## 1

**Double Mutations and Glycine Receptor**

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The purpose of study is to understand functionality of the glycine receptor (GlyR). This pentameric ligand gated chloride channel protein receptor provides inhibitory neurotransmission in spinal cord and brain stem. The double mutation allows ivermectin to be a ligand that binds efficiently to the glycine receptor, while increasing the sensitivity of the receptor. The purpose of our single and double mutations is to understand how agonist and ivermectin sensitivity can be used to target areas of pain in the body. The double mutations are made to GlyR in a pcDNA3 plasmid, useful for transfecting human kidney cells. The development of the mutant will allow ivermectin to be administered via pill form and to target only those recombinant glycine receptors at the location of pain.

## 2

**Study of the effects of varying ligand substituents in copper mediated Atom Transfer Radical Addition using various tetradentate pyrazole-based ligands**

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The addition of polyhalogenated compounds to alkenes, developed in the 1940s, is known as Atom Transfer Radical Addition (ATRA) Typically these reactions were catalyzed using transition metal complexes. However, the principal drawback was the relatively large amount of transition metal catalyst needed (10-30 mol%). The solution to this problem was found through the use of free radical initiators, such as 2,2-azobis(2-methylpropionitrile) (AIBN).? One particularly active complex in ATRA is the complex of tris(pyridin-2-ylmethyl)amine (TPMA) with copper halides; however, the ligand is difficult to synthetically modify making it unsuitable for substituent studies.? Pyrazole-based ligands with electron donating (methyl)/withdrawing ($CF_3$) groups can be easily synthesized, and are therefore more appropriate for such studies. Specifically, tris((pyrazol-1-yl)methyl)amine ($TP_z$MA) and tris((3,5-dimethylpyrazol-1-yl)methyl)amine ($TP_z$MA-2Me) were synthesized in high yields.? These ligands complexed to copper were found to undergo a reversible reduction process and when applied to ATRA perform with moderate success.

## 3

**The Engineering of Aβ-Selectivity of Neprilysin Enzyme by Phage Display for the Treatment of Alzheimer's Disease**

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Duquesne University

A novel approach for the treatment of Alzheimer's disease entails the clearance of amyloid-beta by a soluble mutant form of neprilysin with enhanced specificity through the use of polypeptide engineering via phage display. A pathological feature of Alzheimer's disease involves the formation of amyloid-beta plaques in the brain where there is a failure to degrade or an overproduction of the amyloid-beta protein. It is essential to purify and modify a soluble form of the protease neprilysin, which is a zinc dependent neuronal membrane protein, for an amyloid-beta cleaving specificity because it exhibits promiscuity in proteolysis of important neuropeptides. The method of phage display allows for the fusion of the active fragment of the neprilysin gene to a particular bacteriophage protein coat gene for polypeptide expression. Random mutations introduced to the active site of neprilysin that are specific for amyloid-beta can be selected via an affinity support column.

## 4

**Ligand Substituent Effect Through 'Click' Chemistry Synthesis of Novel Tris(alkyltriazolylmethyl)amine-Copper Complexes**

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Duquesne University

Copper or ruthenium Huisgen 3+2 cycloaddition was one of the first reactions to achieve 'click' status – a set of criteria for clean, green, and economical synthesis developed to meet the demands of modern chemistry. Robust, versatile, and facile, the copper catalyzed cycloaddition of alkyl azides with tripropargylamine results in the formation of poly-1,2,3-triazoles suitable for complexation with copper halides and subsequent use in atom transfer radical addition (ATRA). The high functional group tolerance allows a wide structural variety of azide starting materials and leads to the production of a family of novel ligands bearing different substituents ranging from highly electron donating (t-butyl) to withdrawing (cyano). All ligands in the series were successfully synthesized, characterized, complexed with $Cu^{II}Cl_2$, $Cu^{II}Br_2$, and $Cu^{I}Cl$, undergo a reversible redox process centered around $E_{1/2}$ = -200 to -100 mV, and show at least moderate activity in ATRA.

**5**

**Comparing Experimental Computed Free Energy of Protein/Substrate Complexes**

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Whenever a protein binds with something, either another protein or a smaller organic or non-organic substance in the cell, the energy state of the complex that results from this binding is measured as free energy. The free energy for many such complexes has been found in experiments, using techniques such as isothermal titration calorimetry. There are also ways to calculate the free energy of protein/substrate complexes using physics; Adaptive Poisson-Boltzmann Solver (APBS) software implements one such approach, commonly known as continuum electrostatics. To allow for quick comparison of APBS's calculated free energy to the experimentally found free energy of protein bindings, the Molecular Operating Environment (MOE) program will be extended to automatically perform APBS calculations on protein/substrate complexes that are stored in a MOE database. The experimental free energies of these protein/substrate complexes will be obtained from online databases that store protein structure and information, such as MOAD and BindingDB.

**6**

**Effect of Sodium and Potassium Chloride on Glutamic Acid**

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Duquesne University

It has been shown that salt solutions can affect proteins in different ways. In particular, polyglytamic acid adopts two conformations in salt solutions. The goal of this project is to see how glutamic acid interacts with sodium and potassium chloride in 0.2 and 2.0M solutions. From previous research on the topic, it was predicted that the different salt concentrations will affect the backbone of glutamic acid. It was also predicted that salt ions will impact the hydration of the peptide leading to the different conformations. Molecular dynamics simulations of glutamic acid in salt water will be used to test our hypothesis. The simulation results will be examined in terms of ion and radial distribution functions. The results of these simulations will be presented in the poster.

**7**

**Solid State Synthesis and Characterization of Mn Doped Silver Indium Selenide for Application in Dilute Magnetic Semiconductors**

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Duquesne University

Mn 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 Mn dopant, and synthesis routes to phase purity. Samples were created of Mn concentrations ranging from 0% to 15%. Stoichiometric ratios, heat treatments, and annealing were investigated 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 to verify Mn's inclusion into the chalcopyrite structure. A Scanning Electron Microscope (SEM) coupled with Energy Dispersive Spectroscopy (EDS) was used to further investigate undesirable secondary phase formation. The band-gap energy (Eg) of the material was determined with a UV-Vis-NIR Spectrophotometer.

**8**

**Characterization of Various Phosphonic Acid Self-Assembled Monolayers on Titanium**

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Duquesne University

Titanium is commonly used in orthopedic implant devices, although one major concern is the possibility of post-operative infection by *Staphylococcus aureus.* Surface modification is widely studied in order to improve the biocompatibility of metal implants. In this study, self-assembled monolayers (SAMs) of octadecylphosphonic acid and (11-hydroxyundecyl) phosphonic acid were formed on titanium using a TLC sprayer and nitrogen stream. Infrared spectroscopy and Matrix-Assisted Laser Desorption Ionization Time of Flight Mass Spectrometry (MALDI-TOF) were used to characterize the deposition and ordering of the SAMs. Peaks generated with Infrared Spectroscopy were recorded at 2916 $cm^{-1}$ and 2850 $cm^{-1}$, which are characteristic of ordered alkyl chains. Peaks generated with MALDI-TOF were recorded at 335.18 m/z, indicating ordered monolayers on the titanium surfaces.

## 9

**A Mathematical Model for DNA Overstretching**

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University of Pittsburgh

DNA overstretching is a phase transition that occurs when DNA is stretched to a length that is ~70% greater than its physiological B-form contour length. This transition occurs rather suddenly, at 65pN force for torsionally unconstrained DNA and at 110pN for torsionally constrained DNA. The mechanism behind this transition is not well understood; specifically, does DNA undergo a transition from B-DNA to S-DNA or does it experience force induced melting? This study focuses on constructing a mathematical model that quantitatively investigates the force-induced melting picture of the DNA overstretching transition in conjunction with recent empirical results. The model I consider is represented mathematically using the Hamiltonian formulation of mechanics from which the equations of motion for the system are derived. My investigation of these equations, both numerically and analytically, serves to determine the viability of the force-induced melting picture.

## 10

**Polystyrene-*b*-poly(ethylene oxide) Nanostructures: The Effect of Spreading Concentration**

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Washington & Jefferson College

Polystyrene-*b*-poly(ethylene oxide) (PS-PEO) is an amphiphilic diblock copolymer that spontaneously self-assembles into orderly nanostructures when applied to an air/water interface. These nanostructures can serve as polymer templates, with applications in semiconduction and particle growth. A series of six polymers with varying compositions of PS and PEO were studied at low (0.1 mg/mL), intermediate (1.0 mg/mL), and high (5.0 mg/mL) concentrations using a Langmuir trough. Langmuir-Blodgett films were transferred at 2 mN/m and imaged using an atomic force microscope (AFM). Various nanostructures resembling continents, spaghetti, dots, and mesh were observed. The nanostructures were analyzed in terms of height and width as well as surface density in order to assess the effect of spreading concentrations. Isotherm plots of mean molecular area vs. surface pressure obtained during compression were also interpreted. This study allows us to better understand PS-PEO interactions at the air/water interface and thus better control the resulting nanostructures.

## 11

**Structure and Function of the Glycine Receptor**

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Single point mutation of alpha 1 glycine receptor (GlyR) gene was performed and verified to aid in the understanding of conformational changes of the receptor. The purpose of this project is to understand the extracellular domain in the GlyR in its different states to aid in the understanding of how the protein adapts its structure to function as a ligand-gated ion channel. The goals of this project were to create single-residue GlyR mutants using Quickchange site-directed mutagenesis kit to verify the presence of desired mutant residues by Genewiz sequencing. The mutated GlyR genes were moved to bacmid virus using Bac-to-Bac Baculovirus Expression System. Finally, SF-9insect cells were infected with the virus to over express GlyR. This aids in the understanding of other similar channels in the cys-loop receptor super family.

## 12

**The effects of the 5-$HT_{1A}$ and 5-$HT_7$ receptors on behavioral recovery after traumatic brain injury**

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Previous data has shown that the 5-$HT_{1A}$ receptor agonist 8-OH-DPAT improves behavioral recovery after experimental traumatic brain injury via that receptor. However, because 8-OH-DPAT also has partial agonist activity at the 5-$HT_7$ receptor, it is possible that this receptor may be involved in the benefits. To elucidate this possibility, we evaluated the effects of antagonists for the 5-$HT_{1A}$ and 5-$HT_7$ receptors. Sixty-eight rats received either a controlled cortical impact or sham injury and were randomly assigned to these groups: 8-OH-DPAT (0.5 mg/kg), 8-OH-DPAT + SB 269970 HCl (5-$HT_7$ antagonist; 2 mg/kg), 8-OH-DPAT + WAY 100635 (5-$HT_{1A}$ antagonist; 0.5 mg/kg), or saline vehicle (1 mL/kg). Each group was tested on motor and cognitive tasks on days 1-5 and 14-19. 8-OH-DPAT alone, or when combined with the antagonists showed cognitive improvement relative to vehicle controls, but there was no statistical difference among the groups. The data did not provide the clear cut distinction of what receptor is mediating the benefits observed with 8-OH-DPAT.

## 13

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

Burkholder, Sydney; Cavanaugh, Jane E.; Monlish, Darlene
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Duquesne University

Each year approximately 500,000 women succumb to breast cancer making it the second leading cause of cancer-related death among women. Extracellular signal-regulated kinase 5 (ERK5) is an intracellular signaling protein that has been shown to increase breast cancer cell growth. This study is designed to further investigate the role of ERK5 in breast cancer cell proliferation using novel inhibitors of ERK5 activation. This study investigated how benzimidazole compounds can act as inhibitors of ERK5 signaling in MDA-MB-231 and human (BT-474) breast cancer cells. Cells were treated with the putative inhibitors of ERK5 and then subject to western blot analysis to investigate ERK5 expression and activation. These studies will advance our knowledge of the role of ERK5 in breast cancer progression and may lead to developments of novel therapies for breast cancer.

## 14

**The Effects of Salts on Amino Acid Leucine**

Chuong, Chris; Litzenberger, Emily; Asciutto, Eliana K.; Madura, Jeffry
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Duquesne University

Through study and experimentation, it has been observed that salt solutions effect a change in both the chemical and physical properties of amino acids. Leucine, a neutral charged amino acid, has been chosen to be studied for the different conformations it can undergo in salt solutions. It is believed that salt ions impact the hydration of the peptide leucine, leading to the different conformations. This project is used to observe whether salts sodium chloride, potassium chloride, and sodium perchlorate at concentrations of 0.2M and 2.0M affect the side-chain conformations and hydration of leucine. Molecular dynamics simulations of leucine in salt solutions will be used to examine the ion and radial distribution functions, testing the hypothesis. The results of these simulations will be presented in the poster.

## 15

**Synthesis and Characterization of Copper and Cobalt Complexes with Dithione Ligands**

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Duquesne University

Dithione ligands are found in biological systems. The goal of this research is to synthesize a series of copper and cobalt complexes with dithione ligands in order to study the influence of these ligands in the chemistry of the set of transition metals along with their physical and chemical properties when coordinated with transition metals. In this research copper (I), copper (II), and cobalt complexes with dithione ligands have been synthesized and characterized. The copper (I) complexes were synthesized by reacting $Cu(CH_3CN)(ClO_4)$ with N,N-diisopropyl piperazine dithione($^{i}Pr_2$-Pipdt) and N,N-dimethyl piperazine dithione ($Me_2$-pipdt), while the copper (II) complex was synthesized from $CuCl_2.6H_2O$. The characterization was done by using UV-Vis and cyclic voltammetry.

## 16

**Optimization and Parameterization of IR and Simple Reaction Mixture Analysis in ATRA**

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Duquesne University

ATRA is a process which carbon-carbon bonds are formed by means of a metal catalyst. An alkyl halide reacts with a copper (I) catalyst to form a primary radical and copper (II). The radical reacts with an alkene forming a secondary radical which abstracts a halogen atom from copper (II) to regenerate copper (I) and a monoadduct. Recent advances in this field have found that addition of a reducing agent can be used to dramatically reduce copper concentrations, making this method more attractive to synthetic chemists. Traditionally, analysis has been conducted via $^{1}H$ NMR spectroscopy, which is inaccessible to smaller research facilities. This study investigates application of gas chromatography and IR spectrophotometry to analysis of these reactions.

## 17

**Modeling the $^{13}C$ Chemical Shift of Polymorphic Pharmaceutical Compounds with DFT Plane Waves**

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Washington & Jefferson College

Proper characterization of polymorphic forms of drugs is essential for patent proposals by pharmaceutical companies. Many drugs consist of a flexible carbon chain that enables dihedral angle changes to occur in the formation of various polymorphs. The carbon chemical shift is sensitive to such changes in this angle leading to dramatic shifts in spectral peaks. Thus, solid-state NMR has become a leading tool to characterize polymorphs. Here, using DFT plane-wave shielding calculations, we model the $^{13}C$ chemical shift and chemical-shift anisotropy of pharmaceutical drugs that exhibit polymorphism. The polymorphs of cimetidine and ranitidine, both histamine H2-receptor antagonists, are model drugs for solid-state NMR studies because crystallization of samples suitable for diffraction studies proves difficult. Spectral peak assignments are established by magnetic shielding calculations. DFT methods that utilize plane waves (GIPAW) efficiently incorporate the full lattice structure of crystalline systems, allowing accurate predictions of chemical shifts.

## 18

**Fluorinated Natural Oil Nanoemulsions for Drug Delivery**

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Duquesne University

Celecoxib is a nonsteroidal anti-inflammatory drug and a selective COX-2 inhibitor that is insoluble in water and possesses low bioavailability. This study proposes the first fluorocarbon-based nanoemulsion designed for celecoxib delivery. This study investigates the optimization of concentrations and ratios of three nonionic surfactants, Zonyl FSO-100, Zonyl FSN-100, and F68, within natural oil nanoemulsions prepared by sonication and microfluidization. Nanoemulsions with a minimized particle size increase the potential viability of this formulation as a drug delivery agent *in vivo*. The amphiphilic surfactants studied possess both hydrophilic and lipophilic regions, thus stabilizing the oil/water interface through a reduction in surface energy and preferential molecular orientation. It was found that olive oil o/w emulsions prepared using either Zonyl FSO-100 alone or a predetermined ratio of the Zonyl FSO-100 to Pluronic F68 yielded relatively stable formulations. Stability was assessed based on the modal distribution of relative particle sizes through Dynamic Light Scattering analysis.

## 19

**Building a Pt/γ-$Al_2O_3$ model heterogeneous catalyst and study of γ-$Al_2O_3$ support effects on Pt nanoparticles**

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University of Pittsburgh

A heterogeneous catalyst showing outstanding performance such as in fuel cells and oil-refining is platinum nanoparticles (NPs) deposited onto a γ-alumina support. Our goal is to create a Pt/γ-$Al_2O_3$ model heterogeneous catalyst and understand the γ-$Al_2O_3$ support effects on the structure and stability of the Pt. Epitaxial growth of (111)γ-$Al_2O_3$ thin film was done on (110)β-NiAl, where the film quality and the epitaxial relationship between β-NiAl/γ-$Al_2O_3$ depends on the oxidation temperature and the film thickness. Transmission electron microscopy (TEM) techniques are used to image the interface of Pt/γ-$Al_2O_3$, while electron energy loss spectroscopy (EELS) is used for understanding the chemical and electronic changes at the interface. Such detailed information of the Pt/γ-$Al_2O_3$ is needed to directly compare with theoretical simulations, which assume a certain crystallographic orientation of the substrate and no impurities. The direct correlation between experiments and theory is critical to understand how supports affect structure and catalytic properties.

## 20

**Synthetic Strategies for Precursor Z**

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Molybdenum cofactor deficiency (MCD) can cause death in patients lacking the molybdenum cofactor (Moco). Our research goal is the synthesis of Precursor Z or Compound Z, which is a precursor to the Moco. Successful synthesis may serve as a drug for patients suffering from MCD. To accomplish this, we first synthesized 2-amino-6-(1,2,3,4-tetrahydroxybutyl)pteridin-4(3H)-one (**1**) to create the pyrimidine and pyrazine units, and the initial framework of Precursor Z. Preliminary experiments were conducted using a simplified model compound. We also reacted galactose phenyhydrazine with o-phenylenediamine in an attempt to get the tricyclic ring structure. The resulting compound will be phosphorylated with PO(OEt)Cl2 to produce a compound that can undergo an Amadori rearrangement to yield our target compound.

## 21

**In-Silico Inhibitor Design for β-Catenin/BCL9**

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β-catenin is a protein involved in cell-adhesion, the Wnt signaling pathway and other biological functions. It has also been implicated in pathological processes, including different types of cancer. β-catenin interacts with numerous different proteins, including BCL9, which is required for the transcription of the Wnt pathway genes. The interactions between these two proteins have been seen as a good target for drug discovery, ever since the crystal structure of this complex was resolved. Our hypothesis is that small molecules that inhibit the binding of β-catenin to BCL9 can be developed using the existent interactions between the two proteins. We have developed a structure-based pharmacophore model that mimics these interactions, followed by a virtual screening using this model against commercially available databases of drug-like molecules. The resulting hits were prioritized using *in-silico* ADME/Toxicity filtering, and molecular-docking, to determine the higher affinity hits. Compounds that emerge will be proposed for biological testing.

## 22

**Slot-Blot Analysis of 3-NT Antibodies in the Spleen of Mice Treated With Adriamycin**

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University of Pittsburgh

Adriamycin, an anti-cancer drug, is known to lead to the formation of free radicals. These free radicals can modify existing proteins and cause cellular dysfunction. One such modification is the nitration of proteins (referred to as nitrosative stress). 3-Nitrotyrosine (3NT) antibodies are common markers of nitrosative stress and can be measured using slot-blot analysis. Two groups of mice spleen are used: a control group and a group treated with adriamycin. Each sample is prepared so that 1µg of protein is loaded into each well of a slot-blot apparatus. The samples are then incubated with primary and secondary antibodies. Upon development, the slots with more 3-NT will turn darker in color. The results are analyzed with Scion Image and assessed for statistical significance. The relative concentrations of 3-NT in the spleen of mice can provide insight into how adriamycin affects the immune system.

## 23

**Nutritional Supplement Contamination Analysis by Traditional and Speciated Isotope Dilution Mass Spectrometry using Liquid Chromatography Inductively Coupled Plasma-Mass Spectrometry**

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The goal of this project was to evaluate the contamination of a nutritional supplement which was tainted with antimony. First, quantification of 64 elements using Inductively Coupled Plasma-Mass Spectrometry (ICP-MS) was performed by calibration curve to find other potential sources of contamination. Next, Isotope Dilution Mass Spectrometry (IDMS) was used to quantify the concentration of zinc and antimony. The speciation of antimony was explored focusing on three species – inorganic forms, Sb (III) and Sb (V), and an organic species, trimethyl antimony chloride using Speciated Isotope Dilution Mass Spectrometry (SIDMS). Sb (III) and Sb (V) are highly toxic whereas organic species of antimony are not nearly as harmful. Ion-exchange Chromatography-Inductively Coupled Plasma Mass Spectrometry (IC-ICP-MS) was used to determine the antimony species in the samples. Mass balance of species, species identification, and quantification by SIDMS allows for the best toxicological assessment from the antimony contamination to correct manufacturing processes.

## 24

**From Genes to Protein: Dissecting the Biology of Malaria Parasites**

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Malaria, a disease that causes more than 500 million clinical cases each year and kills more than 1 million worldwide, is caused by *Plasmodium* parasites that are transmitted by infected mosquitoes. There is an urgent need for a protective malaria vaccine and new anti-malarials to combat the increasing prevalence of drug resistant parasites. We have used molecular biology techniques to construct recombinant plasmids for use in *Plasmodium* transfection studies in order to understand the function and localization of *Plasmodium* proteins of interest. Transfection of these plasmids into the Plasmodium parasites would allow for the disruption as well as the modification of the genes of interest. Transfection and phenotypic analysis of the resulting transgenic parasites would reveal when these genes and the proteins they encode are expressed, where they localized in the parasite and whether they are essential for the development of the parasite in various stages of its life cycle.

## 25

**Modification of Steel 316L and Analysis of Fibrinogen Attachment**

Camera, Katie; Kruszewski, Kristen; Gawalt, Ellen S.
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Duquesne University

Stainless steel 316L (SS316L) is a common alloy that has many biomaterial applications, such as medical implants. However, problems arise due to bacteria and protein attachment to the surface, which can cause the device to fail. Therefore, modification of the SS316L surface is one possible solution to improve its biocompatibility. The surface of SS316L was modified with both self-assembled monolayers (SAMs) of perfluorooctodecanoic acid (PFOA) and polypentafluorostyrene (PFS), which was polymerized from the surface. The surfaces were analyzed using diffuse reflectance infrared fourier transform spectroscopy (DRIFT). Once the surfaces were modified, the samples were immersed in a solution of fluorescently tagged fibrinogen (0.2 mg/mL) for 2, 6, and 24 hours. The adhered fibrinogen was then analyzed using a Zeiss Axioskop. Five images were taken on each sample and the amount of protein attached was quantified using AxioVision software.

## 26

**Searching for Transiting Extrasolar Planets at the University of Pittsburgh**

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University of Pittsburgh

The search for extra-solar planets has become extremely exciting field of research in the past ten years with the number of known extra-solar planets jumping from only a few to nearly 470.The STEPUP team was assembled with the goal of observing transiting planets while providing a meaningful research experience for undergraduates. The various aspects of our project include data analysis and collection, programming, observatory mechanics, and public outreach/education. To date we have observed eight known transiting planets and three potential targets. Using these data, we have helped confirm the existence of several known extra-solar planets and constrained their orbital parameters. We have just begun the analysis of data from an international collaboration for the planet HAT-P-13b in search of transit timing variations. These variations may lead to the discovery of a third planet in this system.

## 27

**Finding associations between protein-annotations in the context of protein-protein interactions**

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University of Pittsburgh

We assembled information pertaining to proteins, such as pathways, associated drugs and disease associations from several different databases. Our goal is to find latent relations between the different genetic, biological and environmental factors. After gaining an understanding of the biological aspects that connect these factors, I am currently working on finding dependence of phenotype factors of disease with genetic and environmental factors. I worked to replicate a previous work in which the authors clustered two separate databases to find the relationship between genes and diseases as well as the relationship between environmental factors and diseases. This analysis when completed would reveal the interrelation of genetic and environmental factors in the context of disease manifestation. Replication of this work gave me the ability to automatically compute and analyze the said relations and also provided a starting point on which to add other factors for further study.

## 28

**Characterization of monolayers on the surface of a Copper Nickel Alloy**

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Duquesne University

Copper Nickel alloys are often used in underwater pipes and marine vessels. The problem with these surfaces is that they are readily corroded. It is proposed that modifying the surface with a self-assembled monolayer (SAM) will prevent oxidation. Metal substrates of cupronickel (55Cu/45Ni) were modified with octadecylphosphonic acid (ODPA) and characterized using diffuse reflectance infrared fourier transform spectroscopy (DRIFT), atomic force microscopy (AFM), and Matrix Assisted Laser Desorption Ionization Time of Flight Mass Spectrometry (MALDI-TOF MS). Initially it was shown using DRIFT that stable films formed and remained through solvent rinse sonication. The deposition conditions were altered in attempt to form an ordered monolayer film on the surface.

## 29

**Creation of Continuous Droplet Flow Using Microfluidics**

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Duquesne University

Microfluidics is relatively new to the field of chemistry and has certain advantages including the ability to control the behavior of fluids at microscopic levels. Microfluidics can be used to contain small numbers of cells which can better our understanding of biologic processes. The main goal of this project is to obtain continuous droplet flow using a variety of different ratios. Different size microdroplets will be generated using various flow rate ratios of oil to aqueous phase. The oil, or mobile phase, perfluorodecalin is a fluorinated hydrocarbon that is immiscible in aqueous and organic solvents. The aqueous phase is comprised of two 5 milliliter syringes full of methanol and another syringe full of dye.

## 30

**Characterization of Cobalt Oxide**

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Duquesne University
*Slippery Rock University

Cobalt alloys are an important metals used in medical applications specifically implant devices. Other metals that make up the alloys have been characterized and modified with organic acid monolayers in an effort to prevent bacterial adhesion however pure cobalt has never been examined. The bare surface of pure cobalt metal was analyzed using Atomic Force Microscopy (AFM). The surface of the native oxide was then modified with organic acid monolayers of octadecylphosphonic acid and stearic acid. Infrared spectroscopy, Matrix Assisted Laser Desorption Ionization Time of Flight Mass Spectrometry (MALDI-TOF MS) and AFM were used to characterize the substrates.

## 31

**Mathematical Model of 5-Fluoro-2'-Deoxycytidine (FdCyd) and its Metabolites**

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Abstract: 5-fluoro-2'-deoxycytidine (FdCyd), a DNA methyltransferase inhibitor, has been shown to allow re-expression of tumor suppressor genes. However, *in vivo*, FdCyd experiences rapid metabolic conversion by cytidine deaminase (CD) to active cytotoxic metabolites 5-fluoro-2'-deoxyuridine (FdUrd), 5-fluorouracil (FU), and inactive 5-fluorouridine (FUrd). Preclinical studies coadministering FdCyd with a cytidine deaminase inhibitor, tetrahydrouridine (THU), slowed the conversion of FdCyd to its metabolites. In these studies, different combinations of FdCyd and THU were administered orally to male $CD_2F_1$ mice, and the concentrations of FdCyd and its metabolites were recorded at various times up to 1440 minutes. We are constructing a compartmental based pharmacokinetic model of FdCyd and its metabolites in the presence, and absence, of THU to assist in the design of combination therapy dosing strategies for patients with advanced malignancies of the lung, head and neck, bladder or breast.

## 32

**Temperature Effects on Nanocrystallization of FINEMET Alloy**

Herchko, Steve
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The effects of temperature on the FINEMET compound FeCuNbSiB are examined in this paper. Using Mössbauer spectrometry and X-ray diffraction as well as differential scanning calorimetry on the substance annealed throughout a wide temperature range, the point at which nanocrystallization begins can be seen as the amorphous components become more defined structures. Through these methods the properties of the amorphous and nanocrystalline phases can be determined as well as the specific stages of crystallization. The decomposition of the amorphous matrix can be seen as more sub-spectra become defined as the temperature is increased to a maximum of 750 degrees Celsius. The FINEMET compound was also tested again with the addition of a stainless steel foil to determine the recoilless fraction.

## 33

**Structural characterization and investigation of iron complexes as catalysts for atom transfer radical addition**

Biernesser, Ashley B.; Eckenhoff, William T.; Pintauer, Tomislav
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The process of atom transfer radical addition (ATRA) is a fundamental reaction used to add halogenated compounds across carbon-carbon double bonds by a radical process. Regeneration of the catalyst by using small amounts of a reducing agent allows for a significant decrease in the amount of catalyst required. Although this methodology has been highly effective for copper and ruthenium mediated ATRA, iron catalyzed ATRA has not been explored to a great extent. Iron(III) complexes with nitrogen and phosphorus containing ligands were synthesized and investigated as catalysts for ATRA, and structural aspects of these complexes were examined. Many structures contained $FeCl_4$ counterions, indicating there may be two active species present. The complexation of $FeCl_3 \cdot 6H_2O$ with ethylenebis(diphenylphosphine) resulted in the oxidation of the phosphine ligand by the $FeCl_3$ hydrate, which may relieve steric strain. Computational optimizations were performed to determine the stability of this complex in the absence of oxygen.

## 34

**A Computational Economic Analysis of Needle-Free MMR Vaccine Technology**

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Despite convincing eradication statistics, the measles virus continues to threaten the health of US citizens. Advancing medical technology has afforded an alternative aerosol spray of the measles, mumps, rubella (MMR) vaccine that provides superior levels of immunity at competitive prices. We developed a decision-analytic computational model using TreeAge Pro software—fueled by researched probabilities, costs and utilities—that features the widely accepted intramuscular injection and the innovative aerosol vaccine, to compare the economic value and effectiveness of each presentation. The generated outcomes will facilitate in the execution of nationally implemented aerosol vaccination efforts with regard to cost-effectiveness and health related results. This primitive model, based in the US, provides a sound foundation for future expansion with the intention of global reach. Ideally, introducing needle-free technology to developing countries will drastically reduce and potentially eliminate the risk of needle-stick injuries and complications associated with supplemental immunization activity.

## 35

**Predicting Observable Signals from the Electroweak Phase of the Early Universe**

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In some extensions of the standard model of particle physics, the electroweak phase transition is first order, in which bubbles of the low-temperature phase nucleate, expand, and merge in the primordial plasma. If this is the case, resulting magnetic fields and relic gravitational waves may be observable today. We aim to simulate the plasma motions in a first-order phase transition using the PENCIL code for magnetohydrodynamic fluid mechanics. I will input initial conditions and parameters into the program to create a simulation on the scale of $1024^3$ grid points. Our ultimate goal is to predict signals for future experiments such as the proposed Laser Interferometer Space Antenna in order to understand the mechanism driving the electroweak phase transition.

## 36

**Effect of Cues on Smoking Behavior among Intermittent Smokers**

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Smoking continues to be the leading cause of preventable death in the United States, and a new faction of smokers has begun to emerge. Intermittent smokers (ITS) comprise 15-33% of US smokers, and do not smoke daily but exhibit difficulty quitting and maintaining abstinence. The Smoking Research Group (SRG) has been studying ITS in attempt to better understand their smoking patterns, using laboratory cue-exposure methods. ITS and daily smokers participated in a study in which they viewed six panels of pictorial cues (positive affect, negative affect, smoking, alcohol, non-smoking, and neutral), rating craving level before, during, and after cue-exposure. Participants were also given the opportunity to smoke, and smoking behavior was later coded for latency and puffs. This study has the potential to inform theories of nicotine dependence, and suggest directions for intervention both with ITS and with regular daily smokers.

## 37

**The Weakest Link: Detecting and Disrupting Interactions between Polß and XRCC1**

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Cancer affects over 11 million people in the United States. Multiple forms of chemotherapy damage cellular DNA to induce cell death. DNA polymerase ß (Polß) is an essential enzyme for repairing DNA damage induced by chemotherapy. The protein XRCC1 binds to Polß and may be required to recruit Polß to sites of DNA damage. Our goal is to disrupt the interaction between Polß and XRCC1 by mutating Polß at specific amino acids that are essential for binding to XRCC1. Preventing Polß binding to XRCC1 should eliminate the repair activity of Polß and sensitize cells to chemotherapy. We have made four Polß mutations and will determine if the interaction domain of Polß with XRCC1 is a potential drug target in cancer cells. This could prohibit the interaction in tumor cells, prevent DNA repair and be a useful adjuvant to chemotherapy.

## 38

**Modeling dynamics of gap junction internalization**

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Gap junction-mediated intercellular communication is critical to the functions of most cells of the body. The assembly of the gap junction channels that allow for this communication has been extensively studied, but the mechanisms involved in the disassembly of gap junction plaques are not well understood. The removal of gap junctions from the cell surface results in the formation of annular gap junction vesicles in the cytoplasm of one of the two contacting cells. This project elucidated the regulation and directionality of this process. We built a computational model of fluorescence microscope time series of gap junction dynamics in living cells. The model helped us to determine patterns in the motion of annular gap junctions and to test the hypothesis that their motion is guided by cytoskeletal elements. This project has increased understanding about the unique gap junction internalization process.

## 39

**Exploring the Use of CUDA GPU Programming for High Performance 3-D FFT Applications**

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The purpose of this project was to take advantage of graphic processing units (GPU) to compute fast Fourier Transformations (FFT). The GPU cluster, Lincoln, at the National Center for Supercomputing Applications, allows the use of the Compute Unified Device Architecture (CUDA) programming model. Lincoln is home to 192 compute nodes (Dell PowerEdge 1950 III dual-socket nodes with quad-core Intel Harpertown 2.33GHz processors, 16GB of memory) and 96 NVIDIA Tesla S1070 accelerator units (345.6 gigaflops of double-precision performance, 16GB of memory per unit). We accessed one CPU node and one Tesla unit. CUDA provides a library to compute FFT, which was compared to the standard FFTW C package running on CPUs. At the maximum memory limit of 16GB for 3-D FFT transformations, CUDA performed with double the speed of a threaded version of FFTW. The CUDA architecture can more than double the performance for FFT calculations with applications in astrophysics.

## 40

**Qualitative and Quantitative Analysis of Mercury Species in Human Blood SRM966 and Crude Oil by GC-ICP-MS**

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The primary focus of this research project was to determine the species of mercury present in blood and crude oil. Methyl, ethyl, and inorganic mercury were qualitatively and quantitatively analyzed using Gas Chromatography-Inductively Coupled Plasma-Mass Spectrometry (GC-ICP-MS). Human blood was spiked with a known concentration of mercury species, Microwave assisted extraction was performed using EPA Method 3200, and centrifuged. The supernatant was collected and analyzed by GC-ICP-MS. The crude oil samples were prepared in the same manner. Blank samples qualitatively contained high amounts of inorganic mercury creating skewed SRM and crude oil concentrations. The ammonium acetate buffer that was used was determined to be the source of contamination. Once contamination was resolved, mercury species were quantified in blood samples by GC-ICP-MS and specialized methods were developed to achieve these measurements using Speciated Isotope Dilution Mass Spectrometry (SIDMS).

## 41

**Lowering the Detection Limits of Primary Fatty Acid Amides**

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Primary fatty acid amides (PFAMs) are lipids found in trace amounts in mammalian tissues. They behave similarly to hormones in that they are responsible for biological processes such as fluid regulation, the inhibition of cancer cell growth, and are thought to be responsible for affective disorders. PFAMs come in various carbon chain lengths and may be saturated or unsaturated. PFAMs ranging from twelve to twenty-two carbons in length were analyzed using gas chromatography/mass spectrometry (GC/MS). Serial dilutions of amide standards were used with GC/MS to determine the limits of detection. This data can then be compared with biological samples to identify and quantitate PFAMs found in mammalian tissue. Being able to discern the differences between stearamide (C18:0), oleamide (C18:1$^{9}$) and linoleamide (C18:2$^{9,12}$) at increasingly lower concentrations is a step toward more accurately diagnosing clinical disorders.

## 42

**Protocol Development for Achieving Simultaneous Quantification of Chromium (III) and Chromium (VI) for Mass Balance**

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In order to determine the toxicity or benefit from the chromium in dietary supplements, chromium (III) and chromium (VI) must be measured and verified with mass balance (sum of both species equaling the total chromium). This is necessary because chromium (III) is an essential trace element for metabolism while chromium (VI) is a toxic carcinogen. In dietary supplements, chromium is labeled as chromium (III) but interconversions between chromium species can cause the toxic chromium (VI) to be present. Because of complexation within the supplements and further interconversions during experimentation, protocol development for recovering all of the chromium involved modifications of Method 3060A. Microwave extraction and Speciated Isotope Dilution Mass Spectrometry (SIDMS) with Ion-exchange Chromatography-Inductively Coupled Plasma-Mass Spectrometry (IC-ICP-MS) were used to account for interconversions. These techniques were adjusted with variations in temperature and addition of a complexing agent in an ongoing attempt to stabilize both species in the same solution.

## 43

**Particle Separation of Cohesive (Wet) Granular Systems**

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Particle separations techniques, in large part, exploit differences in particle properties in a decidedly low tech way; sieves use varying grid spacing to separate particles by size, while fluids are used to separate particles by density. Such processes, however, have a number of issues that make them less than optimal. Sieving/screening is an energy intensive and inefficient process, as the screen must be continuously "unclogged" via high energy vibration; fluid-based separations are both energy inefficient (due to the subsequent requirement for drying) and environmentally unfriendly, requiring either surfactants and/or density-modifiers. In this project, we aim to create a novel separation technique by exploiting the interparticle cohesion caused by introducing a small amount of fluid to a granular mixture. Using both a Particle Dynamics simulations and experimental data, we examine whether differing cohesive forces in a vibrated conveyor can lead to a low energy and environmentally benign technique for particle separation.

## 44

**The Development of a New Matrix for the Fluorescent Lead Sensor, Leadglow (LG).**

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Lead toxicity is one of the most common environmental concerns in the United States, as it can affect almost every soft tissue in the body. Fluorescent based sensors have been of interest for their sensitivity and simplicity. Leadglow is a highly sensitive and selective fluorescent lead sensor and when in the presence of lead the emission band shifts with a fivefold increase in the fluorescence intensity, thus it acts as a turn on sensor. [1] In order to improve the usage, in the case of portable detection, new matrices have been tested. Hydrogel materials have been an important component in numerous biomedical applications ranging from drug delivery systems to tissue engineering scaffolds and have also been used in stabilizing many fluorescent molecules. Here in we show the adaptation of Leadglow to a hydrogel matrix.

[1] L. Marbella, B. Serli-Mitasev, P. Basu, Angew. Chem. Int. Ed. 48 (2009), 3996–3998.

## 45

**Analysis of long range kissing interactions essential in the replication of the Hepatitis C virus**

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The Hepatitis C virus (HCV) is a major cause of chronic liver disease, infecting about 170 million people worldwide. Researchers continue to search for a cure, but none has been discovered yet, partly due to the fact the virus has a high mutation rate. However, it has been discovered that a 55 nucleotide region of the virus' RNA genome (named X55 RNA in this study), is 100% conserved in each of the six genotypes. This X55 RNA fragment has been proposed to be involved in long range kissing interactions with another part of the HCV genome (named 5BSL3.2_short), located in its coding region. The goal of this study is to produce the two HCV RNA fragments and to characterize their proposed kissing interactions by native gel electrophoresis and NMR spectroscopy.

## 46

**Effect of Oxygen-containing Functional Group in the Carbon Source on the Synthesis of Carbon Nanotubes Catalyzed by Fe-Mo Nanoparticles.**

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The vast potential applications of carbon nanotubes (CNT) due to their unusual properties of high stiffness, electrical conductivity and light-weight had led to intensive research of their controlled synthesis. A promising method to produce CNT is through the vapor-liquid-solid mechanism using a carbon source and catalyzed by a metal nanoparticle. Our past research demonstrated that a bimetallic catalyst, such as Fe-Mo, is more effective in producing a larger yield. Our focus currently is the effect of the presence of oxygen/water in the carbon source because oxygen is believed to enhance CNT growth by suppressing aggregation of catalyst particles and oxidizing coke formed on catalyst particles. We used two liquid hydrocarbons with similar structure but different functional groups, toluene and benzyl-alcohol, as our carbon source. We will investigate the effect of the oxygen-containing functional group in benzyl-alcohol as compared to toluene on the yield, selectivity and purity of the CNT.

## 47

**Synthesis of Bicyclic Nitriles**

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Bicyclic ring systems often prove quite useful in the total synthesis of pharmaceuticals and natural products. Zinc in the presence of LiCl is readily inserted into various alkyl-iodotosylates that are subsequently trans-metallated with CuCN·2LiCl to the corresponding Knochel-Cuprate. This cuprate then undergoes conjugate addition to cyclic α,β unsaturated ketonitriles. The resultant then undergoes an intramolecular dimethyl sulfoxide oxidation-cyclization forming functionalized bicyclic nitriles. This reaction is thought to proceed first by a Kornblum oxidation followed by a Mukaiyama aldol cyclization.

## 48

**Neural Blood Pressure Control**

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It is important to maintain blood pressure at consistent levels. Doing so requires adjusting blood flow to different body regions to meet metabolic needs, as well as adapting to perturbations such as postural changes. Blood pressure (BP) is controlled by a part of the brain called the Rostral Ventrolateral Medulla (RVLM). The RVLM receives input from BP detectors called baroreceptors, as well as other signals including vestibular inputs that adjust blood flow during postural changes. Interestingly, RVLM activity has not been studied in intact animals that are free from anesthesia, which can greatly alter responses of neurons to stimuli. Our goal is to understand how RVLM neurons respond to changes in BP and posture in conscious animals. To this end, we compared RVLM neuronal activity during different phases of the cardiac cycle, during tilts in different directions, and before and after damage to the inner ear to remove vestibular inputs.

**49**

**MAT Homologue LeuT Transport Mechanism and Conformational Sampling with Principal Component Analysis**

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Monoamine transporters, a class of Neurotransmitter Sodium Symporters (NSS) involved in the reuptake of substrates such as dopamine and serotonin that regulate neuronal functions, are highly homologous in structure and function with the bacterial leucine transporter (LeuT). The symporter uses an electrochemical gradient formed with sodium to fuel the not fully understood transport mechanism. Three 250ns accelerated molecular dynamics simulations were performed with LeuT in a membrane system: one with the sodiums and the leucine substrate, one with the sodiums but without the substrate, and one with neither the sodiums nor the substrate. The conformational changes caused in LeuT by each component of transport will be highlighted in order to better understand the transport mechanisms of NSSs. Trajectories from the simulations using the AMBER forcefield were analyzed using principal component analysis (PCA). The PCA revealed six primary conformations, three of which have currently been undiscovered.

**50**

**Development of a Method for Arsenic Speciation by Speciated Isotope Dilution Mass Spectrometry (SIDMS)**

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Arsenic is a ubiquitous element that comes in many different species. In cases of arsenic contamination or exposure, it is vital to know the species involved because they are of varying toxicities, with $LD_{50}$s varying from 4.5-10,000 mg/kg. For the analysis of elemental species, Speciated Isotope Dilution Mass Spectrometry (SIDMS) is a standard method adopted by the EPA as Method 6800. This method uses man-made, non-natural isotopically-enriched forms of each species to determine interspecies conversions that may take place during testing of labile forms. Arsenic is monoisotopic, making the traditional method unfeasible. To apply Method 6800, $^{18}O$ was used to enrich the most toxic species, As (III). With these spikes, SIDMS is being applied using Microwave Assisted Enzyme Extraction (MAEE), followed by Ion-Exchange Chromatography-Inductively Coupled Plasma Mass Spectrometry (IC-ICP-MS), and Time of Flight (TOF) mass spectrometry.

**51**

**Data Mining of PDB Database for Fragment-based Drug Design**

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Fragment-based drug design is a new approach that uses X-ray crystallography or other physical techniques to successfully screen fragment libraries for specific binding to a target protein. The knowledge of where specific chemical fragments bind to a protein is readily available through protein data bank (PDB) and Relibase. Querying the PDB using Relibase allow for the discovery of thousands of small molecule fragments that bind to specific active sites of any proteins giving way to creating higher affinity compounds. Two prominent fragments for drug-design are piperazine and para-chlorobenzyl motifs. Chemoinformatic studies of the databases give hundreds of ligands that contain either of those two fragments. The further investigation provides how the fragments are interacting with specific amino acids on target proteins. This study will give the insight of new directions for drug design based on these two fragments.

**52**

**Computational Modeling of Cytoplasmic Dynein Heavy Chain 1 Motor Domain and Binding Sites of Potential Inhibitors**

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Cytoplasmic dynein transports organelles along microtubules and is involved in other intracellular processes. No high resolution NMR or EM results exist for cytoplasmic dynein. Therefore, its structure remains largely unknown. Homology modeling coupled with the best possible matching to the low resolution EM results is how cytoplasmic dynein has been modeled. The computer programs MOE and MODELLER were used to produce, new models of the cytoplasmic dynein heavy chain 1 motor domain of *Homo sapiens* based on models homologous to regions of this large (~0.5MDa) protein. MOE was also used to examine potential binding sites for inhibitors by the running of docking simulations with experimentally tested inhibitors of dynein to find most likely binding sites. The overall goal of this work was to find computational, chemical and/or biological tools that can eventually be used to develop pharmaceuticals to treat the diseases that have been linked to cytoplasmic dynein.

**53**

**Novel Synthesis of Drug-Like Compounds with the Innovative Modification of the Ugi Reaction**

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Multicomponent Reactions (MCRs) are a highly efficient class of reactions in which three or more starting materials are reacted all in one step to produce a single product. One particular MCR is the Ugi reaction, which is of great value for drug discovery because variations of the starting materials can yield a library of compounds with great diversity. A variation of the classic Ugi reaction is the Ugi-4-centered-5-component reaction (U4C5CR) in which an amino acid, an aldehyde, an isocyanide and a nucleophile are reacted in one step. Herein we report a library of a new adaptation of the U4C5CR where we add an additional point of diversity to the scaffold by using an amine in trifluroethanol instead of methanol. Previous reports to make these products in two steps gave a racemization of the stereocenter. This new method is not only done in one step but also retains the stereochemistry.

**54**

**The Fragile X Mental Retardation Protein: Translation's Frenemy?**

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Fragile X Syndrome is the most common form of inherited mental retardation, being caused by the loss of expression of the fragile X mental retardation protein (FMRP). FMRP binds to specific messenger RNAs (mRNA) and regulates their translation via its arginine-glycine-glycine (RGG) box domain. The microtubule associated protein 1B (MAP1B) mRNA, has been shown to be an *in vivo* target of FMRP, been shown to fold *in vitro* into a G quadruplex structure, and be is bound *in vitro* with high affinity and specificity by the synthetic FMRP RGG box peptide. In this study, we inserted the G quadruplex forming sequence of MAP1B mRNA into the 5'-untranslated region of a luciferase reporter gene to analyze the translation regulation activity of FMRP. Our bioluminescence spectroscopy results indicate that FMRP acts as a potent translation repressor by binding the G quadruplex structure located in the 5'-untranslated region of the luciferase reporter gene.

**55**

**Fibroblast Cytotoxicity on Modified Stainless Steel**

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Bacterial infection is one of the leading causes of medical implant failure. Recently, the modification of these implants surfaces has attracted growing interest. This research examines the use of perfluorooctadecanoic acid (PFOA) and pentafluorostyrene (PFS) to modify the surface of SS316L, stainless steel, a common medical metal. The biocompatibility of these modifications to fibroblasts, cells that make up connective tissue in the body, was also investigated. Fibroblasts were attached and grown for three different time periods, 1 day, 4 days and 7 days. The samples were stained with an ethidium homodimer and calcien AM, two fluorescent tags. The samples were then imaged using a fluorescent microscope, from which the toxicity was then determined.

**56**

**Osteoblast Proliferation on a Modified Calcium Aluminate Surface.**

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Providing an optimal tissue scaffold is critical for the regrowth of bone at a major injury site. In this study, calcium aluminate (CA) surfaces were investigated as potential bone tissue scaffolds. Furthermore, CA was modified with melatonin (N-acetyl-5-methoxytryptamine) in an effort to enhance cell proliferation. Cell proliferation of human osteoblasts on these surfaces was measured. Melatonin was attached to the CA surface via a two-step process and attachment was confirmed using Diffuse Reflectance Infrared Fourier Transform spectroscopy. To ensure sterility, all CA samples were autoclaved prior to cell adhesion. Osteoblast proliferation on CA surfaces was quantitatively measured at growth points of one, four, and seven days. Due to the high degree of variability in the auto-fluorescence exhibited by CA, a standard proliferation assay could not be performed. Rather, a cell viability stain was performed and cell growth was hand-counted using a Zeiss Axioskop.

**57**

**Transfer of DNA: using different transfer methodologies for obtaining "Touch DNA"**

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Touch DNA has gained international attention as a forensic methodology for obtaining DNA profiles from epithelial cells shed during normal activity. Touch DNA has been confused with low-copy number DNA (>100 pg), however the former has been accepted in US courts since 2005, while low-copy number is still controversial due to variation in amplification. The present study examines collection methodologies using two surfactants (20% SDS and water) and two different commercially-available swabs (traditional cotton and CEP) for the collection of DNA from a live-scan prism surface. The extracted DNA was amplified using RT-PCR to determine DNA concentration. After RT-PCR, samples were subsequently amplified using a 5 STR mini-plex panel (AW12106) for genotyping. To date, partial profiles have been obtained, however work is underway to obtain full profiles without resorting to "extraordinary measures" such as pre-amplification or longer injection times, which are not in accordance with the current legal and scientific communities.

**58**

**Solvothermal Synthesis of Novel Semiconductors Based on the Tris(2-aminoethyl)amine Ligand**

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Solvothermal synthesis techniques using the tren ligand (*tris(2-aminoethyl)amine*, $C_6H_{18}N_4$) were used to prepare the novel materials $(tren)_2Sn_2S_6$ and $[Zn(tren)]_2Sn_2S_6$. The previously reported compound $[Co(tren)]_2Sn_2S_6$ was also prepared in the same manner. Materials were characterized by powder X-ray, single crystal X-ray, DTA and UV-VIS/IR spectrophotometry. A series of experiments explored the impact of reagent stoichiometry, reaction time and the use of water as a co-solvent on the synthesis of $(tren)_2Sn_2S_6$. The reaction is both rapid and robust, producing the desired product within 24 hours and across a range of conditions. Anhydrous $(tren)_2Sn_2S_6$ crystallizes in the monoclinic space group $P2_1/c$, while crystals of $(tren)_2Sn_2S_6 \cdot 2H_2O$ are triclinic P-1.

**59**

**De novo prediction of the DNA binding Interface of tandem repeats of TAL Type III effectors**

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The DNA binding region of TAL-Type III transcriptional activators is made up of a domain of tandem repeats. Two variable residues allow each repeat to bind a specific DNA base pair. While the relative specificities of the variable residues are known, no structural models of TAL proteins exist. We predict the binding mode of the two residues contacting the base pairs computationally. The optimal structure for bound repeats was determined by sampling positions, selecting for those that provided favorable molecular interactions. Optimizations for all repeats were combined to find an optimal orientation for their common backbone. Validation was performed using an explicit solvent free energy scoring function. The relative affinity of each repeat predicted by the scoring function agrees well with observed binding frequencies to each of the four base pairs, revealing the molecular basis of recognition for this important class of factors.

**60**

**A Comparison of Lead, Barium and Antimony Isotope Concentrations in Gunshot Residue Using ICP-MS and SEM**

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Gunshot residue (GSR) evidence may directly link an otherwise unknown subject to an environment of weapon discharge. A bulk analysis of Pb-208, Ba-137 and Sb-121 concentrations in acetate, cotton, nylon, polyester and rayon fabrics containing GSR was done by Inductively Coupled Plasma-Mass Spectroscopy (ICP-MS). Then a total evaluation of all the particulate present in the fabrics was done by manual Scanning Electron Microscopy (SEM) to determine if the potential particles were consistent with GSR. ICP-MS results showed that acetate and nylon retained the fewest amount of GSR, while rayon, cotton and polyester retained the most GSR. Contrastingly, SEM results indicated that polyester had a multitude of particulates composed of Pb-Ba, but only a single unique GSR particulate. A quick backscatter method for the detection of GSR on fabrics using SEM was also developed during analysis of the different types of fabrics.

## 61

**Membrane Pore Model of Benzophenone-Containing Compounds and Critical Intermolecular Interactions that Stabilize the Heptamer Pore**

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Antibiotic resistant bacteria have been a cause for rising concern in hospitals, and communities. It has been found that benzophenone compounds demonstrate good kill kinetics and limited capability for resistance. The mechanism by which these compounds work has not been identified. It is thought that seven compounds and magnesium assemble to form a pore in only the bacterial cells leaving human cells unharmed. In this study, increasingly sophisticated model pores were constructed to evaluate intramolecular interactions necessary for its formation using semiempirical methods and density functional theory. Each pore started as a heptamer of benzophenone units in $D_7$ symmetry. The symmetry constraints were relaxed as each monomer was extended to include more functionality. Key interactions, such as between the benzophenone phenyl rings and the nitrogen in the pyrrole ring, are responsible for pore stability, which is an important first step in understanding the mechanism of the antimicrobial activity.

## 62

**The Effects of Persistent Cyclic Tension on Mesenchymal Stem Cells.**

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A primary objective of tissue engineering is to create functional tissues tailored to a patient's needs. Bone-marrow derived mesenchymal stem cells (MSCs) provide an ideal source of autologous pluripotent stem cells within the adult body. Tissues engineered from autologous stem cells may negate the need for immunosuppressive therapy in the context of transplants. Complex cell matrix interactions play a vital role in the homeostatic regulation and are likely required for cell viability and proliferation. Electrospun poly (ester urethane) urea (ES-PEUU) provides an ideal platform with which to study micro scale force transduction, while also replicating tissue level mechanical properties exhibited by native tissues. Cellular integration into ES-PEUU scaffolds is accomplished by concurrent electrospraying of MSCs during fabrication. Cell seeded scaffolds are subjected to cyclic tensioning for both two and four week periods. Cellular differentiation and biosynthesis of structural proteins are examined.

## 63

**A MATLAB implementation of a self-gravitating massless boson field**

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Computer simulations are very important tools when it comes to investigating the physics of compact stars and black holes. Computational physicists use languages such as Fortran and C to simulate such systems. Unfortunately, a steep learning curve has made these practices inaccessible to undergraduate students. However, in recent years a user-friendly language named MATLAB has become widely available at the college level and in engineering applications. Using the coupled Einstein-Klein-Gordon system in spherical symmetry, and integrating numerically by the finite-differences method, our research resulted in a MATLAB code that accurately simulates the evolution of a boson field. The simulation moves in time showing the intensity of the boson field as a function of position. We are able to demonstrate that individual components of the code, such as boundary placement, high-frequency noise control and initial field amplitude, have a critical effect on the quality of the simulation.

## 64

**Comparing Plaque Assays for Viral Quantification to Study RSV Pathogenesis**

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Respiratory Syncytial Virus (RSV) infects nearly all children by the age of two. According to the World Health Organization, RSV is responsible for 64 million infections and 160,000 deaths annually. Currently, there is no effective treatment. RSV infects lung epithelial cells causing cell death and airway inflammation. Mature alveolar macrophages function to remove cellular debris upon activation. Infants have functionally immature alveolar macrophages, which may contribute to RSV disease. To study RSV pathogenesis, RSV must be quantified for use in mouse models. Plaque assays are the gold standard for virus quantification, yet variability among assays contributes to variability in animal doses. The two most commonly used plaque assays were optimized, compared, and their linear range of quantification established. Understanding variability in plaque assays will improve consistency among animal models. We hypothesize there will be a significant difference among RSV titers between these two plaque assays.

## 65

**Fabrication of Superhydrophobic and Superhydrophilic Surfaces Using Nanoparticles**

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Composite nanoparticles with well-defined structures and surface morphologies characterized by a hierarchical dual-size roughness have received increasing attention due to potentialities such as the fabrication of superhydrophobic surfaces. The experimental procedure found in literature regarding the fabrication of superhydrophobic surfaces involves surrounding a polystyrene particle core with smaller silica particles, giving a raspberry-like structure. However, the properties of surfaces made from such structures are easily lost with physical wear tests such as rubbing. This study involves the fabrication of more robust superhydrophobic surfaces. Raspberry-like composite nanoparticles with polystyrene particles as cores have been successfully created via a sol-gel method. Alterations to this procedure such as replacing the polystyrene particles with silica particles are now being tested as well as various methods to modify the surfaces of the particles from hydrophilic to hydrophobic. Future experimentation will involve using polymer binders mixed with the raspberry-like particles to fabricate a superhydrophobic surface.

## 66

**Oxide Nanoelectronics: Developing ultra-small electronic structures and characterizing their electronic properties at low temperatures**

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Characterization of nanostructures at the LAO/STO interface in a cold temperature environment minimizes not only the electrical resistance of the system, but the scattering of electrons, as well. The scattering of the electrons is caused by phonons, the quanta of the elastic wave in a crystal lattice. At low enough temperatures, these vibrations basically cease, leaving the electrons a “free path”. If one is able to get the temperature low enough, you begin to witness a change in phase, namely, superconductivity. The goal of this research is to design and build a 10K cryostat. While the temperature of the cryostat constructed will not be low enough to witness superconductivity, quantum dot and single electron behavior may be observed.

## 67

**Analysis of the negative strand genomic RNA in Hepatitis C Virus (HCV)**

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Hepatitis C Virus (HCV) infection is life-threatening, affecting 170 million people worldwide. HCV evades all current medical treatment by virtue of its error prone RNA dependent RNA polymerase used to replicate its genome. The replication of the HCV genome involves the production of a negative RNA strand, complementary to the positive sense genome RNA which further serves as a template for the synthesis of more positive genome RNA. Recently our group showed the ability of the positive genomic RNA to dimerize via a kissing complex intermediate structure. My project investigates if the negative strand of HCV, maintains this ability to dimerize similar to the positive strand genomic RNA. Given that dimerization which is otherwise, a functionally distinct feature of retroviruses such as HIV, is currently the most targeted by effective antiretroviral drugs, analysis of dimerization in HCV could provide potential targets for new drugs.

## 68

**Garlic mustard-invaded forest soils suppress fungal hyphal growth**

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Garlic mustard (*Alliaria petiolata*, Brassicaceae), hereafter GM, is a widespread noxious invader of N. American forests. Like some members of the mustard family, GM increases soil levels of allyl isothiocyanate (AITC), a powerful anti-fungal agent suspected to increase GM’s invasive success. Low AITC concentrations are known to inhibit fungal spore germination *in vitro*, but the effect of GM’s AITC on fungal growth within invaded soils is unknown. Therefore, we buried cellulose membranes in field plots with no GM (control) or with natural densities of GM at three sites for four weeks and then quantified hyphal colonization on the membranes using digital image analysis. We found that total hyphal length is significantly lower in GM vs. control plots, and mean hyphal length/image is significantly lower in GM vs. control plots at two sites. These results show that GM-infested soils suppress vital fungal growth and implicate that AITC produces this effect.

**69**

**Computer Simulation of Cell Mechanics to Model Tumor Growth Using Dissipative Particle Dynamics**

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A better model of tumor cell growth and cell-cell interactions could lead to enhanced understanding of tumor invasion and metastasis. In this work, we use a coarse-grained simulation technique, Dissipative Particle Dynamics (DPD), to directly model mecanical interactions between growing cells and the surrounding tissue. In the DPD technique, three forces (dissipative, conservative, and random) are coupled to capture meso-scale molecular interactions while preserving hydrodynamics and cell boundaries. Our code also includes an additional spring force between cell membrane particles to mimic the dynamic behavior of the cell boundary. Ultimately, our goal is to use this molecular dynamics-inspired approach to capture the behavior of growing and mitotic tumor cells and microtumors. It is expected that with this more precise computer model, we will be able to better simulate diffusion of nutrients and chemotherapeutics across the cell membrane, the mechanics of cell interactions around a blood vessel, and tumor invasion/metastasis.

**70**

**Pharmacophore Modeling Strategies for the Development of Novel Nonsteroidal Inhibitors of Human Aromatase (CYP19)**

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Human aromatase is a cytochrome P450 (CYP19) enzyme that catalyzes the biosynthesis of all estrogens from androgens. Suppressing estrogen through aromatase inhibition allows for the treatment of hormone-sensitive breast cancer. Several classes of inhibitors for aromatase have been developed, but important side effects from prolonged clinical use calls for new, more potent, and less toxic CYP19 inhibitors. Through a combination of structure- and ligand-based pharmacophore modeling approaches, we have developed a “merged” model that was used to virtually screen commercially available databases to identify potential novel inhibitors for aromatase. A docking protocol was also developed to rank compounds based on predicted binding affinity. *In vitro* and *in vivo* testing using zebrafish embryos are currently underway and are expected to show that this combination of approaches can be effectively used to identify the next generation of aromatase inhibitors that are highly specific with less adverse side effects for breast cancer treatment.

**71**

**Gorilla Mitochondrial DNA Diversity: assessing patterns of variation and avoiding numts.**

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Gorillas (*Gorilla gorilla*) are one of our closest relatives, and among the most endangered primates in the world. Mitochondrial DNA (mtDNA) is often used to characterize genetic diversity in wild and captive populations, but can be confounded by the accidental inclusion of “numts”. Numts are sequences of mitochondrial DNA that have transferred into the nuclear genome over the course of evolutionary time. We determined the unique DNA sequence of the D-loop portion of the mitochondrial genome from various gorillas living in U.S. zoos to infer their geographic origin. We also identified previously unknown numts from a gorilla genomic library cloned into bacteria artificial chromosomes (BACs). BAC clones were grown, amplified, and partially sequenced to indentify the genomic location of novel gorilla-specific numts. These results are helping to understand the evolutionary history of gorillas, and have implications for conservation genetics and captive breeding programs.

**72**

**Under Pressure-The Effect of Surface Pressure on PS-PEO Nanostructures**

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Polystyrene-b-poly(ethylene oxide) (PS-PEO) diblock copolymer is an amphiphilic polymer that microphase separates into well-defined nanostructures that resemble dots, spaghetti, and continents. These structures can spontaneously assemble when applied to the air/water interface, and the structures can be used as polymer templates. Of particular interest is learning to predict and therefore control the density, size, and distribution of the nanostructures. This study examines the effect of surface pressure on PS-PEO domain formation. Several polymers with constant PEO chain length and varying amount on PS were characterized as Langmuir films through isotherm data and examined as Langmuir-Blodgett films through tapping-mode atomic force microscopy (AFM). Images were analyzed by measuring the dimensions of the observed features in order to better assess the role that surface density plays in film formation.

## 73

**Recovery and analysis of nuclear DNA from burnt tissue using white-tailed deer (*Odocoileus virginianus*) as an animal model**

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Historically, teeth have been used for identification of badly burned remains largely due to the composition of enamel withstanding the burning process. However, dental records are needed for positive identification and are not always available. This study examined the ability to recover nuclear DNA from both tendon and muscle tissue of white-tailed deer (*Odocoileus virginianus*) legs after they have been subjected to gasoline, kerosene, and lighter fluid treatment burns and a non-accelerant wood burn control. These accelerants were chosen because they have been most frequently used to cover up a homicide in order to make victim identification more difficult. To date, DNA has been extracted, quantified, and amplified from the burned samples. A previously designed STR-marker panel was used to genotype the remains. A genetic profile has been obtained from the majority of samples, and the DNA recovery was much greater in the tendon samples than in the muscle tissue.

## 74

**Phase-Changing Aminosilicone $CO_2$ Absorbents**

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An aminosilicone liquid with a primary amine at each end is very unique in that it is capable of capturing $CO_2$ as a fine, dry, carbamate salt powder that is 18wt% $CO_2$. Two amines are required to capture a single $CO_2$ in the form of a carbamate salt, therefore one can consider the $CO_2$ as a “crosslinker” for neighboring aminosilicones. The reaction between the aminosilcone liquid and the $CO_2$ gas is well suited to occur in a “Spray Dryer” in which the $CO_2$ flows concurrently with a mist aminosilicone generated by a nozzle. The $CO_2$-depleted gas and aminosilicone carbamate salt powder leave the spray chamber and then flow into a cyclone, where the powder is accumulated and the $CO_2$-deplteed gas is vented. This is the first report of a liquid-solid phase change $CO_2$ sorbent, and this study will examine the powders generated with various size nozzles and with several aminosilicones.

## 75

**Charge and Conformations of the Carboxyphosphate (CP) Intermediate of N5-CAIR Synthetase**

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CP is an important short-lived intermediate formed by the enzyme $N^5$-CAIR synthetase. Theory and computation have been used to determine the link between reactivity, conformation, and charge in CP. Calculations identified six dianion conformations, but the sixteen monoanion conformations were more relevant to the reactivity of CP. Specifically, it was found that intramolecular proton transfer depends upon a specific conformation that is only accessible by the monoanion. Furthermore, we show that ground state destabilization through hyperconjugation and steric forces are responsible for these reactions. A second CP conformation, acquired by torsional rotation resulting in a 180° flip of the “trigger” proton, is required for decarboxylation to generate the desired $CO_2$. It was found that the proton acted as a switch to regulate both key reactions with CP. Similar studies were also done on carbamoyl phosphate and phosphonoacetate to validate these results.

## 76

**Energetic Contributions of SERT Residues E493 and E494 to Drug Binding**

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The serotonin transporter (SERT) has been shown to play a key role in maintaining brain chemistry. Its function has been linked to a multitude of mental disorders; it follows that SERT is a target for antidepressants such as citalopram and sertraline. Though inhibition assays have been performed with these drugs, the exact binding mechanism remains unknown. This study seeks to elucidate the contributions of two neighboring glutamic acid residues, E493 and E494, to binding in SERT’s vestibular binding pocket. It is hypothesized that these residues interact to lower the binding free energy. Using alchemical free energy perturbation methods, the E494T mutation, and the E493A mutation with the subsequent E494T mutation were performed. Calculations were performed on SERT:sertraline, SERT:citalopram, and SERT:cocaine complexes in aqueous solution, and with no substrate bound. The results of these simulations, along with comparison to existing experimental data, will be presented.

## 77

**High Performance Liquid Chromatography-Mass Spectrometry Analysis of Organic Compounds in Soil**

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Soil evidence can prove to be key in forensic science cases and contains many compounds that can be analyzed, including organic compounds. Soil samples were obtained from different geographical areas around Allegheny County. An organic solvent, acetonitrile, was used to extract the organic compounds from the soil, and the resulting extract was analyzed using High Performance Liquid Chromatography-Mass Spectrometry (HPLC-MS). For increased sensitivity, an HPLC-MS/MS (HPLC-Tandem Mass Spectrometry) system was also used. Analysis of the obtained data has shown few differences between soil extract samples and extraction solvent blank samples. Presently, various aspects of the analysis method, like the HPLC column and solvents, as well as the extraction solvent, are being modified in an attempt to better distinguish sample components. This should allow the soil extract samples chromatograms to be distinguished from the corresponding solvent blank with the main goal being differentiation between different soil samples.

## 78

**Computational Chemistry in Freshmen Chemistry Laboratories**

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A series of three computational laboratories were designed for the honors freshmen chemistry laboratories at Duquesne University to teach students the basics of chemical structure and thermochemistry. The idea is to correlate laboratory activities with lecture material on chemical bonding. The first laboratory involves the use of GaussView to instruct students how to create three-dimensional models using the program, as well as basic commands for molecular visualization. The second laboratory instructs students on the different theories used in computational chemistry and the different commands used to obtain structural, energetic, and vibrational information from energy minimization to frequency analysis. The final laboratory is designed to understand complicated ideas, such as hyperconjugative forces and conformational analysis in organic molecules. It has been reported that students benefit from a hands on approach to understanding the theory of chemical bonding taught in the classroom.

## 79

**The Conformational Effects of a Lysine Residue in 0.2M and 2.0M Salt Solutions of NaCl and NaClO4-**

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Proteins are typically found in buffered solutions, which are comprised of cations and anions. These cations and anions interact with the protein. This project involved studying part of a protein, specifically a lysine residue's interaction with the salts sodium chloride and sodium perchlorate. It is known that salt affects an amino acid's conformation in two ways, elongation or coiling, due to hydration. Developing from this knowledge, our hypothesis was that the salt ions (Cl-, ClO4-, Na+) impact the hydration of the lysine residue, leading to the different conformations. Molecular dynamics were performed for lysine in a saltwater box of 0.2M and 2.0M concentrations. Radial distribution functions and ion diffusion were used to analyze trajectory data and elucidate the configuration of the lysine residue.

## 80

**Structure, Vibration, and Energy of Benzophenone Complexes as the Basic Unit of Antimicrobial Membrane Pores**

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Due to the over-prescription of antibiotics, methicillin-resistant *Staphylococcus aureus* (MRSA) has developed multiple-drug resistance against commonly used antibotics. This multiple-drug resistance has led to the fear that MRSA may one day be untreatable without the development of a new class of antibiotic. Research indicates that benzophenone compounds in the presence of magnesium ions display good kill kinetics of microbial cells. It is proposed that benzophenone compounds self-assemble into a heptamer pore in the bacterial membrane. Semi-empirical methods, density functional theory (DFT), and *ab initio* methods were used to analyze the structure, vibrations, and energies of seven different benzophenone complexes with magnesium ion(s) and water molecule(s) in vacuum and solution. Each level of theory is critiqued to best decide upon how to construct the full-scale heptamer membrane pore model. Semi-empirical methods were found to overestimate grossly the complexation energies of water and benzophenone; however, they produced accurate results for the complexes with magnesium.

## 81

**Binding Analysis of a Mutated Fragile X Mental Retardation Protein to G-Quadruplex Forming Messenger RNA and Its Link to Fragile X Syndrome**

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Fragile X Syndrome (FXS) is the most common form of inherited mental retardation affecting approximately 1/4,000 males and 1/8,000 females. FXS is linked to overabundant (>200) cytosine-guanine-guanine trinucleotide repeats in the fragile X mental retardation 1 (*fmr1*) gene. Hypermethylation of the cytosines leads to transcriptional silencing of *fmr1* and loss of the fragile X mental retardation protein (FMRP). However, recently a patient exhibited phenotypic signs of FXS while still producing FMRP. Upon further study, a guanine insertion was found in the *fmr1* gene causing a frame shift mutation, which affects the FMRP arginine-glycine-glycine (RGG) box and generates a premature stop codon. Wild-type FMRP has been shown to bind to G-quadruplex forming messenger RNAs via its RGG box. This study analyzes the binding ability of the mutated FMRP-RGG box to G-quadruplex forming human Semaphorin 3F-sh mRNA, which is a shown *in vitro* and *in vivo* binding target for wild-type FMRP-RGG box.

## 82

**Desipramine binding energy in monoamine transporter mutants by free energy perturbation**

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Desipramine, a selective norephinephrine transport inhibitor (SNRI), binds to the norephinephrine transporter (NET) with great affinity while showing little affinity for the dopamine (DAT) and serotonin (SERT) transporters. It has been shown that residues F246, S329, G330, and A261 are crucial to desipramine binding. A significant loss of potency is observed when these NET residues are mutated to their DAT counterparts. However, mutating DAT at these residues to their NET counterparts does not consistently correspond to increased desipramine potency. The NET double mutant S329P/G330L shows a 3000-fold loss of potency where as the corresponding DAT mutant shows no gain of potency, and it is likely that the use of molecular modeling will help identify the cause of this discrepancy. Using the molecular dynamics method free energy perturbation (FEP), changes in the binding energy and interactions of several MAT mutants was investigated. The results of numerous FEP simulations will be presented.

## 83

**Computational Determination of Protein Pockets and Channels**

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The “high” associated with cocaine in humans is due to an abundance of dopamine within the synaptic cleft. This occurs when cocaine binds to and inhibits the proper function of the dopamine transporter protein (DAT). The interactions and binding of dopamine and cocaine at different places within DAT causes conformational changes to the protein. In order to understand DAT’s function and dynamics, the individual conformations need to be elucidated and compared. Investigating 3D models that suggest substrate translocation properties can aid in the understanding of how the protein functions. Using Scientific Vector Language (SVL), a programming language, along with MOE, a program in which the results can be visualized, a program was written to display points that lie outside of a certain radius of atom positions within the protein. This program will help determine the location, size, and nature of pockets and channels within protein models.

## 84

**Computational study of carboxyphosphate in $N^5$-CAIR synthetase**

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$N^5$-CAIR synthetase is an antibacterial drug target. $N^5$-CAIR synthetase generates carboxyphosphate (CP) during its catalytic cycle and we have investigated CP and active site models using a variety of computational methods. Our calculations reveal that CP is initially synthesized as a dianionic, linear molecule that is quickly protonated by Lys353 to generate the monoanion. The monoanion folds into a specific pseudo-chair conformation, which allows for intramolecular proton transfer from the acid to the phosphate group. Rearrangement of the resulting product into a specific conformation allows for decarboxylation that generates carbon dioxide and $H_2PO_4^-$. The activation energies are found to be correlated to CP conformation. The above results represent the first detailed calculations performed on CP and these conclusions have important implications for $N^5$-CAIR synthetase and other carboxylating enzymes.

## 85

**Use of *Anopheles* gut trypsin to release anti-malarial effector peptides**

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Global deaths due to malaria now range from 1.5 to 2.7 million each year. As part of an ongoing initiative seeking to design anti-malarial bacterial strains, this research investigated the utility of a protease cleavage site in releasing highly specific, anti-malarial peptides from their secreted carrier proteins. The trypsin cleavage site, IEGR, was tested for release by placing it C-terminal to a Myc epitope tag. The construct was digested in vitro using bovine trypsin and digestion products were assayed by western blot for the presence of cleaved epitope tags. Ultimately, this cleavage site will be incorporated around anti-malarial peptides and cloned into bacteria so that secreted peptides are released by gut proteases.

## 86

**Homology modeling and membrane insertion of the human reduced folate carrier**

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The functionality of the human reduced folate carrier (hRFC) is important to cell proliferation and DNA synthesis, as its main function is to transport reduced folates. The hRFC protein also transports drug compounds known as antifolates. The antifolate, Methotrexate (Mtx), is used as a chemotherapeutic agent in the treatment of acute lymphoblastic leukemia. For patients on Mtx, reduced levels of hRFC result in decreased Mtx uptake. Thus, the knowledge of the 3D structure and transport mechanism of hRFC will provide further understanding of the reduced potency of antifolates and can provide information to create alternate treatment methods. There is no available model of this transporter to date. A comparative model of hRFC was built based on the structures of homologous transporter proteins: lactose/proton symporter and phosphate/glycerol 3-phosphate antiporter. The hRFC model was then placed into a model lipid membrane to study its dynamics using molecular dynamics.

## 87

**Conformational Analysis of the Inward-Facing Sodium-Hydantoin Transporter**

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The importance of transporters can be attributed to the fact that they are involved in the movement of substrates across membranes. Transporters bring substrates from the extracellular matrix, through the membrane, and release them into the intracellular matrix. In order to transport a substrate through the membrane the transporter must go through three different conformations, which include the outward, occluded, and inward states. Recently, biochemists have taken an interest in the mechanism and conformational structures of transporters. X-ray crystallography shows only a snapshot during transport, leaving some conformations elusive. The objective of this study is to investigate the inward-facing conformation of the Sodium-Hydantoin Transporter through a membrane with a 4:1 molar ratio of POPE:POPG lipids. This will provide insight to the mechanistic pathway of transport proteins. Starting with the x-ray structure, a membrane/protein complex was built using CHARMM. Initial molecular dynamics were done using NAMD.

## 88

**The evolution of transcriptional regulation of transglutaminase 4 in primates.**

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The molecular basis underlying phenotypic adaptation in humans and their close relatives remains largely unknown, including the relative contribution of changes in the protein-coding portions of genes versus changes in gene regulation. One such adaption, the consistency of ejaculated semen, reflects differences among species in their mating behavior. In order to determine if transcriptional regulation drives the evolution of the prostate-specific transglutaminse 4 (*TGM4*) gene, we used PCR, DNA sequencing, cloning into luciferase reporter constructs, and transient transfection into a human cell line to quantify differences in the strength of the *TGM4* promoter to drive transcription in humans, chimpanzees, gorillas, orangutans, and gibbons. We identified numerous differences among species in the DNA sequence of their *TGM4* promoters. We are currently performing experiments to transfect promoter constructs to test the hypothesis that these sequence differences result in different levels of transcription among species, driven by selective pressure related to mating behavior.

## 89

**Alternative Fuels: Metal Hexahydrate Catalysis of Ammonia Borane Hydroylsis**

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Ammonia borane (AB) is a target for hydrogen storage media in commercial vehicle hydrogen fuel cells. In our previous work, we have shown agreement between experimental rates of acid catalyzed AB hydrolysis and activation energies from $S_N2$ pathways between hydronium and methylated AB. In similar reactions, precious metals in the form of nanoparticles are known to be powerful catalysts for AB hydrolysis, yet the mechanism is not known. We assume that the nanoparticles are in equilibrium with the metal hexahydrates. In our investigation, we determine how hexahydrates of precious and nonprecious metals influence the structure and energies of AB hydrolysis using density functional theory and ab initio theory. The influence of the hexahydrates of nickel, cobalt, copper, and palladium upon the $S_N2$ reaction path of AB hydrolysis is reported.

## 90

**Refactoring and Testing for RAE: An interactive web-based biomedical informatics system for pediatric orthopedic patients**

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2 Department of Orthopaedic Surgery, Allegheny General Hospital

The primary aspiration of RAE is facilitation of organized yet dynamic interaction between Orthopaedic physicians and their adolescent patients. Utilizing a MySQL database and PHP scripting, RAE interprets input data and gathers a collection of relevant images and text for each presentation. My primary contribution to the software this year was to prepare the system for clinical trial at Allegheny General Hospital. Preparation included focus on refactoring and unitizing source code as well as executing error testing procedures. Code refactoring improved code readability and allowed for easier maintenance and extensibility for future versions of the RAE software. Unitization prepared the code for automated unit testing, a procedure where each unit (smallest functional element of code) was tested and verified for correct functionality. After exhaustive testing, the software was provided to Allegheny General Hospital for the clinical testing stage of development.

## 91

**Hemoadsorption Column for the Removal of Cytokines Associated with Severe Sepsis**

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This study developed a mathematical model of a hemoadsorption column used to reduce the concentrations of cytokines IL-1B, IL-1 receptor antagonist, IL-6, IL-10 and TNF. These cytokines are key regulators in the pathology of inflammation and play a significant role in the onset and dynamics of sepsis. The hemoadsorption device packed with porous adsorptive beads was modeled as a series of continuous stirred-tank reactors (CSTRs) to approximate a plug flow reactor (PFR). A 3 parameter model consisting of an adsorption rate to the beads, a desorption rate from the beads, and a parameter representing irreversible binding (or pore entrapment) most closely matched experimental data. 20 CSTRs in series provided an accurate approximation to the PFR. Explicit modeling of the reaction-diffusion problem is ongoing, using orthogonal collocation on finite elements for the pore model.

## 92

**Quality Assurance for RAE: An interactive web-based biomedical informatics system for pediatric orthopaedic patients**

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2 Department of Orthopaedic Surgery, Allegheny General Hospital

For over two years, the RAE Project has been crafted to present young patients and their families with an opportunity to learn how to manage their muscular skeletal disorders. RAE is a software system that generates personalized, interactive presentations including visuals of a patient's diagnosis, charts to assess improvement, and second opinion referrals. My central task throughout my internship has been quality assurance. Standardizing the project's database and refactoring (making more efficient) the code of the RAE Project was of the utmost importance so that future system modifications and enhancements could be made with ease. Additional time was also spent manually cataloging and verifying various components of the project. Discrepancies were found and corrected in both the database and the code to ensure that future modifications and testing would be facilitated. Both automated and manual test procedures were conducted to ready the system for clinical use at Allegheny General Hospital.

**93**

**Investigation of the dopamine active transporter: A study in the motion and communication stochastics of transporter proteins in the neurotransmitter sodium symporter family.**

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Understanding the motion of proteins is critical in understanding how they perform tasks, such as transporting matter into and out of the cell. In addition, this data can also be critical in designing drugs to counteract the issues that arise when these proteins malfunction. In this study, we are looking the dopamine active transporter (DAT), which is what controls a person's mood, appetite, and several other bodily processes. To observe the motions of this protein, a course grain Gaussian network model was used to predict the mobility of the individual residues of the protein. Using this data, cross-correlation, hitting time, and communication plots were created in order to determine how the motion of each residue affected another. This data provided some insight into how the ultimately moves so that a prediction of how this protein functions can be made.

**94**

**Using BioNetGen Software to Understand Protein Receptor Dynamics**

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The BioNetGen software tool models molecular interactions using a rule-based mechanism that enables the user to input a set of initial molecule types and rules for them to obey during reactions. Signal transduction in cells can be modeled in detail using BioNetGen software. Using the software allows the user to track the concentration of each molecule or possible combination of the molecules through time during reaction to create a comprehensive model of the process. The erythropoietin receptor (EpoR) and erythropoietin (Epo) system is characterized by degradation of the ligand Epo and replenishment of EpoR. An accurate model of this system has been proposed. We use BioNetGen, first, to reproduce the proposed model and, second, to determine which characteristics of this model are important, which can be discarded giving the same results, whether more should be introduced, and which systems are similar in structure to this one.

**95**

**Development of Nanoscale-Porous Membranes for Levitation of MEMS**

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Crookes radiometer consists of a partially evacuated chamber that contains a mill with four wings mounted on a vertical pivot point. When light impinges on the vanes, the mill starts spinning due to gas-kinetic forces. These forces acting on the device are the result of the temperature gradients that exist between the absorbing and the reflecting surfaces of the vanes. Using the principles behind Crookes radiometer, we used microfabrication and nanofabrication techniques to create a nanoporous membrane where gas-kinetic forces are expected to be greatly enhanced at atmospheric pressure. The gas-kinetic force only act within approximately one mean free path of the edge of a surface, therefore a surface with many edges significantly enhances this effect. We anticipate that a temperature difference across the membrane of less than 1ºC could result in enough force on the membrane to overcome the force of gravity and cause it to levitate.

**96**

**An Optical Test-bed for Broadband, High Resolution Confocal Microscopy**

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The optical emission from a variety of single photon emitters such as quantum dots, fluorescent dye molecules and nitrogen-vacancy centers in diamond covers a wide spectral range and emits in all directions. Collecting and observing this broadband light requires high numerical aperture and wide spectrum achromatic optics. I have designed and constructed a test bed in which to compare the chromatic aberration of objective lenses, reflective optics such as reflective objectives and parabolic mirrors, and any other lens combinations. Reflective optical elements are of particular interest due to their theoretical complete lack of chromatic aberration. The test bed is also capable of measuring the NA of any optical system to compare against manufacturer's data.

## 97

**Biomedical surfaces: Analysis of $TiO_2$ rutile structures using quantum chemistry**

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Titanium dioxide ($TiO_2$) is of significant importance in many science and engineering fields, especially in medical implant technology. The surface of rutile [110] $TiO_2$ was approximated using quantum chemical calculations involving periodic boundary conditions and cluster models at various levels of theory. Hartree Fock (HF) and density functional theory (DFT) using the local spin density approximation (LSDA) and the new meta-hybrid functional M06L with the effective core potential LANL2DZ basis set were used as the levels of theory. Titanium (IV) compounds, $TiO_2$, $TiCL_4$, $Ti(OH)_4$, and $Ti(OBut)_4$, were used to evaluate the performance of the levels of theory against experiment. Systematic problems with implementing periodic boundary conditions have been identified. Three different sized clusters ($Ti_2O_{10}$, $Ti_3O_{14}$, and $Ti_8O_{34}$) have been constructed and terminated as either water molecules or as OH groups. The resulting geometries of the clusters are compared back to x-ray crystallographic results from the [110] rutile $TiO_2$ system

## 98

**Role of Lithium atoms upon a nitrile intramolecular cyclization reaction**

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The intramolecular *5-exo-dig* ring closure of cyclohexanecarbonitrile in the presence of lithium is expected to produce the trans-hydrindane with high selectivity. However, cis-product with high selectivity is produced in our experiments. Semiempirical methods (AM1, PM3 and PM6), density functionals (B3LYP and M06-2X), and second-order Moller-Plesset theory (MP2) were used to rationalize the experimental results. Four models were constructed to disentangle the influence of ions and solvent upon this reaction. In the simplest case, vacuum computations with no ions were performed. The second model involved lithium ions in vacuum. The third case included only solvent (THF) with no ions. In the final, and most realistic model, ions and solvent were included in the computations. Consequently, we find that ions are of primary importance and solvent is of secondary importance that further enhances experimental agreement. Natural Bond Orbital (NBO) was used to explore the balance between electrostatic and stereoelectronic forces delivered by the ions.

## 99

**A Model to Generate Synthetic Neural Images for Testing Digital Reconstruction Tools**

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Neuronal reconstruction models are critical tools for understanding the function of neuronal morphology. Current tools like L-Neuron, NeuroLucida, and Neuromantic create digital neurons by manually tracing dendritic arbors. As opposed to reconstructing the neuron, we are using image analysis techniques to synthesize an image as a whole by analyzing the statistics of given neural images and using the compiled image statistics to create image analysis algorithms to semi-automate dendritic tracing. We have written Matlab code to create simple, neuron-like images. Our analysis of a stack of neuronal images indicates the distribution of image statistics in a section of a given image slice is roughly consistent throughout the entire stack. Although a two-dimensional model does not fully represent the original neuron, it is useful for studying branching pattern characteristics that can eventually be applied to a three-dimensional model and providing ground truth for testing automated computer vision based neuronal reconstruction methods.

## 100

**C-Metalated Nitriles: Diastereoselective Alkylations and Arylations**

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C-Metalated nitriles are powerful nucleophiles that allow for the formation of stereoselective quaternary centers. In the case of C-Zincated nitriles generated by deprotonation with TMPZnCl·LiCl are diasteroselectively cross-coupled with the aid of a palladium/phosphine ligand coupling system to furnish α-arylated nitriles. Alternatively, alkylation of C-Magnesiated nitriles generated by the addition of excess *i*-PrMgCl bearing a remote carbinol center is achieved with carbon and sulfur electrophiles in a diastereoselective manner by means of a cyclic intermediate.

## 101

**Cortical Lamination in Autistic Spectrum Disorders**

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Autism is a developmental neurobiologic condition characterized by variable impairments in social ability, the use of language, and restricted and/or repetitive behaviors. Anatomic and histologic studies have demonstrated a substantially altered postnatal growth trajectory associated with subtle microarchitectural changes such as increased neuronal densities in the frontal cortex of many autistic subjects. These abnormalities point to perturbations in cortical regionalization, neuronal precursor proliferation, and migration/lamination – processes all crucial to the later establishment of properly functioning cortical circuits. Embedded sections of the inferior frontal pole and dorsolateral prefrontal cortex – two areas known to differ histologically and functionally between individuals with ASD and age-matched controls—were Nissl stained with neuronal subtype-specific antibodies such as Fox P1 in order to identify potential differences in both the size of neuronal subtype populations and their relative distributions. This study can give insight into what proportion of neurons are required for properly functioning cortical circuits.

## 102

**The Role of Inflammation in Lung Tumor Formation**

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Inflammation increases tumor numbers in mice lungs. Previous studies have shown that immune cells infiltrate tumor tissue along with an increase in tumor-associated macrophages, but how this phenomenon induces tumorigenesis remains unclear. Treatments for inflammation- associated lung cancer may be enhanced if specific patterns (in location, density and protein expression) for different types of tumors could be identified. To test the hypothesis that inflammation promotes carcinogen-induced tumorigenesis, mice were exposed to cigarette smoke carcinogen NNK with or without chronic inflammation elicited by repeated exposure to LPS. Sixteen weeks after the initial treatment, mice were sacrificed, and tissues were collected for analyses. Lung tumors were counted; their densities, area, radii, distance in respect to airway and tissue periphery were measured. Additionally, lung tumors were stained using immunofluorescence for origin (bronchoalveolar stem cells, alveolar region, or airway), and inflammatory cell expression. Specific characteristics of lung tumors can be targeted for therapeutic application.

## 103

**Gene Silencing in Maize: Optimizing Primers for Sodium Bisulfite Treatment of DNA**

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Epigenetics is a form of gene regulation which involves the change in a phenotype that is caused by something other than a direct change in the DNA sequence. One example of epigenetic gene silencing, paramutation, occurs when one allele in a heterozygote directs the repression of the other. Paramutation is associated with an increase in cytosine methylation in the silenced allele. This research study focused on determining levels of methylation in the maize *r1* locus using sodium bisulfite. Sodium bisulfite will convert unmethylated cytosines into thymines. When genomic DNA is treated with sodium bisulfite, the sequence of amplified PCR products can be compared with the progenitor sequence, providing information on the distribution of cytosine in the genomic DNA. This study involved troubleshooting with PCR using sodium bisulfite primers designed specifically for a region in the *R-r:standard* gene that contains two inverted repeats called S1 and S2. As a result, 2 sets of primers were optimized for the region.

## 104

**Endogenous non-retroviral RNA virus elements in nematode genomes**

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In a recent study (Horie et al. 2010) evidence for the endogenization of non-retroviral RNA virus elements in a number of mammalian species was uncovered. These Endogenous Borna-like N Elements (EBLNs), named for their association with a gene coding for the Bornavirus' nucleocapsid, give credence to viral lateral gene transfer from a much larger source than previously believed. In an effort to find further evidence for non-retroviral endogenization we used computational methods to look for non-retroviral elements in parasitic nematode genomes. By homology searches we have been testing a variety of RNA virus sequences against nematode genomic data. While most of the matches found can be attributed to conserved domains in the convergent evolution of protein functions, a few of the similarities include surface glycoproteins and are being further explored.

## 105

**Studying temporal and spatial cellular expression patterns of RNAs differentially expressed in human breast cancer**

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RNAs that do not code for a protein (non-coding ncRNAs), constitute over 97% of the transcriptome [1]. Recently discovered biological functions of ncRNAs include transcription regulation, gene silencing, and dosage compensation [2]. With such important cellular functions, ncRNAs have been implicated in the development of cancer [2]. From genome tiling arrays in preliminary research, we identified 357 differentially expressed RNAs in normal versus cancer breast tissue. This study focuses on identifying the temporal and spatial pattern of expression of several candidate RNAs that do not code for known proteins, using *in situ* hybridization and real time PCR. Results from this study are expected to provide insight as to which RNAs are up- or down-regulated in breast tumors, and identify the cellular processes that are targeted by these RNAs. These studies may aid in the development of new prognostic/diagnostic tools, creating new therapeutic procedures for breast cancer patients.

## 106

**Chromatography and Fragmentation Assignment for Collision Induced Dissociation Patterns of Various N-Acyl Glycines**

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N-Acyl Glycines (NAGs) are biologically important because they are molecules that signal for a wide variety biological activity including antinociceptive and anti-inflammatory effects. In addition, they have been thought to be precursors in primary fatty acid amides anabolism. N-Oleoyl , Arachidoyl, Linoleoyl, and N-Palmitoyl Glycine were used as standards. The carbon chains of these four standards range from 16 to 20 with varying degrees of unsaturation. All of these standards were monitored in ESI negative mode using the $[M-H]^-$ peak. Using collision induced dissociation (CID) maximum sensitivity of the glycine product ion was seen at 20 eV. Separations were seen using both a C18 and C30 column with the mobile phases being methanol and water with 5 mM ammonium acetate. All NAGs were detected using multiple reaction mode.

## 107

**Strategies to Improve the Release of Cationic Proteins from PLGA Microspheres**

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The controlled release of proteins from poly(lactic-co-glycolic) acid (PLGA) microspheres could lead to a number of efficacious treatments. Yet, a number of such proteins have a net charge that causes ionic interactions with PLGA, thus preventing their release from microspheres. We hypothesize that these interactions could be eliminated by excipients, which lower the pH of the microparticles, thus neutralizing charges and minimizing ionic interactions. Excipients, such as citric acid and sodium citrate, are being tested for their ability to prevent adsorption of BSA (uncharged) and lysozyme (charged) onto PLGA. Because polymer stability may be affected by these excipients, their effect on polymer degradation is being examined via microscopy and chromatography. Together, adsorption and degradation studies show that charged excipients improve the release of cationic protein from PLGA microparticles without compromising their stability. This suggests that such excipients may also enhance the controlled release of other charged proteins with therapeutic value.

## 108

**Time Dependent Effects of Low-affinity Drugs on the α4β2 Nicotinic Acetylcholine Receptors**

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The α4β2 nicotinic acetylcholine receptors (nAChRs,) found abundantly in central nervous system, are ligand-gated ion channels that open upon agonist binding and participate in neuronal signal transduction. It is an important target for general anesthetics. Using the perturbation-based Markovian transmission model, we applied perturbations to the agonist binding sites of halothane-bound and halothane-free α4β2 systems in the open- and closed-channel conformations. In all systems, we find that the perturbation signal flows from agonist binding sites up toward the main immunogenic region, and down through the channel gate. At the extracellular (EC) and transmembrane (TM) interface, we observe that the signal travels sequentially through pre-TM1 domain (R207), Cys-loop (F137, P138, F139), TM2-TM3 linker (P271), and down the channel (L257). However, in halothane-bound and halothane-free systems, signal transductions between aforementioned key residues take different time-steps. Differences in transduction time might also cause anesthetics effects in the α4β2 nAChR.

## 109

**Numerical approach to local cloning of entangled states**

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We investigate conditions under which a set of bipartite quantum states can be locally cloned using quantum entanglement as a resource. Local cloning of quantum states involves copying the state of a bipartite system onto another, when a grouping of the subsystems may be spatially separated from another. An operation is performed on one group of subsystems and the result is communicated to the other. Through a series of such operations, two exact copies of the cloned system are obtained. Preliminary results for 3-level systems suggest that sets must have a very special form in order for cloning to be possible. We are now beginning to study systems with four or more levels, and there is reason to suspect that results may be very different for non-prime dimensions.

## 110

**Probing the birth and evolution of galaxies through the Sunyaev-Zeldovich effect.**

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The Sunyaev-Zeldovich (SZ) effect occurs where cosmic microwave background (CMB) radiation is distorted from its initial spectrum by hot electrons through Compton scattering. One theorized source of the SZ effect is the heated gas surrounding a galaxy that hosts a quasar. We will cross-correlate galaxy density maps from the Southern Cosmology Survey with microwave maps from the Atacama Cosmology Telescope (ACT). The signal will be small and negative, about 1 micro-Kelvin per galaxy per square arcminute pixel, at a frequency of 148GHz. We will filter out the noise, leaving only a signal, if one exists. The noise level in the ACT maps is around 25 micro-Kelvins per pixel, so averaging the cross-correlation in 1000 pixels is sufficient to reduce the noise below the 1 micro-Kelvin. A negative cross-correlation will signify energy output from quasars and galaxies, and provide a clue about the birth and evolution of galaxies.

## 111

**Evaluation of Elemental Contamination in Prescription Nutritional Supplements**

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In this project, numerous prescription nutritional supplements from many of the leading national providers were evaluated for elemental contamination. This project resulted from one of the leading supplement companies announcing that one of their supplements had been contaminated with antimony. Many physicians use these supplements to treat their patients for many diseases including autism. The samples were prepared following EPA Method 3052 by microwave-assisted digestion and analyzed for 64 elements by calibration curve following EPA Method 6020A using Inductively Coupled Plasma-Mass Spectrometry. This analysis included neurotoxins and carcinogens such as mercury, cadmium, aluminum, lead, arsenic, and antimony. Additionally, the supplements were evaluated to see if the nutrient concentrations matched the levels stated on the labels. From this project, contamination can be determined by supplement and manufacturer. This information will allow physicians to choose the best manufacturer in their practice. Additionally, any contamination is reported to manufacturers to upgrade their procedures.

## 112

**Heat Dissipation as Oil Spreads on a Denser Fluid**

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Consider an oil drop placed on the surface of a more dense fluid. As the oil spreads, its kinetic energy is converted to heat at the drop's rim. This release of heat has never been previously observed. Using a motorized stage, an oil-dipped needle is slowly lowered until it touches the surface of a dish containing a fluid. As the oil spreads, a thermal imaging infrared camera reveals surface temperature. This procedure was primarily used to observe the spreading of oleic acid on glycerol. The thermal images indicate a temperature rise that corresponds with the oil's advancing edge. This temperature increase may also be present when oil spreads on the sea, as in the Gulf of Mexico oil spill. If so, the increase may affect phytoplankton which are at the beginning of the food chain in the sea.

**113**

**Potential for Roxarsone Degradation in Vadose, Saturated, and Hyporheic Hydrologic Zones**

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3-nitro-4-hydroxybenzene arsonic acid(roxarsone), is widely used as a chicken feed additive. Roxarsone-containing chicken litter is used as a fertilizer, where it is known to be transformed by microbial processes in soil into more mobile and toxic arsenic species. The goals of this project are to investigate the potential for organoarsenic transformation in the vadose, saturated, and hyporheic hydrologic zones, and to determine what microbial species are involved in the transformation of organoarsenic compounds in watersheds that have been exposed to contaminated chicken litter. Anaerobic enrichment cultures were created from sediment samples, amended with roxarsone and lactate, and sampled over two weeks. Spectrophotometric readings were taken at 400 nm to measure disappearance of roxarsone, and 600 nm for turbidity (e.g. cells). Roxarsone concentration was observed to decrease as OD increased in all three hydrologic zone cultures, as well as in the chicken litter cultures that provided positive control.

**114**

**TEM Investigation of the Effects of Arsenic on Microbiota in the Murine Colon**

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Exposure to excess amounts of As(III) is known to have disastrous effects on the human body. However, the effect of As(III) on the microbiota within the colon is less documented. Colon microbiota play an essential role in host immune response and nutrition, with estimates showing between 5-30% of our daily energy requirement is fulfilled by bacterial fermentation of dietary residues that host enzymes are unable to digest. Our Hypothesis is that exposure to As(III) contaminated drinking water will alter the diversity of microbiota within the gut as well as its organization and structure. Colons from mice exposed to As(III) contaminated drinking water were examined and compared to control mice to look for changes in microbial diversity and organization. Definite changes in the microbial communities organization were observed, with the general loss of some species seen as well as morphological and physiological changes in the remaining bacteria within the experimental group.