (III). A procedure for measuring total chromium content was adapted using potassium permanganate to oxidize chromium (III) to chromium (VI), and diphenylcarbazide to measure the chromium (VI) content. Ferric citrate, a component of the growth media, was found to reduce chromium. Chromium (VI) inhibited the growth of *G. metallireducens* growth, but was rapidly reduced by *S. Barnesii*.

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Synthesis of Novel Cyclic Amino Acids with Basic Side-chains

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The final shape of a protein following the folding process determines the function this protein will perform. Folded peptide chains are stabilized in their three-dimensional structure by various intra- and intermolecular interactions, including disulfide bridging. We are interested in looking at how slight changes in the sequence of several small disulfide-rich peptides (our studies focus on the family of α -conotoxins) affect their folding properties and their biological characteristics. In this study we are attempting to synthesize two novel cyclic amino acids, 4-(2-aminoethyl)-L-proline and 4-guanidino-L-proline. These novel amino acids have the ring structure that proved to be important for the appropriate folding of α -conotoxins tested, and at the same time contain a basic side-chain that was shown to be essential for the higher biological activity of most α -conotoxins reported in the literature.

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Development of a colorimetric method to quantify a his-tagged peptide on submicron particles

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The goal here is to develop a quantitative method to enumerate a his-tagged peptide ligand on particles fabricated from the polyester PLGA and nickel-chelating lipid DOGS-NTA-Ni. The overall objective is to construct nucleic acid delivery systems targeted to antigen-presenting cells expressing MHC class II molecules. The rationale is such systems would be useful tools to modulate immunity in situ by which transplant rejection and autoimmunity can be mitigated. The hypothesis is nickel-decorated particles (PLGA-Ni) would compete with nickel-bound horseradish peroxidase (HRP) for the his-tagged peptide VHA-His6, a ligand of the MHC II molecule I-Ad. The experiment was designed to use the enzymatic activity of HRP as the readout to determine the free VHA-His6 not occupied by PLGA-Ni. In this way, the color reaction can be correlated to the number of VHA-His on PLGA-Ni using a standard curve. If successful, this method may be used to develop targeted drug delivery systems.

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Nucleic Acid Sequencing & Community Level Physiological Profiling of Oligotrophic Bacteria from Tytoona Cave

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Despite their oligotrophic character, caves serve as a habitat for diverse microbial communities; although the method by which microbial organisms sustain themselves in a nutrient poor environment remains largely unknown. Samples collected in Tytoona cave, PA, were used to extract genomic DNA from the bacteria present on the cave ceiling. It is often cited that while ~1% of bacteria are culturable, the vast majority are not culturable but may be identified by their DNA sequence. PCR amplified DNA, representing the 16S and 23S ribosomal RNA genes, was cloned in a plasmid vector using *E.coli* as a host. The variety of PCR products was determined by variations in size of the DNA using gel electrophoresis. Plasmid DNA was submitted for sequencing and DNA sequence information was used to identify and classify cave bacteria. A CLPP study was undertaken to determine the biochemical lifestyle of the bacterial consortium present on the ceiling.

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Development of a ENMR-MoCExSy System for studying Protein Interactions in Proteomic Samples

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A novel method of 2-D Electrophoretic Nuclear Magnetic Resonance Mobility Correlation Exchange Spectroscopy (ENMR-MoCExSy) is developed and implemented. ENMR-MoCExSy is a new method combining current multi-dimensional NMR techniques with electrophoresis for the purpose of studying protein interactions in proteomic samples such as blood or urine. ENMR-MoCExSy will allow for fast screening of protein interactions in a proteomic solution, the most notable application of which is the early detection of cancer cells. We develop a prototype NMR probe, along with a radio-frequency coil and gradient coil for use with a 600Mhz Bruker NMR Magnet in order to test the design. The NMR signals of the proteins from a proteomic sample will be modulated with two independent cosine factors as the two electric field amplitudes are incremented independently. Twice Fourier transformations with respect to E_x and E_y will generate a 2-D ENMR-MoCExSy spectrum illustrating interacting proteins co-existing in the proteomic solution.

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Application of Diffusion Monte Carlo Methods in Chemistry

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Diffusion Monte Carlo (DMC) is a method to solve Schrödinger's equation. Unlike the popular Hartree-Fock and Density Functional Theory methods, it provides more exact particle wave functions. We began exploring the application of DMC to the harmonic oscillator and hydrogen atom. For each case, a program, successfully employing the DMC method, has been written. Next we investigated the impact of more exact particle wave functions on simulated molecular systems such as small water clusters, and compare Diffusion Monte Carlo with other electronic structure methods. We focused our efforts on water clusters $n=2-8$ where n is the number of molecules. We are developing a program to generate the necessary input for Qwalk, a QMC program, from a Gaussian calculation.

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The Science of Design

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Duquesne University, and the Regenerative Medicine Partnership in Education (SEPA) has helped me to build a professional portfolio, and has given me professional work experience in the field of graphic and print design. It has also given me a chance to practice using Photoshop, and to learn new Adobe programs, such as Illustrator and InDesign. Working together with scientists, educators, writers, artists, animators, and other multimedia art interns I have had the opportunity to design posters, cd and dvd covers, and logos for several different projects, including the Immun-ologee online game, The Brain Show movie, and Darwin 2009. The design for these different projects were a significant departure from design work that I have done in the past. Each required much more research and creative thought, and a basic understanding of the biology portrayed, because each had to be artistic and professional, as well as historically and scientifically accurate.

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Darwin 2009: Footprints of Our Past Bridging Our Future

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The Darwin 2009 team has designed innovative educational materials for Pittsburgh cultural institutions that will enhance knowledge of revolutionary naturalist, Charles Darwin. With these materials, visitors will be able to acquire understanding of the biological principles of evolution. We have developed easy-to-use classroom materials for teachers as well as students. Furthermore, we have added new displays and programs to institutions, such as the Pittsburgh Zoo and PPG Aquarium and the National Aviary. Together, these assets will help science content come alive, rather than remain limited to the classroom. Researching the various institutions' goals and meeting personally with educational directors, the Darwin 2009 team has made a collaborative effort to create a multidisciplinary approach to teaching evolution by individualizing all activities to fit each institution's personality. By making science fun and exciting, Darwin 2009 will foster a desire to learn science both in the classroom and out, while simultaneously teaching evolution.

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Transposable Element-Induced Mutations of the Lazy Gene in Maize

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Mutations that disrupt the gravitropic response of maize are termed "lazy". The *lazy-1* gene associated with such behavior was characterized as a simple, recessive mutation. Our laboratory is characterizing mutations of three sources: chemically induced using EMS (Ethyl methanesulphonate), spontaneous, and by transposon mutagenesis. The most widely used transposons in maize, *Mutator* (*Mu*) elements, have conserved ~210 bp terminal inverted repeats but unique internal segments of 1-5 kbp, which determine the family of the particular element. The *Mutator* transposable element system was the source of mutation *lazy^{*}-MTM4659*, a mutation having a phenotype similar to other *lazy-1* mutations. We are characterizing this mutation and *Mutator* elements from the MTM line to identify the type of *Mu* insertion in this allele. By using PCR primers that anchor *Mu* ends to the *lazy-1* gene and analyzing the genomic sequences of the products, the molecular basis of this mutation will be determined.

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Flipping Bits - Electron Spins and Quantum Computers

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It has been proposed that electron spins could serve as quantum bits in a quantum computer. However, much research must be done to learn how we can manipulate these electron spins. We have experimented on the spin lifetime of single electrons in GaAs quantum dots by using a technique known as time-resolved Kerr rotation. In this effect, the linear polarization angle of reflected light is rotated by an amount that depends on the electron spin direction. Measuring this angle as a function of time (or "time resolving" it) enables us to see how electron spin quantum information decays. These measurements provide information about quantum gate operation times and design constraints for a quantum computer.

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SAMs on Stainless Steel 316L Components

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Monolayers are deposited on surfaces to protect the integrity of the surface by inhibiting corrosion. Corrosion is a common problem in water-contacting applications such as stents, docks and pipelines. Here the monolayers of octadecylhydroxamic acid on stainless steel components were studied. Different deposition methods were tested on the components of stainless steel to determine which was most effective in adhering the film to the surface. Variables that affect the adherence of the monolayer are deposition time, solution temperature and monolayer concentration. These were manipulated to find the best deposition method. As concentration and deposition time increased so did the bond strength of the monolayer to the metal surface. Also when the temperature differential between the substrate and monolayer was increased the bonding strength improved. The alkyl chain ordering and bonding were evaluated by infrared spectroscopy, contact angle measurements and MALDI-TOF mass spectrometry.

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Three-dimensional Visualization of the Orientation of the Extracellular Matrix Fibers of Rat Urinary Bladder Wall Tissues

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In recent years, bladder research has increased in popularity due to the high numbers of individuals suffering from bladder related problems. This project examined fiber orientation in decellularized bladder tissue. Bladders that had been injected with silicone were first decellularized, and then their 3D surfaces were scanned using a FARO laser arm. The fiber orientations were determined using a 2D light scattering technique, and the next step of this project will be to develop a means of mapping the 2D data back to the 3D surface map in order to visualize the fiber orientation for the entire organ. By repeating this process with varying silicone volumes, the changes in the fiber architecture will be visualized, as the bladder fills. Eventually, a constitutive model of the bladder wall tissue, including the fiber orientation of the extracellular matrix, will be formulated which will then assist to predict effects of modified variables.

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Mathematical Modeling of Ant Pheromones: Determination of Optimum Pheromone Evaporation Rate and Simulation of Pheromone Tracking Abilities

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Pheromones are a major form of communication and are known to aid in the foraging ability of ant colonies. In an environment with limited food, it would be optimal for the pheromones to evaporate over time to prevent ants from following a trail to a diminished food source. In the case of an unlimited food source, it would be optimal for the pheromone not to evaporate. With a certain probability of food appearing in an environment, it was proposed that there is an optimum pheromone evaporation rate allowing the colony to bring the most food back to the nest. Using NetLogo, a programmable agent based program, it was determined that there is an optimal evaporation rate. This idea was also modeled with differential equations which facilitated the dependence of the optimum on different parameters such as the rate of appearance of the food, colony size, and amount of food.

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Trace Detection of Fluorescently Tagged Primary Fatty Acid Amides (PFAMs) Using HPLC Coupled with Fluorescence Detection

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Lipidomics, the quantitative study of lipids, is inclusive of primary fatty acid amides (PFAMs), which are of great biochemical importance. PFAMs are present in specific areas of the human body including the brain, heart, and fatty tissue, and have been shown to demonstrate a variety of physiological effects such as sleep induction, vasodilation, and anti-cancer qualities. However, PFAM detection is challenging due to their very low concentration in the body (sub-micromolar). In this work, PFAMs are converted to their conjugate amines and subsequently tagged with the fluorophore 3-(2-furoyl)-quinoline-2-carbaldehyde (FQCA). FQCA exhibits strong fluorescence intensity when reacted with amines, and displays a very weak native fluorescence as compared to other fluorophores. A highly sensitive fluorescence detector coupled with HPLC has detected amine separations at nanomolar concentrations and is being optimized for picomolar detection. Once the detection limit has been determined, the future work will involve using microfluidic chip technology.

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Copper Catalyzed Atom Transfer Radical Addition of Chloroform to Alkenes in the Presence of Air

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The process of adding polyhalogenated compounds to alkenes using radical means was first achieved in the early 1940's. This reaction is typically catalyzed using transition metal complexes. Until recently, the principal drawback of this useful synthetic reaction was relatively high amount of transition metal catalyst required to achieve high yield of the monoadduct (10-30 mol%). Recently, the solution to this problem has been found for copper mediated ATRA through the use of reducing agents such as free radical initiators (e.g. 2,2-Azobis(2-methylpropionitrile) or AIBN). This work extends on previously reported methodology for copper regeneration in ATRA and examines the effect of air. Copper catalyzed ATRA of chloroform to various alkenes in the presence of AIBN and air was found to be as efficient as the reactions conducted under air free conditions, indicating that AIBN was capable of not only regenerating the copper(I) catalyst, but also consuming oxygen and other inhibitors from the reaction mixture.

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Ultrafast Optical Measurements

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In many applications involving pulsed lasers, it is important to know the duration of the laser pulse being used. However, determining the intensity profile and pulse length of ultrafast lasers presents a challenge: measuring a fast event in time with good resolution requires an even shorter event. One method of overcoming this obstacle is optical autocorrelation, in which an individual beam is split and recombined with itself; the resulting measurement by a slow detector allows information about the laser's character to be extracted. Here, I apply autocorrelation techniques to probe a Ti:sapphire laser and investigate its femtosecond pulses.

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

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Potassium is a cation important for a properly functioning body, especially for nerves, kidneys, and muscles. The goal of this research project is to determine the concentration of potassium in muscle tissue. It seeks to verify a connection between the concentration of potassium in muscle tissue and previously recorded data gathered through an adaptation of the whole body counting method. Atomic emission spectrometry was utilized to analyze the samples. A method was formulated to digest the meat samples through the use of freezing in conjunction with grinding using a mortar and pestle, followed by soaking the meat in HCl acid. The potassium readings were within the previously reported range of 1.9 g potassium for each kilogram of adipose tissue to 3.1-3.5 g/kg in muscle tissue. We obtained a range of potassium concentration from 2.15-3.14 g K⁺/kg of beef sample depending on digestion time and individual samples.

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Development of a New Fluorescent Lead SensorLauren Marbella, Barbara Serli-Mitasev, Partha Basu
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Lead toxicity is one of the most common environmental problems in the United States.¹ Complications due to lead exposure can affect virtually every soft tissue in the body. Thus, the ability to detect small amounts of lead is of paramount importance. We have developed a new fluorescent molecule, MeLbzSSO, which showed potential as a lead sensor. This molecule has a thiol-based binding site,² and thus differs from other fluorophores with more hard donors such as oxygen or nitrogen. In this presentation, we will discuss the details of the synthetic strategy and characterization, fluorescence efficiency, lead binding affinity, and the selectivity against other ions in aqueous solution.

He, Qiwen; Miller, Evan W.; Wong, Audrey P.; Chang, Christopher J. *J. Am. Chem. Soc.* 2006, 128, 9316-9317.

Basu, Partha; Serli-Mitasev, Barbara. *Composition, Synthesis, and Use of a New Class of Fluorophores*. 2008. Patent pending.

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Speciation of Arsenic and Selenium in Chicken Tissue Using Enzymatic Extraction Followed by IC-ICP-MS

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In this study, a method was developed for the simultaneous speciation of arsenic and selenium in chicken tissue. Extraction of arsenic and selenium was achieved using Protease XIV from *Streptomyces griseus* at pH 7.5 and 37 °C during 20 h. Extracted arsenic and selenium species were separated using an ion-exchange chromatography column and analyzed using ICP-MS. For total analysis on ICP-MS, microwave-assisted acid digestion using EPA method 3052 was used. Analysis of chicken tissue was validated by analyzing CRM DOLT-3 dogfish liver. The total arsenic concentration was 126 ± 12 µg/kg and the total selenium concentration was 723 ± 27 µg/kg for chicken tissue. The extraction recoveries for arsenic and selenium were 45% and 88%, respectively. In all samples, the majority of arsenic present was in the form of arsenobetaine (a non-toxic arsenic species), while the majority of selenium present was in the form of selenomethionine (a selenium-containing amino acid).

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The Using of Computer Module by Health Care Providers in Management of SCD

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Sickle Cell Disease (SCD) is an inherited disease, which has adverse effects on hemoglobin in the red blood cells. SCD is associated with excruciating pain crises. The education of health care providers in treating this disease is vital to the patient's quality of life and also to eliminate the negative stereotypes behind the use of opioids to treat SCD

Materials and methods: Using a computer based virtual patient module for health care providers who are treating SCD patients has been created. This module is being piloted with residents at Children's Hospital of Pittsburgh. Learners are asked to answer identical pre-module and post-module question regarding SCD Patient treatment followed by a questionnaire designed to determine the impact of this virtual module on the knowledge, attitude and practice as related to the management of SCD related pain by health care providers.

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Darwin 2009: A Year of Education and Celebration

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The year 2009 celebrates the 200th anniversary of Charles Darwin's birthday and the 150th anniversary of the first publication of Darwin's *On the Origin of Species*. Through the collaboration of the Regenerative Medicine Partnership in Education (www.sepa.duq.edu), an exhibit is being designed for Phipps Conservatory and Botanical Gardens. The display, "Family Trees," combines the ideas of Darwin, Gregor Mendel, and Reginald Punnett. Planted Punnett squares, plant pyramids, and a chalkboard activity allow patrons and students to learn about basic plant genetics and reproduction. Additionally, pre-visit lessons, post-visit lessons, and docent-led classroom lessons have been created to better convey all of these concepts to the students. Overall, the Darwin 2009 celebration is aimed at educating patrons and students about Charles Darwin and his most important contributions to the world of science. At Phipps Conservatory and Botanical Gardens, this is accomplished through the implementation of the aforementioned display and corresponding lesson plans.

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Destabilization Effects of Sulfate on a Poly-Alanine Peptide

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Peptide-based drugs have been developed to potentially treat various forms of cancer, HIV, and other diseases. The α -helix secondary structure of peptides can access cells via crossing the cell's lipid bilayer. The α -helix is not always thermodynamically stable under physiological conditions. The presence of specific salts can destabilize the α -helix causing it to unfold. In this project (de)stabilization effects of the sulfate ion on a poly-alanine peptide (AP) containing three arginines, AAAAA(AAARA)₃A, were investigated using the AMBER ff99SB force field, which was optimized for alanine peptides. Three 100 ns long molecular dynamic simulations were performed for AP in 0.2M sodium sulfate solution. A destabilization effect was found; the α -helix started to unravel at approximately 4.8 ns. The mechanisms of this destabilization were investigated through ion-distribution functions, phi-psi relationships, and VMD. Initial ion distributions are similar to that observed in vacuum-liquid interfacial simulations.

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Improving Science Literacy at Pittsburgh Educational Institutions

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Science is an important part of every child's education. Unfortunately, the educational system in the U.S. is doing little to prepare students for careers in science. The U.S. is ranked 29th out of 57 in science and math literacy, well behind other developed nations (Programme for International Student Assessment, 2006). In order to increase the U.S.'s science literacy rate, new steps must be taken to develop informative and effective curriculum. The goal of my work this summer is to provide teachers with alternative lesson plans or teaching methods that fit the government issued standards, while also providing a fun and effective learning environment that fosters science literacy. The lesson plans being created this summer will focus on Darwin's fundamental principle of biology, evolution. Through research and collaboration with Pittsburgh educational institutions, it is my hope that the materials I am developing will help science educators meet government standards and improve science literacy.

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Atmosphere Characterization and Removal in the Atacama Cosmology Telescope

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The Cosmic Microwave Background (CMB) is a source of blackbody radiation at a mean temperature of 2.7 degrees above absolute zero with nearly equal intensity from all sky directions. One of the primary pursuits of microwave astronomy over the past decade has been measuring tiny temperature variations with direction, which encode the initial density perturbations in the universe. Current ground-based efforts to map the microwave temperature fluctuations on arcminute angular scales are contaminated by noise in the form of atmospheric turbulence. An algorithm has been investigated and developed to resolve the current dilemma of atmosphere distortion in microwave astronomy. These techniques were applied to data from the Atacama Cosmology Telescope (ACT) which was taken in November and December, 2007.

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Crystal Engineering: Crystal Structures of Metal Complexes as a Function of the β -Diketonate Ligand and the Difunctional Nitrogenous Base

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Coordination compounds containing cobalt(II) hexafluoroacetylacetonate and a bridging ligand are being developed and characterized. A nitrogenous base (such as pyrazine, quinoxaline, or phenanthroline) is reacted with the cobalt(II) hexafluoroacetylacetonate in an attempt to form a polymer chain. The observed products are a function of the nature of the nitrogenous base. The ligand exchange reactions of β -diketonates in the presence of a nitrogenous base also are being investigated. The exchange reaction is used to synthesize and characterize metal complexes (where metal = Mn(II), Co(II), Ni(II), or Pd(II)). Acetylacetonato ligands have been shown to exchange with dibenzoylmethane and 1,3-Bis-(4-methoxyphenyl)-1,3-propanedione. The structures of the resulting complexes were determined by single crystal X-ray diffraction. Reflectance and Infrared spectral data are presently being collected to verify the groups present. Crystallization from mixed solvents by slow evaporation was used to form the complexes.

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Developing Tools for *in vivo* Transposon Mutagenesis of *Streptomyces coelicolor*

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Streptomyces coelicolor is a sporulating soil bacterium with a unique and complex life cycle. The cell division genes of *S. coelicolor* are not required for growth and viability, unlike in other bacteria such as *Escherichia coli*. This unique property allows the isolation of mutants with many interesting macroscopic phenotypes. In our laboratory, previous transposon mutagenesis research has focused on using protoplast transformation to introduce specially constructed suicide vectors into *S. coelicolor* in order to identify mutants with insertion mutations. This system employed mini-*neo* and mini-*apra* transposons derived from Tn5. Conjugation is an attractive alternative method of introducing a suicide vector. Currently, I am modifying previously made vectors with better selectable markers in order to introduce mini transposons via conjugation. These tools can be used to identify new cell division genes in *S. coelicolor* and related species with recently determined genome sequences.

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The Nature of Coordinate Covalent Bonding from a Lewis Base Perspective

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The factors that control the coordinate covalent bond strength have been investigated using Truhlar's new generation of hybrid meta-generalized gradient functionals M05-2X and M06-2X with the 6-311++G(3df,2p) basis set. Weinhold's Natural Bond Orbital Analysis program was utilized to study the stereoelectronic influences (hyperconjugation) that regulate the strength of coordinate covalent bonds formed between boron Lewis acids and substituted carbonyl compounds (Lewis bases). Specifically, the hypothesis that $\pi(\text{C}=\text{O}) \rightarrow \sigma^*(\text{B}-\text{X})$ ($\text{X}=\text{H}, \text{F}$) contributes to the coordinate covalent bond strength as a primary effect was investigated. The results are discussed in terms of a linear combination of the resonance (R) and field (F) constants.

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Mossbauer Study of the $x\text{Cr}_2\text{O}_3-(1-x)\alpha\text{-Fe}_2\text{O}_3$ nanoparticles system

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The $x\text{Cr}_2\text{O}_3-(1-x)\alpha\text{-Fe}_2\text{O}_3$ nanoparticles system was synthesized hydrothermally for $x=0.0$ to $x=0.9$. Mössbauer spectroscopy was performed on the obtained samples as well as for samples subjected to thermal annealing at 550 C for one hour. At $x=0.1$, the as obtained samples began showing superparamagnetism and became completely superparamagnetic after $x=0.4$ concentration. The percent of the sample that was superparamagnetic increased with Cr_2O_3 substitution. This correlates with chromium decreasing the particle size of the powder. The thermally annealed samples appeared to have the hematite structure regrown for concentrations $x=0.1$ to $x=0.4$ with the intensity of the hyperfine magnetic field decreasing with Cr_2O_3 concentration. For $x=0.5$ to $x=0.9$, the percent of superparamagnetic particles increased with Cr_2O_3 concentration, dominating the system by $x=0.8$. This system is believed to have applications in gas sensing and catalysis.

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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. This information includes the surface temperature, the abundances of elements and their ions, the mass of the star, et cetera. Because all of this knowledge comes from a star's spectrum, 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. It is in the event that a star is rapidly rotating that one must find a new way to calculate the star's spectrum. 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 determine through computer modeling how much rapid rotation affects measurements of stellar masses and luminosities.

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Transport coefficients computation in the Van Hove limit and their fluctuations(noise calculations)

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In the Boltzmann theory, transport coefficients are computed from the one-particle Boltzmann transport equation. The distribution function $f(r, k, t)$, in the presence of a field is usually obtained by means of a perturbation procedure. All terms of order higher than the zeroth order (f^0) are neglected in the streaming terms while in the collision terms, the first order (f^1) is retained. The transport coefficients which depend on f^1 are then expressible in terms of the equilibrium distribution f^0 . In contrast to the Boltzmann method, we utilize the many body approach. Using the Van Hove limit, the response of a quantity $B(t)$ to an external field force is expressed in correlation form for the fluctuation $\Delta B(t)$ in the equilibrium system. With the obtained correlation function, the general microscopic expressions are given for the transport coefficients. Utilizing the many body current correlation function $\langle \Delta J(t) \Delta J(t') \rangle$, the $1/f$ noise spectral density is evaluated.

Rule-based Modeling of VEGF SignalingNilgun Yilmaz^{1,2} and James R. Faeder³¹Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA USA²Molecular Biology and Genetics Department, Bilkent University, Ankara, Turkey ³Department of Computational Biology, University of Pittsburgh School of Medicine,

VEGF (*Vascular Endothelial Growth Factor*) is a crucial regulator of angiogenesis, which has an important role in diseases such as cancer and arthritis. Although there are several published models of VEGF binding to its receptors, no models exist that consider events following receptor aggregation. Development of such models may provide comprehensive understanding of the pathway dynamics and assist in developing new anti-tumor drugs and other therapies. Because the number of possible phosphorylation states and signaling complexes can be very large, we develop our model using the BioNetGen software platform, in which objects and their components represent signaling molecules and their functional elements, and rules describe biochemical interactions. We are developing a model including VEGFR phosphorylation sites that couple directly to angiogenesis. The model extends published models for the ligand-induced aggregation of VEGF receptors and co-receptors with the addition of kinase activation, receptor phosphorylation, and recruitment of downstream effectors.

Li₂FeSnS₄: Synthesis of a Quaternary Diamond-Like Semiconductor

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Diamond-like semiconductors (DLS) have attracted increased attention for their potential applications in data storage, computing and optics. Due to their complexity, quaternary diamond-like compounds have yet to be explored to the same extent as their binary and ternary counterparts. Li₂FeSnS₄, a I₂-II-IV-VI₄ DLS, was synthesized using traditional high temperature solid state reactions. A comparison of the product's powder X-ray diffraction pattern with calculated patterns of known DLS structures indicated that Li₂FeSnS₄ crystallizes in space group *Pn*. Additionally, alkali polysulfide flux reactions were carried out to improve the phase purity of the product and obtain single crystals. Characterization of reaction products using X-ray diffraction, diffuse reflectance spectroscopy and thermal analysis will be presented.

Robustness and Statistical Significance of Allosteric Communication Pathways**Derived from Conservation Scores and Markov Propagation Models**Glassford, William J and Chakra Chennubhotla
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University of Pittsburgh School of Medicine

Many cellular processes involve allosteric mechanisms of proteins by which local energetic and conformational changes cooperatively diffuse from ligand-binding site to distal regions across the three dimensional structure. Despite significant efforts, the molecular basis of allosteric regulation remains to be established. Tang *et al* used evolutionary constraints to calculate a set of residues mediating allosteric communication from the binding site of ATP to functionally relevant sites in the protein myosin¹. In this work, we use an alternative method based on Markov propagation of information across the structure². We ascertain the robustness and statistical significance of the proposed pathways by perturbing the network, i.e. how removal of one or more links in the network affect the proposed pathways.

1. Tang, S *et al*. Journal of Molecular Biology. (2007) 373, 1361–1373.2. Chennubhotla, C and I Bahar. Molecular Systems Biology. (2006) 2:36.**Relative Binding free energy for tricyclic antidepressants LeuT.**

Sergile Dostaly, Center for Computational Sciences, Department of Chemistry & Biochemistry, Duquesne University; Jeffrey D. Madura, Center for Computational Sciences, Department of Chemistry & Biochemistry, Duquesne University, Florida Memorial University

Transporters are ubiquitous pumps that harness pre-existing sodium gradients to catalyze the thermodynamically unfavorable uptake of neurotransmitters across the lipid bilayer. LeuT is a leucine transporter from the eubacterium *Aquifex aeolicus* and is the only member of the transmitter sodium symporter family of secondary transporters that has a solved x-ray structure. We applied a free energy perturbation approach to calculate the relative binding free energy of tricyclic antidepressant compounds such as imipramine, desipramine, and clomipramine to the Leucine transporter. We mutated clomipramine to imipramine and imipramine to desipramine to determine the relative binding free energy. We will discuss our results in relation to the experimental data.

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Synthesis, Characterization, and Reactivity of Cu(II) Complexes with Tris-(pyrazolmethyl)amine Ligands in Atom Transfer Radical Addition Reactions

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Copper(II) complexes with tris-(2-pyridylmethyl)amine (TPMA) ligand in the presence of reducing agent such as 2,2'-azobis(2-methylpropionitrile) (AIBN) effectively catalyze atom transfer radical addition reactions with catalyst concentrations as low as 5 ppm. However, structural modification of TPMA typically requires multi-step synthesis. Tris-(pyrazolmethyl)amine ligands are structurally similar to TPMA, and can be easily synthesized in two steps using commercially available reagents. This work has focused on the synthesis of tris-(1-pyrazolmethyl)amine (TPyMA) and tris-((3,5-bis(trifluoromethyl)-1H-pyrazol-1-yl)methyl)amine (TFPyMA), formed by reacting tri(chloromethyl)amine with the corresponding potassium pyrazolate salt. These syntheses resulted in a 47% and 30% yield respectively. The ligands were reacted with copper(II) chloride to form the respective complexes (40% and 32% yield respectively). These complexes were then used for the addition of carbon tetrachloride to 1-hexene in the presence of AIBN, forming the desired monoadduct with a TON as high as 2000.

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Human Macrophage Inflammatory Response to *Mycobacterium tuberculosis*

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Monocytes are involved in many aspects of innate and acquired immunity. These cells are recruited to sites of infection by inflammatory signals and differentiate into macrophages and dendritic cells. The purpose of this study was to define the inflammatory signals produced during infection by *Mycobacterium tuberculosis* that contribute to interferon gamma production (IFN- γ) from human macrophages. Quantitative methods were used to determine whether the cytokine, IL-18, is produced in response to heat-killed *M. tuberculosis* (hkTB) and necessary for the production of IFN- γ . Secreted protein levels of IL-18 and IFN- γ were measured by ELISA, while IFN- γ transcripts were measured by real-time PCR. IL-18 is produced and secreted by human macrophages at a basal level that is increased by IL-12 and hkTB. Likewise, IFN- γ secretion is increased in response to hkTB. Additional experiments are underway to evaluate production of IFN- γ -induced antimicrobial products such as nitric oxide.

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Rigid-body Docking of Mdm2 Antagonists

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The transcription factor p53 is a protein that regulates the cell cycle and has anti-cancer mechanisms. In some cancers, there are increased levels of the protein Mdm2 that bind to p53, inhibiting the body's ability to fight tumors. Mdm2 is an appealing target for small molecule docking, because finding an antagonist could lead to the development of novel compounds to fight cancer. At the interface of a protein-protein complex, one protein has side chains, called anchors, which bury into a cavity of the other protein. X-ray crystallography has revealed three important anchors on p53, residues Phe19, Trp23, and Leu26, which interact with the binding pocket of Mdm2. An antagonist of Mdm2 will mimic these interactions with the binding pocket. We will utilize the molecular design software suite Moloc to rigid-body dock and score four known antagonists to Mdm2. Results and conclusions will be discussed.

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Creating Total Bacterial Profiles for Feral and Domestic Cats to Determine Species Present and Prevalence of Species

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In order to investigate the bacterial species present in feral cats, bacterial profiles for two household and two feral cats were determined. DNA isolated from stool samples was prepped using silica extractions followed by PCR amplification utilizing the universal bacterial primers ITSF and ITSReub to amplify the 16s-23s rrrn region. The intergenic region DNA was cloned into pCR2.1. Purification and sequencing of over one hundred clones from each of the four animals has revealed the identity of the bacteria present in the cats as well as provided insight into the prevalence of these species within the animal. This data will allow us to determine if these animals contain any bacteria that could be hazardous to people and other animals. The information gained will be used to develop a screening protocol for bacteria in a large number of feral cats.

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Methylphenidate-Based Irreversible Ligands for the Dopamine Transporter, the Brain's Cocaine Receptor

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The dopamine transporter protein (DAT) has been implicated in a number of disease states including psychostimulant (e.g. cocaine, amphetamine) abuse. However, despite decades of intense research, no medications are currently available to treat psychostimulant abuse. This tremendous void can be attributed in part to the unsuccessful rational design of DAT-targeted CNS therapeutics due to limited information on the protein's 3-D structure. As a result, high-resolution elucidation of DAT 3-D structure, especially regarding its substrate and inhibitor recognition sites, remains critical. We aim to understand how abused and therapeutic drugs interact with the DAT by using irreversible ligands to map drug-binding pockets at the level of the amino acid residue. To this end, we have begun exploring irreversible ligands based on the attention deficit hyperactivity disorder drug methylphenidate (Ritalin), derivatives of which are currently being explored as medications for cocaine abuse.

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NMR Spectroscopy Analysis of the Hepatitis C Virus RNA 3'-Untranslated Region

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Worldwide, approximately 170 million people are chronically infected with the hepatitis C virus (HCV). The infection has been linked to liver failure, cirrhosis and hepatocellular carcinoma. The viral genome consists of a 9.5 kb single-stranded RNA of positive polarity, containing a 5'-untranslated region, a single open reading frame (ORF), and a 3' untranslated region (3'-UTR). A highly conserved sequence of 98 nucleotides in the HCV 3'-UTR—known as the X-tail—has been shown to be essential for viral RNA replication and to dimerize in the presence of HCV's core protein. This region has also been proposed to form long range interactions with a sequence in the ORF. In this study, we use NMR spectroscopy to characterize the X-tail 55 nt segment implicated in these events.

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Making Graphene

Bertoni, Bridget
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Graphene is a two-dimensional crystal—a one atom thick monolayer of carbon. It forms a hexagonal lattice with sp^2 hybridized carbon atoms and is a zero band gap semiconductor with charge carriers that behave like 2D Dirac massless fermions. Graphene's properties are currently the center of much theoretical interest and graphene has many potential applications as well, especially in nanoscale electronics. Graphene is easily obtainable by micromechanical cleavage verified by Raman spectroscopy, though this method of finding flakes is unpredictable and subject to much human error. Additionally, graphene's electrical properties have been the focus of much research, while its optical properties remain largely unexplored. My project is to improve the cleavage technique of obtaining graphene as well as initiating a further investigation of graphene's unique optical properties.

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Generation of Functionalized Grignard Reagents Using a Sulfoxide/Magnesium Exchange

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The eco-friendly alkylation of thiophenol with chloroacetonitrile affords sulfide 1 which can undergo subsequent oxidation to the corresponding sulfoxide. This sulfoxide can be treated with excess potassium tert-butoxide followed by 1,4-diodobutane to afford a cyclic system 2 which readily undergoes sulfoxide/magnesium exchange. The resulting C-Metalated nitrile 3 can be trapped with various electrophiles to afford highly functionalized products of type 4.

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Development of Detection and Quantitation Method for Arsenicals in Bacterial Culture using HPLC/UV

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Arsenic is a ubiquitous element that is found in atmosphere, in aquatic environments, soil and sediments, and chronic exposure to elevated level of arsenic is linked to a variety of diseases from cardiovascular to diabetes to cancer. Organoarsenicals are being used as pesticides, and one of them, roxarsone, is widely used in poultry industry. The compound degrades to other arsenicals due to microbial activity. To understand the biotransformation of arsenicals it is important to develop a robust method of detection. We are developing a method for identification of several arsenicals in a mixture with other compounds e.g., arsenate, arsenite, dimethylarsinic acid, disodium methyl arsenate, roxarsone, 2-nitrophenol, 2-aminophenol, p-hydroxybenzene arsonic acid, 2-amino-1-hydroxybenzene-4-arsonic acid, lactate, propionic acid, and acetic acid using High Performance Liquid Chromatography (HPLC) with UV detection. We are using reverse phase (RP) chromatography using C18 columns with ion-pairing agents for separating ionic analytes.

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Identification and Analysis of Novel Gorilla Numts

DiMattio, Kelly and Jensen-Seaman, Michael

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Pieces of mitochondrial DNA that have incorporated themselves into nuclear DNA are referred to as "numts". The goal of this study was to identify novel gorilla numts that have recently translocated to their nuclear genome. In order to identify these numts, gorilla-specific probes were designed and hybridized to a gorilla genomic BAC library. Positive BAC clones were then grown up as colonies, amplified using the TempliPhi in vitro amplification kit, and sequenced with BAC end primers. From the BAC end sequencing, the numts were grouped according to the chromosome on which they exist. Numt-specific primers were designed to obtain the complete numt sequence and the flanking genomic sequence. Using this approach, at least six previously unidentified novel gorilla numts were discovered. The junctions were then analyzed to infer a possible mechanism for insertion into nuclear DNA.

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Characterization of the Zebrafish Torsin A protein

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Early onset torsion dystonia (EOTD) is an autosomal dominant movement disorder that results in involuntarily prolonged muscle contractions. EOTD is caused by a glutamate deletion in the torsin A protein, and believed to be related to neuronal imbalances in the basal ganglia during development. The torsin protein is localized to the endoplasmic reticulum, however mutant torsin relocates in cytoplasmic and perinuclear inclusions. This relocation is believed to be related to the ATPase activity of the torsin protein, but the mechanism is unknown. Research has found that zebrafish have a torsin ortholog with high sequence homology and similar relocation patterns when mutated. Zebrafish can be studied during development, making them suitable for an animal model of the torsion mechanism. We have mutated the ATP binding site gene region in the zebrafish to characterize the influence of this binding site on both torsin localization and function of wild type and mutant torsin.

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Quantum/Classical Mechanical Study of Carbon Dioxide Capture to the Carbonate Anion.

Ivancic, Tim; Madura, Jeffrey

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Large-scale producers of carbon emissions are responsible for a significant percentage of the anthropogenic carbon dioxide being released into the atmosphere. Investigations have taken place into the potential capture and of these emissions in saline aquifers. In this project we investigated the potential energy changes associated with the reaction of carbon dioxide with water or hydroxide to form carbonate compounds using quantum mechanical methods to model the reaction mechanism as well as QM/MM calculations to simulate the reaction in aqueous environments such as a confined aquifer. The activation energy of the reaction is relatively high in gas phase calculations, ranging from 41.0 to 67.3 Kcal/mol supporting the idea that capture through a carbonate is inefficient. The potential energy landscape of a carbon dioxide/hydroxide reaction more promisingly indicates that there is no activation energy for the reaction and an enthalpy change ranging from -87.7 to -51.0 Kcal/mol.

The Role of ICAM-1 in Translocation of Smad Proteins into the Nucleus of CD4+CD25- T cells

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SMAD proteins are transcription factors activated by the TGF β 1 signaling pathway. Phosphorylated Smads 2 and 3 (pSmad2/3) form a complex with Smad4, enabling entry into the nucleus of CD4+ T cells. Smads in the nucleus induce expression of Foxp3+ T regulatory cells (T regs). In this study, we investigated the role of the adhesion molecule, ICAM-1 to facilitate movement of pSmad2/3 from the cytoplasm into the nucleus. Previous studies revealed reduced T regs in ICAM-1^{-/-} mice. We hypothesized that ICAM-1 is either required for dissociation of pSmads from the microtubules or that ICAM-1 is required for association of pSmad2/3 with Smad4. We used ICAM-1^{-/-} mice and control splenic CD4+ T cells to test these hypotheses *in vitro* using confocal microscopy, co-immunoprecipitation, and flow cytometry at various time points. Our data suggest that ICAM-1 may play a partial role in movement of pSmad2/3 into the nucleus.

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Effects of Chronically Elevated Corticosterone on Behavior in an Amphibian

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When stressed, animals respond physiologically by releasing glucocorticoid hormones such as corticosterone (CORT) to cope with the stressful situation eventually returning the body to homeostasis. However, chronic elevation of CORT has been shown to suppress reproductive behavior. This stress hormone has been studied primarily in domesticated mammals but less is known about non-domesticated, wild species. To understand behavioral effects of CORT in the male mountain dusky salamander *Desmognathus ochrophaeus*, I surgically administered silastic implants containing low or high doses of CORT. Control animals were given blank implants or received no surgery. No significant difference was found among treatment groups in feeding, mating, or activity in the presence of predator cues. I conclude that mountain dusky salamanders are resistant to chronically elevated CORT. This work is important because it is one of the first studies that measure the effects of chronic elevation of CORT in an amphibian.

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Functional Classification of Inositol-5-Monophosphate Dehydrogenase (IMPDH)

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A protein's sequence provides key information about its physiological role and can be useful for predicting functions of newly discovered sequences. Functional classification using phylogenomic inference is an effective method to detect differences within a protein family and to attribute the distinctions to specific amino acid sequences. IMPDH, the superfamily of interest, is an enzyme responsible for purine metabolism and thus cell proliferation. A complete set of IMPDH sequences were collected and used to produce an accurate global multiple sequence alignment. The alignment was then analyzed using phylogenetic and principle components analyses to identify subfamilies. Sequences within the subfamilies were examined using a cross entropy analysis to isolate key residues unique to each subfamily. Creation of structural visualizations highlighted the special regions and was used to interpret the analysis in terms of known biochemical and physiological properties.

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PrgL Contributes to Hydrogen Peroxide Resistance in *Serratia marcescens*

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Serratia marcescens is a Gram-negative bacterium in the family Enterobacteriaceae. It is a human and plant pathogen commonly associated with keratitis. Host defense mechanisms include the release of hydrogen peroxide which induces oxidative stress, destroying the microbe. Here we tested the hypothesis that a novel gene (*prgL*) predicted to code for a hybrid peroxiredoxin (Prx) and glutaredoxin (Grx) protein contributes to oxidative stress resistance. We compared the effect of hydrogen peroxide on the wild type, the *prgL* mutant, and the *oxyR* mutant using disk diffusion assays. The *prgL* mutant was shown to exhibit a significant increased H₂O₂ sensitivity ($p > 0.01$), as well as the *oxyR* mutant which served as the negative control. Complementation experiments are in progress to show the restoration of H₂O₂ resistance after the *prgL* mutation is reversed. The *prgL* gene may represent a novel oxidative stress resistance factor in *Serratia marcescens*.

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Feline Genotyping by use of STRs to Assert Relationships within a Colony

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Using primers designed to amplify short tandem repeats (STRs) in the feline genome, a genomic profile can be created which is unique for each individual cat. This genomic profile can then be used to identify individual animals and establish relatedness. Complementary studies to determine bacterial disease load in each animal will be coupled with our genotyping studies to examine disease prevalence as it relates to genotype. Each primer requires optimization to a particular set of PCR conditions before a full genotype can be achieved for an individual cat. Three hundred seventy-five samples have been collected from feral cats from colonies surrounding Allegheny County. Once genotyped, allele frequencies can be estimated and used to calculate relatedness between individuals. Complementary studies to determine bacterial disease load in each animal will be coupled with our genotyping studies to examine disease prevalence as it relates to genotype.

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Characterizing Gap Junction Formation in Cell Cultures

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Gap junction channels have been observed to interact with actin cytoskeleton elements, yet little is known of the role of actin in gap junction formation. We propose that the actin cytoskeleton plays a pivotal role in gap junction formation and turnover. To study the relationship between the actin cytoskeleton and gap junction formation immunocytochemical techniques were used in adrenal cortical cell in culture. A significant increase in the number of gap junction plaques occurred between 2 - 4 hours; followed by a plateau between 4 - 8 hours and a final increase between 8 - 24 hours. In cells treated with a RhoA kinase inhibitor, Y-27632, to inhibit actin stress fibers an increase in the size of cytoplasmic annular gap junctions were observed. Our findings provide evidence that the actin cytoskeleton regulates gap junction maintenance.

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Characterization of Steroid Sulfatase in the Human MG-63 Pre-Osteoblastic Cell Line

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Formation and degradation of bone is partially dependent upon steroid hormones, with estrogens playing a particularly important role. Osteoporosis is more prevalent in post-menopausal women, who exhibit low levels of circulating estrogens. However, post-menopausal women have notably high levels of inactive conjugated estrogens. These compounds can serve as precursors to active estrogens, which may support increased bone density. Conversion of sulfo-conjugated estrogens into active estrogens requires the enzyme steroid sulfatase. Steroid sulfatase has not been well documented in bone. Our lab investigated the presence of steroid sulfatase in the human pre-osteoblastic cell line MG-63, using biochemical and immunological techniques. We found that MG-63 cells have significant steroid sulfatase activity. Furthermore, microsomes from these cells also had steroid sulfatase activity and showed the presence of steroid sulfatase protein. These data indicate that bone cells possess the enzyme necessary to convert prevalent sulfo-conjugated estrogens into active estrogens in post-menopausal women.

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The Art in Science Education

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Today's ever evolving graphics technology serve as a growingly important tool for science education, and general public teaching. The Regenerative Medicine Partnership in Education (www.sepa.dug.edu) produces multiple educational projects on platforms that include films, web resources, and print teaching resources. Under the guidance of my colleagues, many projects were produced, including a film that is aimed at educating the older public about osteoporosis, and the modern treatment options. Using detailed visuals to simulate the look of bones, cells, organs, and cell-cell interactions we aim to educate people on the processes of osteoporosis and its treatment by illustrating the actions on screen. Other projects include the preliminary steps in the production of a full-length film to educate heart-transplant kids about the human heart and surgery.

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Effect of Self-Assembled Monolayers on the Adhesion of *Staphylococcus aureus* to Stainless Steel Surfaces

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Bacterial adhesion on stainless steel surfaces is an area of ongoing biomedical research due to the high risk of bacterial infection in orthopedic implants. *Staphylococcus aureus*, a common bacterial strain, is known to readily form bacterial biofilms on stainless steel. These biofilms are difficult to remove due to the formation of an interconnected bacterial network thus leading to increased infection rates. The purpose of this study was to investigate the ability of self-assembled monolayers bound on the surface of stainless steel to retard bacterial adhesion. Stainless steel coupons were modified with methyl-terminated phosphonic acids, and the acid deposition was confirmed using diffuse reflectance infrared spectroscopy and MALDI-TOF mass spectrometry. Control stainless steel coupons and organically modified coupons were exposed to bacteria cultures for 1 and 3 day time periods, and the bacteria growth was quantified using confocal scanning microscopy with live/dead staining coupled with COMSTAT for statistical analysis.

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Investigation and Optimization of Polymer Fiber Analysis through Gas Chromatography-Mass Spectrometry

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Synthetic polymers can be difficult to differentiate when comparing fibers within the same class of material. However, polymers are regularly altered by manufacturers through the inclusion of chemical additives to enhance desirable characteristics such as flexibility and color fastness. Determination of these additives may reveal a way to more readily identify the source of a fiber. In this study, liquid extractions from various carpet fibers were analyzed by gas chromatography/mass spectrometry (GC/MS) in hopes of procuring component characteristics unique to each sample. To obtain the best results for cross-sample comparison, parameter development was necessary and included consideration of sample dilution, variation of ramp time and temperature as well as column polarity. In the future this technique could provide a more effective means of fiber identification than current forensic methods.

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Designing an Algorithm to Study the Evolution Flu Viruses

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Currently, the number of reported transmission of avian flu to humans is small and subsequent human-to-human transitions are of limited virulence. The avian virus' ability to infect humans is dependent on whether it binds to one specific shape of receptor on the surface of human respiratory cells [1]. How these viruses evolve to infect humans is not adequately explained by current research. We are creating an algorithm supplemented by an option in which two different viral strains can infect the same cell and recombine randomly and the overall fitness of the recombined viruses will be taken into consideration. We will start with a flu genome and will generate random mutations according to a mutation rate. Sequences will be selected based on some fitness function and the process will be repeated. After analyzing the mutated sequences, we can predict how the evolution of the avian virus is capable of infecting humans.

[1] Massachusetts Institute of Technology. "Key To Avian Flu In Humans Discovered." *ScienceDaily* 7 January 2008. 8 July 2008<<http://www.sciencedaily.com/releases/2008/01/080106193222.htm>>.

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Development of Novel Methods for Imaging Latent Fingerprints.

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This study utilizes the hydrophobic properties of the latent (un-fumed) and ethyl cyanoacrylate fumed prints in order to investigate novel methods for imaging fingerprints. The hydrophobicity of the fingerprint surface can be increased by fuming with ethyl cyanoacrylate (super glue), as determined by contact angle goniometry and digital image analysis. Carboxylated polystyrene microspheres infused with a fluorescent dye were used to increase the contrast between the fumed fingerprint and the substrate the print was deposited on. Blue light (455 nm) was used to excite the fluorescent dye and white light was used as a way to compare the fluorescent prints to the actual print when imaging. All images were obtained using a camera attached to a zoom stereoscope fitted with an appropriate filter.

Developing an Active Learning Framework for Transmembrane Helix PredictionWehner, Jessica¹; Ganapathiraju, Madhavi^{1,2}¹Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh, Pittsburgh, PA 15261²Department of Biomedical Informatics, University of Pittsburgh

Over 30% of an organism's proteins are membrane proteins¹ (MPs), which play key roles in important functional pathways such as signal transduction. However, experimental determination of MP structure is difficult, making computational prediction desirable. State-of-the-art prediction methods achieve acceptable accuracies for many proteins but perform poorly on uniquely structured proteins like aquaporin. Here, we developed an active learning framework that explores the space of unlabeled sequences and asks for experimentally determined labels for as few data points as possible. The purpose is to develop a strategy of identifying the next protein, which when solved experimentally, would disambiguate the labels of the remaining sequences. We computed features from primary sequence¹ and performed cluster-density driven selection of labels, yielding Q_2 of 74.0% at 280 (1%) selected data points. Further computations are expected to be completed by the end of the project.

1. Ganapathiraju et al (2008) BMC_Bioinformatics 9(1).

Effects of Temperature on Stochastic Gene Expression

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Stochastic expression of the LamB gene in *E. coli* became evident when studying the population dynamics of *E. coli*. The LamB receptor protein is a transmembrane maltose channel protein in *E. coli* that is also exploited by Lambda Phage for attacking the bacteria. If a population of *E. coli* is subjected to high phage pressure, a minority of the population is observed to survive. Studies have shown that the cells of the minority population are a phenotype resulting from LamB expression noise. The regulatory step for transcribing the LamB receptor gene is the formation of a DNA loop required for RNA polymerase to bind to the malKp promoter. Formation of this loop is a statistical event subject to thermal fluctuations. The objective of this study is to determine the extent to which the occurrence of the minority phenotype is a function of the temperature at which the bacteria is grown.

Parameterization of Small Molecules that Interact with the Dopamine Active Transporter

Jonathon D. Gibbons, Center for Computational Sciences, Department of Chemistry and Biochemistry, Duquesne University and Dr. Jeffrey D. Madura, Center for Computational Sciences, Duquesne University.

There are many molecules that bind to the dopamine active transporter (DAT), like antidepressants and narcotics. Some of these molecules block DAT from re-uptaking dopamine from the synaptic cleft. This causes an excess of dopamine to remain in the synaptic cleft, which causes euphoric like feelings. How and why specific molecules bind to and inhibit DAT is of high pharmacological interest. To study the binding of substrates to DAT, parameters were developed for: dopamine, cocaine, mazinol, clomipramine, imipramine, and desimipramine using PDDG/PM3 semiempirical methods for gas phase optimizations as well as single point calculations using the Biochemical and Organic Simulation System (BOSS). The parameterized molecules were then bound to a DAT homolog, leucine transporter (LeuT). Monte Carlo Simulations for Biomolecules (MCPRO) was used to calculate binding free energies of these complexes. Relative free energies of solvation have been calculated for desimipramine to imipramine, clomipramine to desimipramine, and imipramine to clomipramine.

Computational Investigation of the Leucine Transport Mechanism in LeuT_{Aa}

Merchant, Bonnie A.* & Madura, Jeffrey D.; Center for Computational Sciences; Department of Chemistry & Biochemistry; Duquesne University; *Carlow University

Neurotransmitter sodium symporters (NSS) are targets for various medicinal and illegal drugs that affect mood and behavior. Of particular interest are the dopamine (DAT) and serotonin (SERT) transporters. A structure with similarity to DAT and SERT, both in sequence and in function, is the leucine transporter (LeuT_{Aa}). With the X-ray crystal structure of the bacterial homologue from *Aquifex aeolicus* revealed in 2005, it is of interest to determine how leucine is transported through LeuT_{Aa}. This project focused on the transport of leucine through the LeuT_{Aa} using VMD and NAMD. The Adaptive Biasing Force (ABF) method of NAMD was utilized to obtain the free energy for the transport of leucine. From the simulations, we see that as leucine travels through LeuT_{Aa} several of the transmembrane helices move to form a path for the leucine. In particular we see TM 6B move to allow the substrate in from the intracellular side.

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Molecular Dynamics Simulations of LeuT Transport Mechanism Restrained by Normal Modes

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Na⁺/Cl⁻ -dependent transporters play key roles in driving the movement of neurotransmitters, such as dopamine and serotonin, across cellular membranes.

The protein LeuT is a bacterial homologue of these transporters and allows for the select diffusion of the substrate leucine through membranes in *Aquifex aeolicus*. Here, we aim to determine the plausibility of a previously proposed transport mechanism that involves a specific conformational change upon substrate/Na⁺ transfer. We apply a molecular dynamics procedure that uses normal modes derived from anisotropic network modeling (ANM) to harmonically restrain the protein during simulation. Deformations along multiple frequency modes provide an efficient way to sample potential conformational changes in the presence of a water and membrane environment. ANM-restrained simulation is useful in determining a relatively low-energy transport pathway.

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Identifying Unfolding Pathways of G Protein-Coupled Receptor Protein Structures

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G protein-coupled receptors (GPCRs) have important functionality in cell signaling processes by external affects such as light, smell, taste, and hormones. The conformational changes in structures of GPCR's play vital role in signaling processes. The understanding of conformational changes is useful to determine basis of certain diseases that are related to malfunctioning of these proteins. The study of structures of GPCRs, however, is challenging since GPCR proteins are not sufficiently stable for crystallization. In this study a new computational method for analyzing protein structures is proposed to assess their stability. The method is based on computational unfolding of proteins utilizing the Gaussian network model framework that represent protein structure by network of springs. The unfolding of a protein is represented by removal of springs so as to increase the conformational entropy in an appropriate fashion. This new method is tested on several GPCR protein structures to determine their folding cores and important residue-ligand interactions.

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Characterization of Steroid Sulfatase in Mouse MC3T3-E1 Pre-Osteoblast Cells

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Estrogen is a regulator of bone remodeling, a balanced dynamic between osteoblastic bone formation and osteoclastic bone degradation. In post-menopausal women, little estrogen exists in circulation; however, large quantities of sulfo-conjugated estrogen precursors are present. Conversion of these precursors to active estrogens utilizes the enzyme steroid sulfatase. This pathway may be important for bone growth and repair after menopause. Steroid sulfatase has not been well characterized in any bone tissue. Our study was designed to provide information on steroid sulfatase in the mouse MC-3T3-E1 pre-osteoblastic cell line. Using enzyme and immunological assays on whole cells and microsomal cell fractions, we demonstrated that these bone cells possess significant quantities of steroid sulfatase. This finding may be important in understanding the role of steroid sulfatase in maintenance of bone density after menopause.

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Constructing Darwin: Writing to Teach about his Life and Science

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Using sources that go beyond textbooks often makes concepts more accessible and memorable for children. I have worked to create enticing text for both a synthetic interview and a website in preparation for the 2009 "Darwin Days," an event sponsored by the Regenerative Medicine Partnership in Education (www.sepa.duq.edu). The synthetic interview allows visitors to choose a question to ask Darwin and to hear a response with visuals. The web pages contain text and images to supplement content presented at local institutions. While creating web chapters and responses to several high interest questions, I repeated the process of researching, writing, and revising. I found that integrating direct quotations from Darwin's autobiography and letters into the material allowed Darwin's voice and character to show through. This created a man behind the fundamental principle of biology and a story behind the fame, which may allow people to get past preconceived ideas about evolution.

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Measuring the Effect of B Lymphocyte Activation on the Expression of DC-SIGN and Co-Stimulatory Molecules with Fluorescence Tagged Antibodies

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Human immunodeficiency virus type 1 (HIV-1) can be transmitted from antigen-presenting cells such as dendritic cells (DC) and a subset of B lymphocytes to CD4+ T cells in *trans*. It has been shown that transmission can occur via the C-type lectin receptor DC-specific ICAM-3 grabbing nonintegrin (DC-SIGN). Some studies demonstrated that activation of B cells induces the expression of DC-SIGN; however, others have shown that high expression levels of DC-SIGN on some cell lines cannot efficiently transfer the virus. Thus, it is uncertain whether DC-SIGN is solely responsible or if co-stimulatory molecules play a role in the transmission. This study will measure the expression levels of DC-SIGN and co-stimulatory molecules using flow cytometry for activated B cells with LPS, CD40L, and BAFF. Results from this study will help evaluate the role of DC-SIGN and co-stimulatory molecules in the transfer of HIV-1 from B cells to T cells.

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Copper Catalyzed Atom Transfer Radical Addition of Carbon Tetrachloride to Alkenes in the Presence of Air

Matthew J. Taylor, William T. Eckenhoff and Tomislav Pintauer, Department of Chemistry and Biochemistry, Duquesne University

Atom transfer radical addition (ATRA) is one of the fundamental reactions in organic synthesis. In the past, ATRA has not been an economical method for the formation of carbon-carbon bonds for two reasons: (a) relatively high catalyst loading required (typically 10-30 mol%) and (b) system's low tolerance for contamination by air. In this work, copper catalyzed ATRA reactions of CCl₄ to alkenes in the presence of 2,2'-azobis(2-methylpropionitrile) (AIBN) and limited amounts of air were performed. It was shown that free radicals generated by AIBN were able to constantly regenerate the catalyst, which allowed for much lower catalyst loadings (<<1 mol% relative to olefin), and actively remove oxygen from the reaction mixture. Using this method for ATRA of CCl₄ to 1-decene in the presence of 1×10⁻⁵ mol% catalyst and 15% mol AIBN, TON as high as 9000 was achieved. In addition, an array of alternative reducing agents for these reactions is being investigated.

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Pharmacophore Model Development for the Identification of Novel Acetylcholinesterase Inhibitors

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Clearly established as one of the successful computational tools in rational drug design, pharmacophore modeling has become an integrated part of drug discovery. The work described herein focuses on the use of ligand-based pharmacophore modeling to identify novel acetylcholinesterase inhibitors against Alzheimer's disease. Starting with a small training set of known dual inhibitors of the *Torpedo californica* acetylcholinesterase (TcAChE), we generated a series of ligand-based pharmacophore models using the Molecular Operating Environment (MOE) software. The models were further used to screen the lead-like subset of the ZINC database. The top 100 molecules will be virtually screened against the TcAChE three-dimensional structure using Molegro Virtual Docker in order to prioritize hits for experimental testing.

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Anti-Bacterial Activity of Calcium Aluminates

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Hydrated calcium aluminate cements cast quickly at room temperature, making them potentially useful in repairing critical defect wounds in bones. A major problem with implants, in general, is the high risk of infection due to bacteria present at the site of the wound and also on the implant itself. The purpose of this project is to examine the binding of ampicillin to the surface of the calcium aluminates and their interaction with *E. coli* (strain MG1655). The effect of the material and the ampicillin on overall bacteria growth and on attachment of bacteria to the surface of the material was studied. Results show that ampicillin modified hydrated calcium aluminates do not have a large effect upon the growth of bacteria. Unhydrated calcium aluminates, however, create a pH change and cause the bacterial growth to slow down.

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Cytochrome c Electrochemistry: Determining the Effects of Self-Assembled Monolayer Composition in the Protein Formal Potential and Electron Transfer Rate

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Cytochrome *c*, a solution protein, transfers electrons between two inner membrane redox partners, cytochrome *c* reductase and cytochrome *c* oxidase located in the mitochondria. The opposing charges of the two surfaces facilitate the interactions between the two proteins. A self-assembled monolayer can be utilized to recreate the interactions between the proteins. The SAMs were prepared with varying compositions of carboxylic acids to acquire the change in formal potentials and electron transfer rates for cytochrome *c*. The electron transfer rates of the most widely studied system containing amine terminated thiols (-NH₂) remained static demonstrating ideal nonideality.¹ Solutions variations will be explained. Three and four component SAMs were prepared to greater mimic monolayers found in living systems. The surface charge of cytochrome *c* was changed using the addition of two modification devices, poly-L-lysine and maleic anhydride.²

¹Ooi, Y.; Hobara, D.; Yamamoto, M.; Kakiuchi, T.
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²Aviram I.; Myer, Y. P.; Schejter, A. *Journal of Biological Chem.*, **1981**, *256*. 5540-5544.

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Correlation of CaMKII Activity to Synaptic Strength by Fluorescent Imaging

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Changes in synaptic strength are considered important cellular mechanisms by which one can understand learning and memory. Ca²⁺/calmodulin-dependent kinase II (CaMKII) is an important protein kinase that is highly enriched at the postsynaptic site of neurons and is known to be activated when the synaptic strength increases. The activity of CaMKII is believed to be correlated to the synaptic strength upon Ca²⁺ input. We used the fluorescent probes of CaMKII to measure its activity under conditions that are likely to induce increase in synaptic strength. We will test whether the changes in CaMKII activity indeed corresponds to the changes in synaptic strength. It is also known that one of subtypes of NMDA receptors (NR2A) is more responsible to the increase in synaptic changes. We will test whether the changes in CaMKII activity is affected significantly by blocking NR2A receptors.

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

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This study was conducted in order to extract, purify, and characterize the novel pigments produced by two species of fish in the genus *Etheostoma*. Unlike most other vertebrates, these two species do not utilize structural refraction to display blue or green color. The blue coloration exhibited by the rainbow darter (*E. caeruleum*) and the green coloration exhibited by the greenside darter (*E. blennioides*) during their mating season are due to true chromoprotein pigments (related but not identical between the two species). Extraction of these pigments was accomplished by performing multiple freeze/thaw cycles on each of the specimens. The purification process consisted of gravity filtration, ammonium sulfate fractionation, size-exclusion chromatography, and ion-exchange chromatography. Polyacrylamide Gel Electrophoresis and a Bradford Assay were carried out to analyze the purity and concentration of the pigments. Ultimately, characterization will involve protein sequencing and comparative biochemistry of the chromophore.

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Peptide Folding Effects of the Cyclic Amino Acid Proline

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Evaluation of the role of disulfide bridges plays an important role 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, α -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.

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Day in Life of Mycobacteriophage Bre19

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Bacteriophages are estimated to be the most widely distributed and diverse entities in the biosphere with an estimated 10^{31} in existence, many with unique characteristics. With growing numbers of bacteriophages being discovered, a large genomic database is needed to characterize and organize newly discovered bacteriophages' genomes. The tremendous diversity of bacteriophages in the current genomic database gives hope for possible break through in the research of diseases, such as *Mycobacterium tuberculosis*. In the concrete dirt behind Crawford Hall at the University of Pittsburgh, mycobacteriophage Bre19 is one of the newest mycobacteriophages discovered. Through proper isolation and purification of Bre19, the lytic growth cycle and small to medium plaque morphology were observed on its host *Mycobacterium smegmatis*. Currently, DNA is being extracted to allow for DNA sequencing of mycobacteriophage Bre19. Bre19, along with other mycobacteriophages, provide possibilities for innovative progression in the diagnosis and treatment of mycobacterial diseases present and future.

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Analysis of Data from MINOS, a Long Baseline Neutrino Experiment

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I describe a method of analyzing neutrino oscillation data from MINOS. MINOS is a long baseline neutrino beam experiment whose primary purpose is the study of atmospheric neutrino oscillation parameters and CPT violation. My purpose is to determine the ideal region of the detector area for taking ν_{μ} charged current event data with reduced systematic errors. The effects on the neutrino energy spectrum of choosing various detector areas are also investigated. Such neutrino oscillations violate the Standard Model of particle physics and therefore have resulted in a quest for new physics beyond that model. Additionally, neutrinos are known to play a huge role in solar nucleosynthesis and the early Universe and are the likeliest candidates for the composition of dark matter. Results are pending at this time.

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Fluorescence Spectroscopy Analysis of the Fragile X Mental Retardation Protein RGG Box Arginine Methylation upon Binding to G-Quadruplex RNA

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Fragile X syndrome, the most prevalent inherited mental retardation, is caused by the absence of the fragile X mental retardation protein (FMRP). The RGG box domain of FMRP, which has been shown to bind to neuronal target RNAs that form G-quadruplex structures, can be post-translationally methylated on arginines. In this study the FMRP RGG box domain was *in vitro* methylated by the protein arginine methyltransferase 1 and its binding properties to a G-quadruplex forming RNA were tested by fluorescence spectroscopy. In doing this, the binding affinity of the methylated arginines within the FMRP RGG box was compared to that of the non-methylated version of the peptide. Thus, our results should confirm whether the methylation of the RGG box attenuates or amplifies its binding to G quadruplex forming RNA *in vitro*.

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Protein-Protein Interaction Between HIV GP-41 and Human Protein LCK

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Treatment for HIV/AIDS has proven difficult due to the high mutation replication rate of the HIV virus as well as the high mutation rate of the HIV genome. Current treatments for HIV consist of multiple drugs, generally all targeted at the enzyme *reverse transcriptase*, but these treatments are far from perfect; and the discovery of new drug targets could lead to more effective treatments or even a cure for HIV/AIDS. To this end, we have used computational models to predict binding between the HIV virus proteins and the human body proteins, and we have utilized other such methods to select an unknown interaction that we believe may be crucial to the HIV life cycle, the GP-41-LCK interaction. We have ordered these proteins and are testing in the lab to determine the pattern of interaction between these two proteins, which holds promise to lead to new HIV drug targets.

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Optimization of NAMD for Use with the Cell Broadband Engine

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Currently, most molecular dynamics simulations are run on expensive supercomputers, but with the use of the Cell processor, simulations can become both cheaper and faster. Testing of the Cell processor against standard processors used today shows a massive jump in the efficiency of computation intensive programs. I will rewrite NAMD for use with the Cell processor. Once the code has been rewritten, I will test the speed of the optimized NAMD software. Hopefully, this optimized code will allow molecular simulations to be done cheaply and efficiently. From what I have achieved so far, it seems like the Cell processor will allow simulations and other computation intensive code to be run quickly and without the need of expensive alternatives.

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Educating Third World Farmers on Soil, the Scientific Method, and Using Technology

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Bioinformatics

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People in third world countries lack the knowledge regarding impact of soil conditions on crop yield. We designed an experiment using the XO laptop and Vernier probes to test and measure specific soil conditions and their impact on plant growth. To measure its effectiveness, the experiment was designed and executed locally (Houston, PA), with the intentions of also doing the experiment in Africa. Our experiment has flexibility to test for different variables on plant growth and uses technology and common household items. Preliminary results show promise that this experiment will be effective for educating third world children about using science and technology for improving soil conditions. This research in educating children about science and providing technology can have a major impact on reducing world hunger.

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Development of a Method for Extracting Organic Content from Soils

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Extraction methods and gas chromatography-mass spectrometry (GC-MS) analysis parameters for the organic content of soil have been studied, which eventually may be used, in conjunction with other methods, to definitively characterize the location that a particular soil may have originated from. Previous research has led to an extraction procedure involving heating and sonicating in methylene chloride. More current research was focused on finding the minimum amount of soil necessary for the extraction and optimizing the GC-MS parameters. One important parameter that was being tested was the type of GC column used. Initially, a nonpolar polysiloxane column was used; a nonpolar polysiloxane column capable of higher temperatures and a polysiloxane column of intermediate polarity were also tested. The data has yet to reveal compounds that are uniquely identifiable to a particular soil.

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ProMessis: Software for Farmers on Small Computers

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Saint Vincent College

This part of the Isidore project focuses on using technology to help farmers both here and worldwide. Right now many farmers, including those in the United States have to do much if not all of their planning by hand. Although this finishes the job, it is not the most effective or most useful way to accomplish this work. To solve this dilemma we have built a computer program which can keep track of past information on the fields as well as suggest plans for the future. This program will also be portable enough to use in 3rd world countries on cell phones and XO laptops, which are distributed by One Laptop Per Child to assist in education in 3rd world countries. We will build the application and distribute it locally to find out its effect. Once fully developed I believe that this program will greatly enhance the yield of farmers around the world.

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The Isidore Project: Using Probes to Increase Crop Yield

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World hunger is one of the greatest challenges faced by society in the 21st century. In third world countries people are often forced to become self-sufficient farmers in order to survive, but are often plagued with low crop yields. The soil in most places does not lack nutrients, but the problem lies within the pH of the soil. However, with today's technology we are able to produce efficient soil probes that can be used to test soil pH and help increase crop yield. By performing a small experiment involving soils with different pH, and a pH probe used in Lowe's Garden Center the results of farming using a probe to first test soil can be easily seen. Soil probes have the potential to not only help the modern farmer, but to also help self-sufficient farmers in poor areas survive and enjoy larger crop yields.

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System Architecture for RAE: An interactive web-based biomedical informatics system for pediatric orthopedic patients

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To automate the process of creating personalized patient education presentations, PHP, XHTML, and MySQL are used in a modification of the standard three-tiered architecture. The web-based user interface (top tier) allows pediatric orthopedic physicians to input patient information (including the patient's age, height, weight, gender, x-ray image). The entire patient presentation, composed of individual HTML pages, is then automatically generated. The input interface links to a web server (middle tier) that operates PHP scripts to store the patient's information into a MySQL relational database (bottom tier). Additional PHP scripts retrieve information from the database to write HTML pages and store the pages in a patient-specific directory (a modification to the three-tiered architecture). The presentation is then viewed via a web browser by the patient and physician. An initial prototype was developed and sample presentations produced.

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Image Architecture for RAE: An Interactive Web-based Biomedical Informatics System for Pediatric Orthopedic Patients

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The purpose of this project is to create an interactive web-based biomedical informatics system to assist Dr. Mark Sangimino to teach his young patients how to cope and manage their muscular skeletal disorders. The system, nicknamed RAE, will automatically create an educational presentation individualized to the patient's disorder and interests in hopes of engaging the child in his/her own daily care. RAE's personalized presentations will work by minimizing word usage and maximizing inspirational images. One key aspect of the project was completed by identifying the possible resources for appropriate images on pain, deformity, and function. Various image rights and privileges were explored for utilizing the required images. Proper indexing was developed to retrieve the images from the database. In addition, a layout template and test-run presentation were developed. Dr. Sangimino's hope for the future is that the Bioinformatics System will be used in pediatric orthopedic practices nationwide.

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Data Design & Flow for RAE: An interactive web-based biomedical informatics system for pediatric orthopedic patients

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An interactive web-based biomedical informatics database has been developed to produce presentations that will help pediatric orthopedic surgeons educate their patients on how to cope with and manage their conditions. These presentations will provide patients and their families with the necessary information to allow for a complete recovery of the patient while minimizing complications due to mis-interpreted follow-up care. A personalized presentation will be produced based upon input from the database involving the individual needs and interests of the patient. Initially, a conceptual schema was constructed that mapped the relationships between the various concepts to appear on the presentation pages. A MySQL database architecture is being designed based on the conceptual schema (see William Kunkle's poster). Finally, an initial design of the web page templates was developed in HTML.

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A New Pilot Program at Duquesne University for High School Chemistry Teachers

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Duquesne University

The American Chemical Society (ACS) Summer Research Fellowships for High School Chemistry Teachers is a new pilot program administered by the ACS and sponsored by Motorola. The program is being piloted in only three locations across the country. Through this program, three teachers worked at Duquesne University this summer under the guidance of a faculty mentor and were provided the opportunity to participate in a cutting-edge research project. The experience serves to update their content knowledge and provide them with the opportunity to experience academic culture and college life, which will translate into success for their own students in their home districts.

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Characterizing Mn doped AgInSe₂ for Use as a Dilute Magnetic Semiconductor

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Manganese doped AgInSe₂, a diamond-like semiconductor with chalcopyrite structure, has potential uses including nonlinear optics, photovoltaics, and spintronics devices. This system has been investigated to determine the solubility limit of the manganese dopant, phase purity, and its potential application as a dilute magnetic semiconductor (DMS). Samples were created of manganese concentrations ranging from 0% to 10%. Stoichiometric ratios and heat treatments were refined to improve the phase purity of the material. Powder X-ray diffraction (PXRD) was used to characterize the phases present and adherence to Vegard's Law. A Scanning Electron Microscope (SEM) coupled with Energy Dispersive Spectroscopy (EDS) was used to further investigate undesirable secondary phase formation. The band-gap energy (E_g) was determined with a UV-Vis-NIR Spectrophotometer.

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Doping of Latex Polymer Microspheres with Near Infrared Dyes

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Cyanoacrylate fuming has been used to detect and develop fingerprints by covering the fumed fingerprints with a near infrared dye solution. These fumed fingerprints can be viewed by exciting the dye with a laser. Near infrared dyes are useful in the detection of fingerprints since few natural materials fluoresce in the near infrared region. The purpose of this study is to explore methods to dope latex polymer microspheres with a near infrared dye. These doped microspheres will then be applied to latent fingerprints to enhance the detection of latent fingerprints on various surfaces that would have unacceptably high fluorescent backgrounds when viewed under ordinary visible or UV radiation, such as plastics.

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A Comparison of the Trends Regarding Concentration of Tannins From Five Forests and Seven Different Elevations in Pennsylvania

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Oak tannins (soluble polyphenols) are the most abundant compounds extracted from wood during the wine aging process. Twenty samples of oak cores from five different forests in Pennsylvania were analyzed via an oak soak of one, two and three weeks to determine tannin concentration and permeability. Oak powder from seven different elevations was also evaluated for tannin concentration. The purpose of this investigation is to note any trends in tannin concentration with regards to location and elevation of oak trees. Different studies and hypotheses regarding the concentration of tannins and their influence on wine flavor during the aging process are reviewed and conclusions are drawn as to the effect of tree location and tannin concentration in American Cooperage Oak.

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Project SEED Program at Duquesne University

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Project SEED is a program cultivated by the American Chemical Society (ACS) that plants economically disadvantaged high school students in a laboratory setting for eight weeks during the summer. Applications harvested from area high schools are sifted through by grade point average, teacher recommendations, and student essay to reap the cream of the crop. The students blossom as they work independently on a cutting edge research project under the nurturing guidance of their faculty supervisor and graduate student mentor. The students continue to grow by interacting with other research students and by participating in many enriching activities. Financial assistance for this year's summer program at Duquesne University was subsidized by the ACS and various local patrons; such as, R.J. Lee Group Inc, Acucis, Respirationics, and the Spectroscopy Society of Pittsburgh.

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Solid-State Microwave Irradiation of Intermetallic Compounds

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Intermetallic compounds can exhibit a wide variety of useful properties such as, superconductivity, shape-memory and magnetoresistance, among others. They are traditionally synthesized via high temperature solid-state reactions. Solid-state microwave synthesis of intermetallic compounds is a relatively new and unexplored application of microwave irradiation that possesses a number of benefits compared to other synthetic methods. Reaction times are shorter, 10 to 20 minutes for the microwave method, compared to multiple days for some traditional preparations. Shorter reactions save both time and energy. However, the solid-state microwave synthetic method is not well understood. A number of variables have been identified including, grinding time of reactants, sample volume, irradiation time and sample geometry. Microwave experiments in a number of intermetallic systems including Bi-Ni, Ni-Sn and Ni-Fe have been performed and analysis of the products will be discussed.

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Studying Monolayers on Alloys

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For this project, we studied monolayers on Stainless Steel (SS316L). It is important because many doctors use SS316L on patients who need implants. Sometimes the body rejects the implant and it can lead to very harmful effects. Solutions of 2mM Octadecylsulfonic acid (ODSA) and 1mM Octadecylphosphonic acid (ODPA), in tetrahydrofuran were prepared. The SS316L substrates were dipped in the solution of either ODPA or ODSA for 2 hours at room temperature and the substrates were put into an oven overnight at 120°C. Then Diffuse Reflectance Infrared Spectroscopy was performed to determine whether the monolayers stayed on. The peaks were less than 2918 cm^{-1} indicating that the monolayer is ordered on the SS316L surface. Parameters such as time of dip and temperature of the solution were altered to form well ordered monolayers.

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Conformational Analysis Using MOE Software

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

