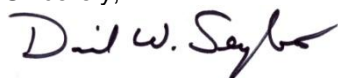


Welcome to the 2011 Summer Undergraduate Research Symposium!

It is a pleasure and privilege to welcome you to today's **14th Annual Summer Undergraduate Research Symposium** at Duquesne University. Each year the number of student participants, as well as the quality and breadth of the research presented at this symposium, continue to grow. The abstracts in this year's program highlight the remarkable quality of the student research that we will see and discuss at today's symposium. In an era in which we hear persistent concerns regarding our nation's ability to sustain global competitiveness and global pre-eminence in the STEM disciplines, events such as today's conference validate the superb caliber of the scientific research and training that is occurring in our colleges, universities and research centers. Today's gathering of student researchers reinforces our conviction and confidence that we are preparing an emerging cadre of scientific leaders who will possess the creativity, motivation, and intellect to meet and solve the challenges that lie before our society. On behalf of the faculty, students, and staff of the Bayer School and Duquesne University, I offer our sincerest congratulations to each of the student researchers participating in today's symposium and our best wishes for continued success in your academic and professional careers!

Sincerely,



David W. Seybert
Dean, Bayer School of Natural and Environmental Sciences

Schedule:

9:00 AM	Registration and Poster Set-Up Continental Breakfast	Mellon Patio, Academic Walk Side Rotunda, Bayer Learning Center
10:00 AM	Welcome and Keynote Address	Pappert Hall, Bayer Learning Center
11:00 AM	Plenary Session (Student Presentations)	Pappert Hall, Bayer Learning Center
1:00 PM	Picnic Lunch	Mellon Patio, Bluff Street Side
2 – 4:00 PM	Poster Session	Mellon Patio, Academic Walk Side

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Instructions to Authors:

Authors presenting posters should locate their abstract number in the index of this program and then find the poster board space marked with that number. Authors with even numbered poster assignments must be present from 2 p.m. to 3 p.m. to answer any questions. Authors with odd numbered posters must be present from 3 p.m. to 4 p.m.

Authors presenting talks during the Plenary Session should report to Pappert Hall no later than 9:15 a.m. A tech assistant will be available to download your PowerPoint presentation.



**Plenary Session Schedule
Pappert Lecture Hall
Bayer Learning Center**

10:00 AM	Welcome	David W. Seybert, Ph.D., Dean, Bayer School of Natural and Environmental Sciences, Duquesne University
10:10 AM	Keynote Address	Eric Beckman, Ph.D., Swanson School of Engineering, University of Pittsburgh <i>“Opportunities for Sustainable Innovation”</i>
11:00 AM	Student Presentations	
	Jared Romeo	Modified Calcium Surfaces as Optimal Tissue Scaffolds Department of Chemistry and Biochemistry, Duquesne University
	Anne Clark	Nowcasting the Incidence of Infectious Disease: Improved Inference through the Combination of Multiple Data Streams Department of Computer Science, Carnegie Mellon University
	Thomas Ribelli	The Effect of Various Substituted TREN based ligands for use in Atom Transfer Radical Addition (ATRA) Department of Chemistry and Biochemistry, Duquesne University
11:45 AM	Short Break	
	Nwamaka Onyeozili	Determining the Binding Affinity of <i>Toxoplasma</i> ROP Proteins to a Membrane Using Free Energy Calculations Department of Computational & Systems Biology, University of Pittsburgh
	Bernandie Jean	Search for a Selective Serotonin Re-uptake Inhibitor Department of Chemistry and Biochemistry, Duquesne University
	Luke Tedesco	Characterization of Bovine Mitral Heart Valve Remodeling During Pregnancy Department of Computational & Systems Biology, University of Pittsburgh
	Sara Katrancha	The Effect of a Fragile X Syndrome Causing Mutation in the Fragile X Mental Retardation Protein Concerning Its Binding Interactions with the G Quadruplex Forming Semaphorin 3F mRNA Department of Chemistry & Biochemistry, Duquesne University
	Session Moderator	Ralph Wheeler, Ph.D.; Professor and Chair, Department of Chemistry and Biochemistry, Duquesne University

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1

Progress toward the synthesis of poison dart frog alkaloid 237I

Stultz, Eric T; Leonard, Michael S.
Department of Chemistry
Washington & Jefferson College

The skin glands of poison dart frogs contain a diverse set of alkaloids that afford a measure of chemical defense against predation. These compounds are of interest because of their unique molecular architectures and because of their biological activity. A painkiller 200 times more potent than morphine has been isolated from poison dart frogs, and other isolates include muscle relaxants, heart stimulants, and appetite suppressants. Poison dart frog alkaloid 237I, a 4,6-disubstituted quinolizidine, appears to be among the isolates whose biological activity remains to be fully explored. To that end, progress toward the total synthesis of this compound and its analogues is presented herein.

3

Effect of Homocysteine on Peroxisome Proliferator Activator Receptor Gamma Signaling

Vance, Sabrina; Robel, Izabela; Soukup, Maria; Bridges, Kristie
Department of Biomedical Sciences
West Virginia School of Osteopathic Medicine

Homocysteine (Hcy) is a molecule produced in the methionine metabolic pathway that is frequently elevated in the follicular fluid of women with polycystic ovary syndrome. Mice treated with Hcy have been shown to produce fewer oocytes. However, the mechanism through which Hcy affects ovarian function is not understood. It has been proposed that Hcy alters signaling through the gamma isoform of the peroxisome proliferator activator receptor (PPAR γ) which is required for ovarian function. The goal of this work was to determine if Hcy decreases expression of PPAR γ or impairs its function. Because ovarian cell lines were not available, 3T3-L1 adipocytes were used as a model system. Treatment with Hcy slightly decreased PPAR γ stimulated lipid accumulation in these cells but this effect was not statistically significant.

2

Progress toward the synthesis of poison dart frog alkaloid 245F

Warmbrodt, Taylor A.; Leonard, Michael S.
Department of Chemistry
Washington & Jefferson College

Poison dart frogs are replete with a variety of alkaloids that provide defense against predation. Many of the greater than 800 compounds isolated from these frogs have interesting structures, as well as sometimes potent biological activity. A potent painkiller has been isolated from poison dart frogs, and other isolates have activity as muscle relaxants, heart stimulants, and appetite suppressants. Poison dart frog alkaloid 245F is purportedly a dehydro-5,8-disubstituted indolizidine; however, the structural assignment remains tentative. A synthesis of the proposed structure would allow verification of the molecular architecture, as well as exploration of the biological activity. To that end, progress toward the total synthesis of indolizidine alkaloid 245F is presented herein.

4

Characterization of Uric Acid Test Strips

Hower, Margaret; Robel, Izabela; Soukup, Maria; Bridges, Kristie
Department of Biomedical Sciences
West Virginia School of Osteopathic Medicine

Patients with cardiovascular disease or metabolic syndrome often have elevated serum uric acid levels. We have found that there is a linear relationship between serum and salivary uric acid making it a potential non-invasive biomarker for monitoring disease risk. This approach would be improved by the development of point-of-care methods for measuring salivary uric acid. A previous study demonstrated that uric acid could be detected at high concentrations in the saliva of patients with kidney disease using colorimetric test strips based on bicinchoninic acid chemistry. The goal of this project was to determine if the same method could be used to detect uric acid at the lower levels our preliminary studies suggest are associated with cardiovascular disease risk. Several modifications to the method were tested but the lower limit of detection could not be improved. The effect of inflammatory molecules on uric acid metabolism in adipocytes was also investigated.

5

Synthesis and Characterization of Lithium-containing Quaternary Diamond-like Semiconductors

Henline, Kylie M.; Rosmus, Kimberly A.; Aitken, Jennifer
Department of Chemistry and Biochemistry
Duquesne University

Diamond-like semiconductors (DLSs) are materials that have crystal structures related to diamond. One reason that these materials are of interest is their potentially useful nonlinear optical properties such as second harmonic generation. Due to their chemical complexity, many DLSs have not been researched thoroughly; however, this composition flexibility can be exploited for physical property tuning. Here, new lithium-containing DLSs were synthesized using molten flux syntheses at temperatures of 650 and 750°C. Different ratios of starting reagents and various heating profiles were explored in attempt to synthesize the desired products. The products which consisted of crystalline powders were ground and characterized by X-ray powder diffraction. By comparing the diffraction patterns of the products to the calculated patterns of known DLSs, it was determined that one new quaternary material has been prepared thus far. Scanning electron microscopy and energy dispersive spectroscopy were used to study sample composition and morphology.

7

Molecular Cloning of the Periplasmic Nitrate Reductase (NapA) without His-tag from *Campylobacter jejuni*

Nassif, Samih; Sparacino-Watkins, Courtney; Stolz, John; Basu, Partha
Department of Chemistry and Biochemistry
Duquesne University

Campylobacter jejuni is a pathogenic, gram-negative bacterium which relies on nitrate reduction for growth via a periplasmic nitrate reductase (Nap). The catalytic subunit, NapA, is a pterin-containing molybdenum enzyme that has 4Fe-4S unit as a prosthetic group. Heterologous expression of *C. jejuni* NapA has been carried out in *E. coli* in our laboratory, using a plasmid containing *napA* with a 6x-Histidine tag, and a second plasmid containing *napLD*, proteins that aid maturation of NapA. Kinetics of the recombinant protein shows a low affinity for nitrate (2.2 mM), especially when compared to native *Sulfurospirillum barnesii* NapA (0.29 mM). In order to understand the role of the 6x His-tag in the protein, herein we describe the molecular cloning of *napA* without His-tag expression. The expression plasmid, pET21-a(+), was cut with a different restriction enzyme, Bam-HI, to prevent His-tag incorporation. Colony PCR, restriction digest and directional PCR confirmed presence of the new plasmid.

6

Distinguishing Between a Gamma Particle and an Electron in a Segmented Plastic Scintillator Particle Detector

McGinley, William; Paolone, Vittorio
Department of Physics and Astronomy
University of Pittsburgh

Electrons and gamma particles may have distinguishable characteristics when traveling through a fully active particle detector made of segmented plastic scintillator planes and strips. As a gamma particle interacts with plastic scintillator an electron and a positron is formed which should deposit more energy per unit length than a single electron does. In addition once a gamma interacts and forms an electron and a positron pair the transverse width of the gamma shower is expected to be greater when compared to the width of an electron shower. These variables, along with others, have been used to study the distinguishing characteristics of electron and gamma showers using this type of particle detector. Presently I am studying several other variables of gamma and electron interactions to improve the efficiency and purity for gamma and electron separation.

8

Crystal Structure, Optical Band Gap, and Thermal Stability of Li_4GeS_4 , Li_4SnS_4 , and Li_2SnS_3

¹Massi, Danielle M.; ¹Rosmus, Kim A.; ¹Gentile, Taylor A.; ¹Brunetta, Carl D.; ²MacNeil, Joseph H.; ¹Aitken, Jennifer A.

¹Department of Chemistry and Biochemistry, Duquesne University

²Department of Chemistry, Chatham University

Lithium sulfides have potential use in lithium battery development due to their high lithium ion conductivity, yet few have been synthesized and characterized. Li_4GeS_4 , Li_4SnS_4 , and Li_2SnS_3 were synthesized using polychalcogenide flux and/or high temperature solid state methods. The structure of Li_4SnS_4 was determined for the first time and found to be isostructural to Li_4GeS_4 , which has been previously published. Differential thermal analysis showed that Li_4GeS_4 and Li_4SnS_4 are thermally stable until approximately 850 °C and 920 °C, respectively; the Li_2SnS_3 showed no thermal events until approximately 740 °C. Rietveld refinement of x-ray powder diffraction data of Li_4GeS_4 showed a phase pure material with a χ^2 of 5.656 and a R_p of 0.0771. The optical band gaps of Li_4GeS_4 , Li_4SnS_4 , Li_2SnS_3 are 4.13 eV, 3.54 eV, and 2.49 eV, respectively.

9

Synthesis and Characterization of Chromium and Manganese Complexes with Dithione Ligands

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Duquesne University,

Ligands are used in coordination chemistry to synthesize metal complexes through coordination of the ligand(s) to a central metal atom. They can be attached to the metal center by one (monodentate), two (bidentate) or more (tridentate etc.) non-contiguous donor sites. When bound to transition metals, such as chromium and manganese, complexes are formed that present various optical, magnetic, and chemical properties. These transition metal complexes have exceptional uses in areas including catalysis, biological systems, photochemistry, and materials. In this research, a 1,4-dimethyl-2,3-piperazinedithione (Me₂Pipdt) ligand was synthesized by first refluxing *N*¹,*N*²-dimethylethane-1,2-diamine with diethyl oxalate in toluene. Then the product was refluxed with Lawesson's Reagent in toluene to form the Me₂Pipdt ligand. The ligand was then attached to chromium and manganese atoms. Each compound was characterized by NMR and FT-IR spectroscopy, cyclic voltametry, and mass spectrometry.

11

Unpacking Fracking: How Industry Framing Could Determine Pennsylvania's Future

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Environmental Studies
University of Pittsburgh
Advisor: Dr. Stanley Kabala, Center for Environmental Research and Education, Duquesne University

Pennsylvania is in the middle of a natural gas drilling boom, sparked by technological advancements in the practice of hydraulic fracturing ("fracking"). The process is steeped in controversy, and the issues associated with drilling represent almost every major political issue of our time.

My research looks at the framing of the natural gas industry's advertisements and public statements. The framing of hydraulic fracturing is particularly interesting because of the different stories the industry tells to serve its interests, at times selling itself to free-market capitalists, middle-class Pennsylvanians, and even liberals and environmentalists.

Using scholarly literature on framing as a guide, I will classify the industry's different frames on the issue, then explore what these frames mean, what political issues they reference or mirror, the validity of these frames based on the realities of drilling. Using survey data from Penn State, I will also evaluate the effectiveness of the frames.

10

***N*¹-(substitutedphenyl)-7-(3',4',5'-trimethoxybenzyl)-5*H*-pyrrolo[3,2-*d*] pyrimidine-2,4-diamines as Inhibitors of Receptor Tyrosine Kinases Design and Synthesis**

Gentile, Taylor; Gangjee, Aleem; Pavana, Roheeth Kumar
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Angiogenesis, the formation of new blood vessels, is crucial for tumor growth. Inhibition of angiogenesis is a well documented concept for combating cancer. RTK pathways have been implicated in tumor angiogenesis, proliferation, and metastasis. Hence, inhibition of receptor tyrosine kinase (RTK) signaling pathways is a promising area of research for the development of novel anti cancer agents. A series of *N*¹-(substitutedphenyl)-7-(3',4',5'-trimethoxybenzyl)-5*H*-pyrrolo[3,2-*d*] pyrimidine-2,4-diamines were designed in order to create potential RTK inhibitors. The designed compounds can have multiple binding modes which perhaps can have affinity for multiple distinct binding sites. This in turn could furnish inhibitors of multiple RTKs and allow for circumventing or at least delay the occurrence of resistance. The design and synthesis of these analogs will be presented.

12

Molecular dynamic simulations of the norepinephrine and serotonin transporters in a lipid bilayer membrane

Rocco, Sarah C.; Madura, Jeffrey D.
Chemistry Department, Center for Computational Chemistry
Duquesne University

The norepinephrine and serotonin transporters (NET and SERT) have been reported to play a role in neurological cases such as depression and drug abuse. These transporters are integral membrane proteins that function in the reuptake of norepinephrine and serotonin from the synaptic cleft back into the presynaptic nerve using a Na⁺/Cl⁻ gradient. Previous research shows that the neurotransmitter transporters follow the alternating access mechanism. There is little information available to provide insight into the molecular mechanisms and pathways involved with NET and SERT, which would support this theory. Using the molecular dynamic studies on the leucine and dopamine transporters as a guide, NET and SERT models have each been placed into a POPE lipid bilayer membrane. Molecular dynamic simulations were then used to follow substrate movement along the protein's permeation pathway. The results from these simulations will be discussed.

13

Molecular dynamics simulations to predict the structures of amyloid beta (A β) and its aggregates implicated in Alzheimer's disease.

Pierre, Kamau*; Nguyen, Bao-Linh; Wheeler, Ralph A.
 Department of Chemistry and Biochemistry
 Duquesne University
 Florida International University*

Alzheimer's disease is a degenerative disease characterized by the presence of deposits of aggregates (fibril and plaques) of the human amyloid beta (A β) protein. Although the nature of this protein is α -helix rich, both the fibrils and the plaques are comprised of β -sheet-rich structures, whose exact molecular structure is unknown. Successful determination of both the minimized geometries and the mechanism of protein aggregations would lead to effective drug design based on inhibiting the formation of the A β aggregates associated with the disease. Utilizing molecular dynamics simulations with an implicit solvent model, the mechanism of amyloid aggregation as well as the molecular structures was explored. With secondary structure constraints applied to various initial structures containing both parallel and anti-parallel β -conformations, a simulated annealing protocol was employed to facilitate the effective structure characterization of globally minimized A β protein systems. The resulting minimum-energy structures of small aggregates of A β -derived peptides will be described.

15

The Effect of a Fragile X Syndrome Causing Mutation in the Fragile X Mental Retardation Protein Concerning Its Binding Interactions with the G Quadruplex Forming Semaphorin 3F mRNA

Katrancha, Sara; Mihailescu, Mihaela Rita
 Department of Chemistry and Biochemistry
 Duquesne University

Fragile X Syndrome (FXS) is the most common form of inherited mental retardation and the best-understood single-gene cause of autism. FXS is linked to the expansion of cytosine-guanine-guanine trinucleotide repeats in the fragile X mental retardation 1 (*fmr1*) gene causing hypermethylation of the cytosines and leading to transcriptional silencing of *fmr1* and loss of the fragile X mental retardation protein (FMRP). However, one patient who phenotypically expressed FXS was found to still produce FMRP. Further studies revealed a frame shift altering guanine-insertion in the *fmr1* gene, which subsequently created a premature stop codon and affected the major G quadruplex binding site of FMRP, the arginine-glycine-glycine (RGG) box. In this study we have used different biophysical methods to characterize the binding activity of the newly discovered mutated FMRP RGG box to the G quadruplex forming human Semaphorin 3F-sh mRNA, which is a shown binding target for wild-type FMRP RGG box.

14

Analysis of Interactions in the Hepatitis C Virus Positive Sense Genome Involving 5BSL3.2sh and X55

Hennessey, Brianne; Mihailescu, Mihaela-Rita
 Department of Chemistry and Biochemistry
 Duquesne University

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, which consists of a single stranded positive sense 9.6 kB RNA. Despite its highly mutational rate, several sequences in the genome have 100% conservancy among the six different genotypes. Among these 5BSL3.2, a stem-loop located in the coding region, is particularly significant for replication, as any alteration of its sequence has been shown to greatly diminish or prevent HCV replication. The goal of this project was to transcribe and purify the twenty-five nucleotide upperstem of 5BSL3.2, named 5BSL3.2sh, and analyze any interactions it has with another conserved region of the HCV genome, X55 located in the 3'-untranslated region (3'-UTR) of the HCV genome. Analysis of these interactions could provide potential RNA targets for new drugs.

16

Predicting bulk properties of butyl-3-methylimidazolium hexafluorophosphate using molecular dynamics simulations

Beck, Rory, Boesch, Scott E., Wheeler, Dr. Ralph A.
 Department of Chemistry and Biochemistry
 Duquesne University

Butyl-3-methylimidazolium hexafluorophosphate is a room temperature ionic liquid, or RTIL, with potential applications in carbon dioxide sequestration or electrochemistry, and it can also be used as a solvent. This study used molecular dynamics to examine the bulk properties of butyl-3-methylimidazolium hexafluorophosphate. Molecular dynamics, or MD, simulations are useful for predicting trends in the bulk properties of liquids such as self-diffusion coefficients, ionic current, and ionic conductivity. Calculated results will be compared to existing experimental data.

17

Quantification of Elemental Contamination in Commercially Available Dietary Supplements by ICP-MS

Roeske, Liz; Zinn, Greg; Kingston, H.M. "Skip"
Department of Chemistry and Biochemistry
Duquesne University

The primary goal of this research project was to analyze dietary supplements for detrimental elemental contamination and actual content compared to listed values. Contamination, from elements such as heavy metals, can have adverse health effects among users. Ingested heavy metals accumulate in the body, leading to damage of the nervous system along with other irreversible damage. It is important to make sure the listed content is in the supplements to provide the proper nutrition value. In this project, standard reference material (SRM 3280) from National Institute of Standards and Technology (NIST) and various over-the-counter dietary supplement samples were digested in a microwave using EPA Method 3052. Analysis was performed using EPA Method 6020A with an Agilent 7700 Inductively Coupled Plasma-Mass Spectrometer (ICP-MS). Contamination from heavy metals was found in many dietary supplements analyzed.

19

High Resolution Solid-State NMR Spectroscopy of Polymorphs

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Washington and Jefferson College

The study of polymorphs and polymorphism is crucial to the pharmaceutical industry. The majority of drugs ingested orally are crystalline that have to be dissolved by the body to work effectively. Dissolution rates though are dependent on the form of the polymorph. The polymorphic form must be identified for proper administration of the drug. High resolution solid-state nuclear magnetic resonance (NMR) spectroscopy is beneficial in obtaining structural information of crystals, especially when analyzing compounds that exist as polymorphs. To acquire high resolution spectra, magic angle spinning, cross-polarization, decoupling are essential. Furthermore optimal parameter settings are necessary to maximize signal. This poster will cover how to operate a solid-state NMR spectrometer properly, experiments to optimize parameter settings, a nutation curve, and spectra of the polymorphic antihistamine drug Cimetidine

18

Molecular Crystal Structure through NMR CASTEP Calculations

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The most common method for determining molecular crystal structure is through diffraction methods. By combining solid-state NMR spectroscopy and quantum chemistry, NMR Crystallography is an alternative method for determining crystal structure. This is a relatively new and still growing field. Using Accelrys' Materials Studio, CASTEP geometry optimizations were performed on powder diffraction structures of naphthalene, acetaminophen and adenosine. The CASTEP generated structures are compared to neutron diffraction structures. Moreover, NMR CASTEP calculations of these structures are in excellent agreement with ^{13}C solid-state NMR spectra. It was found that GGA-PW91 and GGA-PBE density field theory methods produced identical results while the LDA-CA-PZ method produced structures of lesser quality. Based on NMR CASTEP and experimental NMR data, crystal structures reported in the literature for cimitidine A and ambuc acid were improved using the CASTEP geometry optimizations.

20

The Ease of Unfolding Ubiquitin by Localized Compression and Expansion using Computer Simulations

Seemiller, Joseph; Salari, Reza; Chong, Lillian T.
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The University of Pittsburgh

A recent technique for developing molecular switches is to fuse two proteins through a domain insertion (the guest protein is inserted into the host protein). When the two fused proteins fold with mutual exclusivity, a virtual tug-of-war ensues. A more stable host protein will unfold the guest through compression, while a more stable guest protein will unfold the host through expansion. Here, we examine the model proteins ubiquitin and titin. Ubiquitin, made of alpha helices and beta sheets, binds to proteins and labels them for destruction. Titin, made of beta sheets, gives muscles their elasticity. It is nearly impossible to experimentally measure the unfolding of a protein through compression, so computational methods are necessary. In order to test ubiquitin and titin's design as a molecular switch at the atomic level, we computationally determine their ease of unfolding through localized compression and expansion by changing the distance between their terminal ends.

21

Developing CGenFF Parameters for NorepinephrineLi, Yan^{1,2}; Immadisetty, Kalyan²; Madura, Jeffrey D.²¹State University of New York at New Paltz²Center for Computational Chemistry; Department of Chemistry and Biochemistry
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The drug-like properties of norepinephrine (NE) have been studied extensively in the past although the binding site in the norepinephrine transporter (NET) has yet to be determined. Through the use of a CHARMM General Force Field (CGenFF) for NE, NET-NE interactions can be better understood. CGenFF parameters were developed for NE following the method of Vanommeslaeghe *et al.* The force field parameters for the NE molecule were used in a NET-NE simulation to calculate the binding free energy. The results of the force field parameter development and binding free energy calculations will be discussed.

23

Nowcasting the Incidence of Infectious Disease: Improved Inference through the Combination of Multiple Data Streams

Clark, Anne; Rosenfeld, Roni

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Carnegie Mellon University

Yearly influenza epidemics place a large burden on nations' health and economies. Epidemiologists have developed models to predict the course of severe influenza epidemics or pandemics to inform policy decisions on mitigating the impact, but these models rely on accurate counts of individuals currently becoming infected. A method is presented for inferring the incidence of infectious disease in a human population by combining all available data streams, including doctor's office visits, internet searches, and over-the-counter drug sales. The computational model was applied to data generated from statistical rules, as well as available real-world data. It was found to accurately infer the incidence of infectious disease, with greater accuracy accompanying the inclusion of more data streams. Results of combining data streams with differing temporal granularity will also be discussed. This inference method could be used with existing models to improve real-time predictions of epidemic curves.

22

Simulation of Glutamic Acid in Salt SolutionsKrawczak, Mary; Gaborek, Timothy J; Madura, Jeffrey D.
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The study of protein solubility dates back to the 1880's with Hofmeister's discovery that salt solutions can either increase or decrease a protein's solubility. Despite this, much is still unknown about the effects of salts on proteins. The study of protein solubility is important because proteins are found in buffered solutions, which contain anions and cations. These ions interact with the protein, affecting its hydration. The change in hydration can cause elongation or coiling of the peptide. The impact of sodium and potassium ions have on the hydration of blocked glutamic acid in water was studied using molecular dynamic simulations. The trajectory data, which was analyzed using the radial distribution function, ion density map, and Kirkwood-Buff integrals, will be discussed.

24

Biochemical and Biophysical Analysis of SYT5 and TACR3 mRNA G-quadruplex StructuresMcAninch, Damian S.¹; Evans, Timothy L.¹; Mihailescu, M. Rita²¹Department of Chemistry, University of Pittsburgh at Johnstown²Department of Chemistry and Biochemistry, Duquesne University

Certain guanine-rich sequences of DNA and RNA have been shown to fold into the G quadruplex secondary structure and regulate certain processes. In particular, the G quadruplex structure located in the messenger RNA (mRNA) 5'-untranslated region (5'-UTR) may serve as a translation regulatory element. Moreover, bioinformatics analyses have predicted that 2334 guanine-rich sequences from the 5-UTRs of protein-coding human mRNAs could form the G quadruplex structure. We have selected several human neuronal 5'-UTR mRNA sequences predicted to fold into the G quadruplex structure for *in vitro* analyses of structural properties and comparison of *in silico* predicted and *in vitro* thermodynamic stabilities. Initial analyses are focused on the sequences from Synaptotagmin-5 (SYT5) mRNA and neuromedin-K receptor (TACR3) mRNA. These mRNAs were transcribed *in vitro* and purified via electrophoresis and electroelution. Circular dichroism spectroscopy, ¹H-nuclear magnetic resonance spectroscopy and UV spectroscopy were utilized to characterize the G quadruplex structure of these mRNAs.

25**The Hydration of a Lysine Residue in 0.5M, 1.0M, and 2.0M Salt solutions**

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Chemistry Department; Center for Computational Sciences

Duquesne University

Franz Hofmeister discovered that salt ions increase or decrease the solubility of a protein ("salting in" or "salting out"). The original hypothesis focused on changes in the entire water network. The new hypothesis is that the hydration of protein residues leads to protein solubility. To prove that this hypothesis specifically affects the hydration of the protein's backbone and side chains, simulations on individual amino acid residues, peptides and a protein are constructed. This project involves studying a lysine residue's interaction with the salts NaCl, NaClO₄, and Na₂SO₄ under various concentrations. Molecular dynamics simulations were performed for lysine in those salt solutions. Radial distribution functions, ion density maps, and Kirkwood Buff integrals are used to analyze trajectory data. This analysis also allows for the examination of the amino acid's hydration.

27**Development of a New Generation of Fluorescent Sensors**

Deibler, Kristine and Basu, Partha

Department of Chemistry and Biochemistry

Duquesne University

Metal ions are essential for maintaining cellular homeostasis; disruptions in their optimal concentrations can lead to numerous human disorders. Thus accurate determination of their intracellular concentration as well as their in vitro concentration is of great interest. Small fluorescent molecules that can selectively bind to a specific metal ion and thereby changing the fluorescent properties offer a means to examine metal ions trafficking in real time, which then can lead to the basic understanding of biochemical properties and/or disease state. We are interested in developing selective sensors for alkali metals. Crown ethers are known to coordinate alkali metal ions. We envisage that a known fluorophore can be altered by the addition of a crown ether that can also bind alkali metals. Herein we show the progress of the design, synthesis and characterization of such fluorescent molecules.

26**The Impact of Polarizable Force Fields on Peptide-Salt Interactions**

Trout, Colin; Gaborek, Timothy G.; Madura, Jeffrey D.

Department of Chemistry and Biochemistry

Duquesne University

Computational investigation of complex systems require very accurate force fields to obtain results comparable to experiments. A particular complex system, aqueous salt solutions, calls for the introduction of polarization into the force field. Polarization has been introduced using the drude oscillator model and implemented in both CHARMM and NAMD molecular dynamics programs. NAMD with polarization was used to study the properties of 0.5 M, 1.0 M, and 2.0M solutions of sodium chloride and potassium chloride in comparison to traditional fixed charge models. To illustrate the importance of polarization on protein systems, a model for poly- α -glutamate (AEAAAEA) was tested, incorporating drude polarization. The results of these simulations will be discussed.

28**Wireless Sensory System for PerMMA Robotic Gripper**

Ohiri, Ugonna; Houston, Elaine; Cooper, Rory, PhD.

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University of Pittsburgh

Power-motored wheelchairs with external mobility devices attached have played a major role in the field of assistive technology. This paper presents the robotic gripper used as an extended functionality of the MANUS robotic arm. In our study, we used both force and temperature sensors on the PerMMA gripper to obtain proprioceptive feedback as the arm manipulated common objects. The effect of this study is to show how effective this device can eventually be for people with disabilities, especially people with both upper and lower extremity impairments. The arm would have the ability to assist in more complex tasks and provide more information on the objects it manipulated. Future work should focus on continuing to improve the PerMMA interface as a unit.

29

Optimization of labeling conditions for the Glycine receptor (GlyR)

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Neurotransmitters transfer chemical signals from the synapse of a nerve cell to a target cell. A major superfamily of receptors for these chemical signals is the Cys-Loop superfamily. It is a ligand-gated ion channel whose major constituents are nicotinic acetylcholine, 5-hydroxytryptamine, γ -aminobutyric acid, and glycine receptors. The glycine receptors are anionic-specific channels that typically hyperpolarize neurons upon activation. There are three states of the glycine receptor: open; desensitized; and closed. By using mutant proteins with only one reactive thiol group such as: K206C; H419C; and 290C, it is possible to run accessibility studies to determine under which conditions are best to chemically modify the receptor. Upon site-directed modification by photoreactive crosslinkers, one can identify sites of photo-crosslinks using mass spectroscopy to determine the distance between specific amino acids in the glycine receptor. After this the structure and protein subunits can be modeled from this information.

31

Solvothermal Synthesis and physical characterization of the series $[M(\text{tren})]_2\text{Sn}_2\text{S}_6$ ($M = \text{Mn}^{2+}, \text{Fe}^{2+}, \text{Co}^{2+}, \text{Ni}^{2+}, \text{Cu}^{2+}, \text{Zn}^{2+}$).

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Solvothermal synthesis techniques promote the formation of novel metal-organic compounds using non-aqueous solutions and moderate temperatures. The template organic amine ethylenediamine (en) is now widely reported in the literature, but far less is known about the chemistry that can be achieved when using more structurally complex solvents. The synthesis of a series of first-row transition metal thiostannates with tris (2-aminoethyl)amine (tren) as a solvent has been patterned on the known complex $[\text{Co}(\text{tren})]_2\text{Sn}_2\text{S}_6$. The novel complexes $(\text{tren})_2\text{Sn}_2\text{S}_6$, $(\text{tren})_2\text{Sn}_2\text{S}_6 \cdot 2\text{H}_2\text{O}$, and $[\text{Zn}(\text{tren})]_2\text{Sn}_2\text{S}_6$ have been characterized by single-crystal x-ray diffraction, PXRD and UV/Vis/NIR bandgap measurements. The preparation and physical characterization of the Mn, Fe, Ni and Cu analogs has proven more challenging. Progress towards their solvothermal syntheses will also be reported. In addition, we are exploring the solvothermal conditions required to prepare a new series of $[\text{Sn}_2\text{S}_6]^{4-}$ thiostannate complexes with the template ligand diethylenetriamine.

30

Developing a New Quark Model for Heavy-Light Hadron Interactions

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We created a new quark model describing the entire known heavy-light hadron spectrum, including the B (bd) and Bs (bs) spectra. Modeling both relativistic and nonrelativistic hadron particle interactions between heavy and light quarks via computer simulation has shown that spin-dependent interactions and relativistic kinematics are essential to the new model. Hadrons are particles made up of quarks, the building blocks of all other matter, and gluons, the strong force carriers. "Heavy" hadrons' quarks are the charm, bottom, or top while "light" ones refer to the up, down, and strange varieties. Our model is intended to supplement the existing constituent quark model, in which heavy quarks interact nonrelativistically, that is most successful when applied to limited hadron spectra regions (i.e., charmonium states). Results are pending at this time. The model can be extended to predict heavy-light mesons discovered by experiment at B-factories and the LHC.

32

Developing Force Field Parameters for Sulfate and Phosphate AnionsKrizon, Evan M.^{1,2}; Madura, Jeffrey D.²¹Thiel College²Center for Computational Sciences; Department of Chemistry and Biochemistry,
Duquesne University

The conformation of a peptide is dependent upon what salts are present in its surrounding medium. Current computer simulations of peptide conformations in some salts are in disagreement with experimental results. Currently, only fixed charged force field parameters are available for most anions. Without polarization, the fixed charge approximation for complex ions may be a cause of the discrepancy between experimental and computational results, e.g. sulfate and phosphate anions. Electronic structure calculations using TeraChem 1.57 of the sulfate and phosphate anions in water will be used to generate data for the development of improved fixed-charged force field parameters. The results from classical molecular dynamics simulations with the improved fixed-charge force field parameters will be discussed.

33**Characterizing druggable sites in protein-protein interactions**

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Protein-protein interactions (PPIs) are an emerging class of targets for drug discovery. To better understand the design principles of small molecules (SMs) that perturb PPIs, we have developed a database of SMs in the Protein Data Bank (PDB) and analyzed the changes in their binding sites relative to the unbound, protein-protein, and protein-ligand structures. Our analysis shows that SMs do not create new cavities but overwhelmingly bind in the pockets identified in the PPI, even though there are significant changes between the protein and ligand bound structures. A distribution of the root mean squared deviation between unbound-ligand bound and protein bound-ligand bound interface further confirms more conformational changes between the unbound and ligand-bound interface than in the protein-bound interface. Our findings suggest that conformational change can play a key role for a PPI binding SM, but for the most part the druggable site is well defined by the PPI structure.

35**Exploring Monoamine Transporter Substrate Translocation Properties**

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The monoamine transporters (MATs) are important in terms of neuronal activity. For example, the serotonin transporter plays a role in depression by regulating amounts of serotonin in the synapse. Understanding the process of substrate translocation is important to the study of how regulation occurs. One possible mechanism for translocation is the formation of a channel through the transporter. MAT molecular dynamics trajectories were analyzed using dxTuber to locate water channels. The results from the dxTuber analysis will be discussed

34**Characterization of Bovine Mitral Heart Valve Remodeling During Pregnancy**

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Pregnancy is a terrific example of a change in hemodynamic stresses on the cardiovascular system of an organism *in vivo*- cardiac output and blood volume increase up to 50% in humans. Although other cardiovascular elements have been shown to remodel in response to pregnancy, it has been debated if the mitral valve has the capacity to do so even though the tensile stress on the mitral valve increases significantly. Recently, however, mitral valve growth was observed in pregnant cows. This study furthers previous research by using Small Angle Light Scattering (SALS) techniques to characterize overall collagen fiber orientation in pregnant and non-pregnant cows. It is expected that the fibers will become more aligned to reflect the increased tensile stress. The results of these scans of pregnant and non-pregnant bovine mitral valves will be presented in the poster.

36**Importance of Pseudochair Conformations of Carboxyphosphate**

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Wayne State University

Carboxyphosphate (CAP) is an important intermediate formed during the catalytic activity of the members of the ATP-grasp carboxylase family. The 70 ms half-life of CAP prevents experimental observation, demanding a computational approach to understand its structure and properties. DFT conformational analysis revealed two novel monoanionic pseudochair conformations that differ in the positioning of the hydroxyl group on the phosphate side. Both are stabilized by intramolecular resonance-assisted hydrogen bonding (RAHB); however, RAHB has been found to be enhanced in one particular pseudochair conformation. From NBO analysis, it was found that $\sigma(\text{P-O}_{\text{HBA}})$ to $\sigma^*(\text{P-O}_{\text{OH}})$ and $n(\text{O}_{\text{OH}})$ to $\sigma^*(\text{P-O}_{\text{HBA}})$ interactions weaken the $\sigma(\text{P-O}_{\text{HBA}})$ bond relatively more in one pseudochair compared to another. This change increases the polarity of the $\sigma(\text{P-O}_{\text{HBA}})$ bond, which increases the diffuseness of the lone pairs of HBA. The result is a strengthening of the $n(\text{O}_{\text{HBA}})$ to $\sigma^*(\text{O}_{\text{HBD}}-\text{H})$ interactions. Structural analogues of CAP were investigated to better understand the RAHB in CAP.

37

Developing Building Blocks for *de novo* synthesis of the Molybdenum Cofactor

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With more than 50 enzymes, pterin-containing molybdenum enzymes constitute an important class of molecules that are essential in life and environmental processes such as sulfur detoxification and purine catabolism in mammals. In these enzymes, the molybdenum cofactor (Moco) lies at the catalytic heart. In humans, defects in the synthesis of Moco lead to a condition known as Molybdenum Cofactor Deficiency (MCD). Patients suffering from MCD typically have progressive neurological damage that results in early childhood death caused by a buildup of toxic sulfite that damages the brain and other organs. Recently, we have been able to synthesize a new model compound that resembles Moco. In order to make a closer analog of the cofactor we have designed a new building block harboring additional components. Herein we describe the design, synthesis and characterization of this new building block as a stepping stone towards a more complete analog of molybdenum cofactor.

39

Investigating the pKa's of molecules within the protein complex cytochrome bc₁

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Cytochrome bc₁ (cytbc₁) is found in all living organisms, and plays a vital role in energy storage. When this protein malfunctions in humans the host is known to develop diseases like cardiomyopathy. The two main molecules in cytbc₁ that are being studied are ubiquinol and ubiquinone. PKa is the acid dissociation constant, so if it was determined then it would be possible to alter the protein by removing one of the molecule's bonds. Since cytbc₁ has different conformations in mammals and bacteria, it would be possible to replace ubiquinol with a drug harmful to bacteria and not to mammals. Making a virtual model of the molecule is the first step. Once the molecule is made, it is then entered into a super computer which simulates how it reacts in certain environments and phases. This yields the pKa of whatever molecule was entered into the program.

38

A Benign Novel Approach towards the Synthesis of Copper(I) Cyanide Coordination Polymers

De Fratti, Marissa; Kaur, Rajbhupinder; Pintauer, Tomislav
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The field of coordination polymers is rapidly growing because of their wide application, which includes heterogeneous catalysis, semiconducting properties, and gas absorption. The commonly used route for synthesizing these polymers is solvo-thermal method, which requires elevated temperature, pressure and prolonged reaction times. The novel approach affords a more economical and environmentally friendly alternative for synthesizing these polymers. Various copper(I) cyanide coordination polymers are obtained by reduction of copper(II) complexes with amino acids by AIBN and ascorbic acid, which are elucidated by IR, UV and single crystal X-ray crystallography.

40

Forensic Analysis of Hairs: Identifying Styling Product Residues on Hairs by GC-MS

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Forensic analysis of residues found on hairs is an important crime scene investigative tool. To help identify these unknown residues on a hair a Gas Chromatographer-Mass Spectrometer (GC-MS) is used. Before samples of hair were collected, hair products were mixed with different solvents such as Acetone, Hexane, Isopropanol, and Methanol. Then these samples were sonicated to extract soluble residues, and then analyzed by the GC-MS. After looking at these results from the GC-MS, a solvent was chosen and hair samples were collected. Finally, the ability to extract hair products from a single hair and identify them was tested.

41

Customization Functionality for RAE: An interactive web-based biomedical informatics system for pediatric orthopedic patientsMartin, Josh¹; Sherbondy, Martin¹; Martincic, Cynthia¹; Raab, Mandy¹; Sangimino, Mark²

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2 Department of Orthopaedic Surgery, Allegheny General Hospital

The goal of the RAE system is to facilitate patients' coping and management process when diagnosed with potentially serious musculoskeletal disorders through an interactive educational experience. The RAE software produces a personalized presentation containing disorder-specific and patient-specific information, as well as printable information packets to combat learning attrition. Our contribution to the project involved making the software flexible enough to be used by different physicians without directly interacting with the underlying database and code. A physician can simply select user-level customizations and patient-level presentation templates in order to make the educational presentation experience his or her own. To accomplish this, the existing database architecture was expanded to store physician preference information. The user-interface was refined to create a simple first time user experience and facilitate quick edits of existing customization settings. The future plans for this software include a clinical trial phase followed by distribution to physicians nationwide.

43

Understanding the Biotin Carboxylation Mechanism

DeLozier, Chantelle; Clymer, Traci; Evanseck, Jeffrey D. Department of Chemistry and Biochemistry Duquesne University

Biotin carboxylase (BC) is part of acetyl-CoA carboxylase which catalyzes the first committed step in fatty acid biosynthesis. Although BC has been extensively studied, its mechanism is poorly understood. Because of its role in this crucial step a better understanding of its mechanism could be exploited to treat obesity. The first step is the reaction of bicarbonate with ATP to produce a carboxyphosphate intermediate. However, when this reaction was modeled in vacuum, it had a steep energy barrier of 71 kcal/mol. The residues Lys²³⁸, Arg²⁹², Glu²⁹⁶, and Arg³³⁸ have been implicated in the literature as being crucial to this mechanism and may help overcome this energy barrier. To test the ability of these residues to overcome this energy barrier, docking methods were used to find the placement of bicarbonate in relation to these residues and then simplified quantum mechanical models were developed to evaluate their effect on the activation barrier.

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Further Expansion of RAE: An Interactive web-based biomedical informatics system for pediatric orthopedic patientsSeckar, Aaron; Raab, Mandy; Martincic, Cynthia¹; Sangimino, Mark²

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The purpose of the RAE software project is educating adolescent patients and their parents about the patients' conditions and treatments. The RAE software facilitates interactive educational sessions between orthopedic physicians and patients with the creation of a personalized, informational, and interactive presentation. My contribution to the RAE project is a new section for the patients who are required to undergo surgery. In this section, a virtual tour of the hospital that shows the child the equipment, the rooms, and the hospital personnel that the child and his or her parents can expect to see on the day of surgery. Also added are a number of preoperative and postoperative forms that can be reviewed with the patients and parents and printed for them to keep. Upon completion, the newest addition to the software will enter the clinical testing phase of development.

44

Self-assembled Monolayers on Ti-6Al-4V

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Biomaterials are a subject of increasing interest in the fields of chemistry and medicine. They are used anywhere from prosthetic limbs to contact lenses. The material being examined in this project is Ti-6Al-4V, which is used in hip implants. A multi-functional implant surface, presenting cell adhesion peptides and antibiotics, is the ultimate objective of the project. In order for this to happen surface chemistry must be established on the metal alloy which allows for the immobilization of the organic acids. Octadecylphosphonic acid, 12-aminododecanoic acid, and 16-hydroxyhexadecanoic acid, were used to form self-assembled monolayers. Solution and aerosol spray deposition methods were utilized, and the substrates were analyzed using Diffuse Reflectance Infrared Fourier Transform Spectroscopy.

45

Detection and Quantification of Dextromethorphan in Human Saliva via Solid Phase Extraction and MS-ESI

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Robitussin is a commonly ingested medication to treat ongoing cold symptoms, especially coughing. However, this drug is also commonly abused, as high dosages of the active ingredient- Dextromethorphan- have dissociative psychedelic effects¹. This project develops a method for identification (and eventual quantification) of dextromethorphan in human saliva using Electrospray Ionization-Mass Spectrometry. A dextromethorphan standard was diluted to 0.1 μ L dextromethorphan in methanol. 0.980 mL of human saliva was spiked with 0.02 mL of the diluted dextromethorphan standard and a solid phase extraction was performed. While dextromethorphan in the spiked saliva was (possibly) detected, it was almost invisibly minute compared to the other compounds in the saliva, indicating the probable need for other processing methods prior to ESI-MS^{9, 10} or that the detection limit is higher than was spiked. Ongoing research into the solid phase extraction method is being performed, as well as the possibility of testing this method on human subjects who have (orally) ingested dextromethorphan.

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Characterization of calcium phosphate and antibiotic prophylaxis

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The high cost and limited availability of bone grafts warrants the need to find a low-cost synthetic grafting material. Calcium phosphate serves as a potential synthetic grafting material. Its porous structure allows for protein and bone cell adhesion, which leads to quick and effective healing. However, low structural integrity and the risk of infection at the implantation site deter the use of calcium phosphate. This study characterized the physical and mechanical properties of calcium phosphate through scanning electron microscopy and powder X-ray diffraction. Also, a three-step deposition method was used to covalently link the antibiotic vancomycin to the surface of calcium phosphate in order to reduce the risk of implant-associated infection, and this process was confirmed stepwise using Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFT). The vancomycin-modified calcium phosphate was shown to be equally effective as standard vancomycin at inhibiting the growth of *S. aureus* (UAMS1) over time.

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Cyclic Voltammetry of the Surface of Cupronickel Modified with Methyl- and Carboxylic Acid-Terminated Phosphonic Acids

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Copper Nickel alloys are often used in underwater pipes and marine vessels. An issue with these surfaces is that they are readily corroded. To prevent oxidation, the surface was modified with Self-Assembled Monolayers (SAMs). Metal substrates of cupronickel (55Cu/45Ni) were modified with octadecylphosphonic acid (ODPA) and 16-phosphonohexadecanoic acid (COOH-PA), and characterized using diffuse reflectance infrared fourier transform spectroscopy (DRIFT) and cyclic voltammetry (CV). The modified samples were rinsed and sonicated in deionized water or brine and characterized to determine if the surface remained passive through sonication. A CV of the monolayers indicated that they appeared to remain through sonication in water; however, when sonicated in brine, the surface became less passive, possibly due to the residual salt on the surface of the metal.

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An Investigation of Interspatial Properties of Self-Assembled Monolayers

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The use of Self-Assembled Monolayers (SAM's) for metal substrates is common in many fields: medical, industry, engineering, etc. Van der Waals interactions can have an effect on the frictional properties of the underlying substrate. The carbon chain is responsible for the strength of the Van der Waals forces in the SAM. Longer chains should have more Van der Waals forces, meaning the SAM will be more compact and orderly than a smaller carbon chain. The intent of this research is to determine dependency of interspatial properties on the length of the carbon chain of a SAM. Through atomic force microscopy (AFM) friction response of the SAM's is measured and compared to the bare surface and larger and smaller chains. The less compact and orderly the monolayer, the less friction response is observed.

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3D Homology Modeling and Virtual Screening for Protein Kinase D1 InhibitorsMiller, Rebecca L.^{1,4}; Wang, Lirong^{2,3}; Wipf, Peter³; Xie, Xiang-Qun^{2,3,4}¹ Department of Physics, Rhodes College² Department of Pharmaceutical Sciences, School of Pharmacy, University of Pittsburgh³ Pittsburgh Center for Chemical Methodologies & Library Development (PCMLD) and Drug Discovery Institute, University of Pittsburgh⁴ Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh

Protein kinase D (PKD) is a family of serine/threonine kinases that has recently emerged as a key player in several processes involved in human tumor development. The role of PKDs in protein trafficking, oxidative stress response, cardiac hypertrophy, and angiogenesis promotes our interest in these enzymes as potential chemotherapeutic targets. In this study we focus on the structure of PKD1, one of three high-identity isoforms in the PKD family whose structure is currently unknown. Recently, the three dimensional structure of the related enzyme Protein Kinase C β II (PKC β II) was solved to a high resolution using x-ray diffraction analysis. In order to expand our present understanding of the architecture and dynamics of PKD1, we constructed a homology model of PKD1 using the structure of PKC β II as a template. We then docked a variety of known small molecule PKD1 inhibitors and screened for new potential lead compounds using chemical databases.

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Identification of novel mitochondrial to nuclear translocations in the Gorilla genomeYedla, Haritha; Jensen-Seaman, Michael
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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 identified previously unknown numts from a gorilla genomic library cloned into bacteria artificial chromosomes (BACs). BAC clones were grown, amplified, and sequenced to identify and confirm the genomic location of recent gorilla-specific numts using numt specific primers. We also attempted to isolate numts via Alu repeat consensus-based polymerase chain reaction, also known as ARC-PCR. These results are helping to understand the evolutionary history of gorillas, and have implications for conservation genetics and captive breeding programs.

50

Stress Responses in Plethodontid SalamandersRatay, Katie; Woodley, Dr. Sarah
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Amphibian populations are declining throughout the world yet little is known about the physiological mechanisms mediating amphibian stress responses. Corticosterone is a stress hormone that helps animals cope with stressors. In one study, I looked at the effects of CORT on antipredator behavior in *Plethodontid shermani*. In another study, I looked at the effects of chronic increases of CORT on the brain by quantifying the number of AVT cells present in the brains of *Desmognathus ocoee*. According to the first study, CORT does not have an effect on antipredator behaviors. The results of the second study are still being quantified but will hopefully contribute to the understanding of stress responses in amphibians. Together, this work will help to increase the overall understanding of stress responses in amphibians which may help to end the decline in amphibian populations.

52

Modeling Suboptimality and Complexity in EvolutionCox, Jeffrey; Snoke, David
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In evolution, increased complexity comes at the cost of the creation of both useful and useless biological structures. A computer simulation is helpful in modeling this tradeoff between increased complexity and the necessary cost associated with that increased complexity. This was accomplished by creating a number of pseudo-organisms living on a grid, and then simulating mutations as random paths in a multi-dimensional parameter space. All mutations had a cost associated, and some mutations resulted in the organism being rewarded. Dr. David Snoke created a program to model this facet of evolution using a serial approach, and I have expanded this program, allowing for simulations to be run simultaneously on a cluster.

53

Arsenic Speciation Validation of EPA methods 3110/6870 using 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 LD₅₀s varying from 4.5-10,000 mg/kg. The EPA has developed two methods for arsenic speciation, one for extraction (3110) and one for analysis (6870). These EPA methods do not account for transformation between the inorganic species of arsenic, which are the most toxic. Normally, a method called SIDMS could be used in which the samples are spiked with different isotopic forms of the element of interest. However, arsenic is monoisotopic, making this traditional method unfeasible. Therefore, ¹⁸O is used to enrich As (III). With these spikes and ¹³C for the organic arsenic species, SIDMS is being applied and the sample analyzed by Ion-Exchange Chromatography-Inductively Coupled Plasma Mass Spectrometry (IC-ICP-MS), and Time of Flight (TOF) mass spectrometry.

55

Equilibrium Weighted Ensemble Sampling of Biomolecular Configurations

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Brute force molecular dynamics simulation is an impractical method to find equilibrium ensembles of proteins. As an alternative, the weighted ensemble (WE) method uses multiple trajectories and reweighting to more easily sample the configuration space of a protein. We propose a modification to the original WE method which uses the rate information to continually update the equilibrium probability distribution of the configuration space. We tested this equilibrium WE method using alanine dipeptide, a small molecule often used in testing new methods. To assess the efficiency of the new approach, we compared the computation times and equilibrium ensembles for brute force and equilibrium WE simulation.

54

Modified Calcium Surfaces as Optimal Tissue Scaffolds

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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 (CaAl) and hydroxyapatite, the mineral components of bone, were investigated as potential bone tissue scaffolds. These materials are bioactive, easily synthesized at room temperature, and have been shown to induce *de novo* bone formation. To enhance regenerative properties, the scaffolds were modified via chemical immobilization of bone morphogenetic protein 2 (BMP2), a protein responsible for enhancing bone cell growth and differentiation, and the cell adhesion peptide Lys-Arg-Ser-Arg (KRSR). Viability of both fibroblast, a component of connective tissues, and osteoblast cell lines was examined to determine cell-binding specificity. This study effectively shows that BMP2 functionalized and KRSR functionalized calcium scaffolds selectively increase osteoblast viability as compared to fibroblast viability and enhance cell adhesive properties over unmodified scaffolds.

56

Examining Assembly Formation in Inhibitory Neural Networks

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Understanding and predicting the behavior of neural networks is a key goal of mathematical neuroscience. When coupled, two inhibitory neurons will alternate firing. In larger networks, this activity can give rise to sequentially switching assemblies of neurons, as well as waves of activity. We predict the formation of these patterns of activity based on network topology and connectivity. Groups form among neurons with low connectivity between them, and group size and connection weights influence firing dynamics. We find that dynamics at each network node are insignificant compared to the topology of the network as a whole. This work was supported by NSF Award # 1004555.

57

Obtaining Timing Accuracy Among Transit Data Using Known Asteroids

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We can detect planets around other stars by measuring the change in brightness as a planet passes in front of the star. While we can confirm this by the dip in the lightcurve plot, careful analysis of successive transits and possible transit timing variations can reveal other planets in the system. Since earth sized planets can cause variations as small as one minute between transits, accurate timing of the transit is extremely crucial.

However, it is difficult to obtain accurate timing information when comparing data among different nights and different observatories.

The location of the observatory combined with the time standard used and the accuracy of the computer clocks can all cause false timing variations.

We seek to resolve this issue by creating a program that utilizes known asteroids in our field of view to shift and stack the images. By shifting and stacking the images accordingly with the motion of the asteroid, we obtain a final image where the asteroid appears as a stationary point source while the stars are streaked. By comparing these final images and measuring the discontinuities, we will be able to synchronize the time between sets of data. This accuracy will allow us to measure definitive timing variations that would suggest the presence of an additional planet.

59

Simulation of Leucine in Salt Solutions

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Protein structure and function depends on the aqueous environment composition. All proteins are found in aqueous buffers, which contain salt ions. Hofmeister observed how different salts affected a protein's solubility. Insight into how cations and anions interact with amino acids that make up a protein is poorly understood. This study reports the results for the interaction of NaCl and KCl aqueous solutions with the amino acid Leucine at 0.5, 1.0, and 2.0M. The results from evaluating Kirkwood-Buff, ion-density maps, and radial distribution functions will be discussed.

58

Computational Investigation of the Brucine-Derived Amino Alcohol Catalyzed Asymmetric Henry Reaction

Rooney, Edward; Pakkala, Venkata S.; Kim, Hun Young; Oh, Kyungsoo; Evanseck, Dr. Jeffrey D.

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Department of Chemistry and Chemical Biology
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The enantioenriched Henry products were synthesized and analyzed from the use of metal-ligand complexes generated from Cu(I) and Zn(II) metals with readily available chiral amino alcohol. When using Cu(I) the enantioselectivity of the products generated 78-96% anti-Henry products (R,S) and 92-98% syn-Henry products (R,R). With Zn(II) the enantioselectivity generated yielded 28-60% anti-Henry products (S,R), (R,S) and 52-92% syn-Henry products (S,S). In order to understand the asymmetric origin of our catalysts, computational analysis was undertaken. Initially, the Henry reaction was modeled with aldehyde and nitroethane in the absence of metalated catalyst, to generate 12 plausible asymmetric Henry products. From these calculations four of the chiral products syn-(R,S), syn-(S,R), syn-(R,R), and syn-(S,S) were found to be most stable with the same activation energy. Of interest is on how the catalyst modifies the stereochemistry of the products. This study will highlight the electronic and steric considerations in explaining the role of Cu(I) and Zn(II) metalated brucine-derived amino alcohols in asymmetric Henry reactions.

60

Using Bacterial Spores for Vaccine Delivery

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Spores from unicellular bacteria have been used for vaccine production, probiotics, and biosensors. Spores from filamentous bacteria have not been thoroughly investigated for use in similar applications. SapC is a spore-associated protein of the filamentous sporulating soil bacterium *Streptomyces coelicolor*. The goal of this project is to fuse the gene encoding SapC to the gene encoding the B subunit of the heat labile toxin of *E. coli* to determine if the antigen portion can be expressed and incorporated on the spore surface. If this antigen can be expressed on the spore surface, it could allow for an oral vaccine with an extended shelf life. The toxin fusion gene was inserted into the chromosome to see if it would be expressed and exposed on the spore surface. This procedure will allow for gene fusions of other toxins, including the gene encoding the tetanus toxin with *sapC* or other spore-associated protein genes.

61

Reproduction in the Serranid Reef Fish, *Hypoplectrus*, Using a Molecular Parentage Approach

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Hamlet fish (genus *Hypoplectrus*) are simultaneous hermaphroditic broadcast spawners, theoretically switching male and female roles between each mating bout. The goal of this project is to investigate this mating strategy using a molecular parentage approach and to determine empirically if this proposed strategy is accurate. Maternally inherited mitochondrial DNA will be used to determine which individual contributed the egg in each mating bout. Multi-locus microsatellites markers will be used to determine the distribution of parental alleles between offspring. Fieldwork was performed off of Islamorada, Florida to observe and capture the fish while they were spawning. Mitochondrial primers in the 16S ribosomal subunit, tRNA-Leucine, and ND1 genes were designed to amplify the control region. Microsatellite primers for five loci were used to determine the genotypes of individuals from a small Hamlet population collected off the coast of Florida.

63

Complementarity of the IIIId Region of the Hepatitis C Genome with 5BSL3.2 and Antisense PNA

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Hepatitis C Virus (HCV) infects 170 million people worldwide, causing chronic liver disease and hepatocarcinoma. Currently there is no adequate treatment for HCV, but proposed drug targets include conserved regions of HCV's positive sense RNA genome. Two such regions are the 5' and 3' regions of the genome, which interact with conserved regions within the coding region to facilitate HCV translation and replication. This study characterizes at the molecular level the interactions of a conserved region within the 5' untranslated region (IIIId) with a conserved stem-loop within the coding region (5BSL3.2), interactions essential for the translation of the viral proteins. Additionally, we have analyzed a peptide nucleic acid (PNA) designed against the IIIId region to determine whether the IIIId-PNA hybridization can disable IIIId function, and hence the HCV translation.

62

Ivermectin Sensitive GlyR Mutations

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Studies conducted on the glycine receptor (GlyR) can help us understand the structure and function of not only GlyR but also other receptors like nAChR and 5HT3A, as they all belong to the Cys loop superfamily. The purpose of this project was to put single reactive cysteines in the area that is believed to be the Ivermectin (IVM) binding site of an IVM-sensitive form of the $\alpha 1$ GlyR. These mutations in a cys-null pFastbac background will later be used in crosslinking studies to look at the receptor in different states of its conformation. The specific aims of this project were to create single-cysteine GlyR mutants using Quickchange site-directed mutagenesis kit then to verify the presence of desired mutant residues by Genewiz sequencing. The mutated GlyR plasmid will be moved to bacmid virus using Bac-to-Bac Baculovirus Expression System. Sf-9 insect cells were infected with the virus to over express GlyR protein.

64

Alternative Fuels: Investigation of Ammonia Borane Hydrolysis

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Ammonia borane (AB) is a target for hydrogen storage media in portable fuel cell applications. We have found that density functional theory (DFT) and second-order Moller-Plesset (MP2) theory model the activation of hydrolysis of AB through an S_N2 mechanism to within 3 kcal/mol of the experimental activation energy. AB and dimethyl AB hydrolysis reactions were conducted in order to gather experimental activation energies for validating our model further. In similar reactions, we have investigated metal catalysts in the form of nanoparticles in AB hydrolysis. Using DFT, stable transition metal clusters (TMC) of cobalt were found using B3LYP/LANL2DZ. These TMC are will be used in future investigations of AB and its derivatives. The influence of the TMC upon the S_N2 reaction path of AB hydrolysis, as well as the hydrolysis of AB and methylated AB in the presence of acid at various constant temperatures is reported.

65

Determining the binding affinity of *Toxoplasma* ROP proteins to a membrane using free energy calculationsOnyeozili, Nwamaka^{1,2}, Callenberg, Keith M.³, Boyle, Jon P.²; Grabe, Michael^{2,3}¹Department of Chemistry, Florida A&M University, Tallahassee, FL, ²Department of Biological Sciences, ³Joint Carnegie Mellon University-University of Pittsburgh Ph.D. Program in Computational Biology, ⁴Department of Computational & Systems Biology, University of Pittsburgh, PA.

Toxoplasma gondii is an intracellular parasite that has infected about a third of the world's human population. Infection involves the secretion of rhoptry proteins (ROP) into the host cell during invasion. Some of these ROP proteins associate with a nascent parasitophorous vacuole membrane (PVM), in which the parasite resides. The ability of ROP proteins to associate with the PVM is due to a specific arginine-rich domain consisting of three putative α -helices. We used MARTINI coarse-grained molecular dynamics simulations to elucidate the nature of this interaction between helices from one of these ROP proteins (ROP5) with a model membrane. We went on to use umbrella sampling together with Weighted Histogram Analysis Method to calculate the binding energy of each helix to a model membrane. We predict that helix 2 binds the strongest to the membrane, which is in excellent agreement with fluorescence experiments carried out on ROP5 deletion mutants *in vivo*.

67

The Effect of Pressure on a PS-PEO SeriesMiceli, Lia; Logan, Jennifer
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Polystyrene-*block*-poly(ethylene oxide) (PS-PEO) is an amphiphilic diblock copolymer that phase separates into nanostructures when applied to an air/water interface. Such features can be imaged by transferring the polymer onto a substrate using the Langmuir-Blodgett technique and an atomic force microscope (AFM). In this study, we investigate a series of polymers containing constant PEO but variable PS. We specifically examine the effect of surface pressure to determine the role of surface density in nanostructure formation. Films were prepared at pressures of 2, 6, 10, and 15 mN/m and transferred onto a mica substrate in order to determine if structural formation followed distinct patterns regarding the amount of PS and pressure. Width, height, and percent coverage measurements were obtained. In general, we found that increasing surface pressure leads to compressed features in more hydrophobic polymers and additional aggregation in more hydrophilic ones.

66

PS-PEO Nanostructures: The Effects of Spreading SolventGlagola, Cameron; Logan, Jennifer
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Polystyrene-polyethylene oxide (PS-PEO) is an amphiphilic diblock copolymer whose immiscible components lead to the formation of nanostructures. The resulting structures can be used as templates to incorporate quantum dots or for thin film deposition of conductive metals for electronics. To create these nanostructures, the PS-PEO is dissolved in a solvent and spread along the air/water interface on a Langmuir Trough. The resulting structures are transferred as a Langmuir-Blodgett film and imaged using an atomic force microscope. The spreading solvent's effect on PS-PEO nanostructures was investigated using a series with a constant length of PEO and variable PS with chloroform (v.p. 160mmHg), 1,1,2,2-tetrachloroethane (v.p. 8mmHg), and toluene (v.p. 22mmHg) as solvents. Traditionally chloroform is used though its rapid evaporation leaves PS-PEO kinetically trapped, frozen into certain structures. Our findings, however, show that using less volatile solvents dramatically affect the nanostructures, giving us greater control over the polymer system.

68

Search for a Selective Serotonin Re-uptake InhibitorJean, Bernandie; Manepalli, Sankar; Madura, Dr. Jeffrey
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Duchesne University

The serotonin transporter (SERT) is the primary target in treating depression because it regulates serotonin levels. Selective serotonin re-uptake inhibitors and tricyclic antidepressants are the most widely prescribed medications for clinical depression. These inhibitors block the pathway and uptake of serotonin in the transporter thus alleviating depressive symptoms by increasing levels of serotonin. While effective, these inhibitors have undesirable side effects. A structure-based pharmacophore was developed and virtual screening was employed to identify new compounds that will bind in the high affinity S1 pocket of SERT. The results from the virtual screening calculations will be discussed.

69

Examining the p53-Mdm2 Binding Mechanism By Computer Simulation

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The p53-Mdm2 complex is well-studied due to its implications for cancer. p53, a tumor suppressor is inhibited upon binding by Mdm2, an oncoprotein. Traditionally, protein binding is believed to occur only when both partners are folded prior to binding. A recently proposed “fly-casting” mechanism argues that binding occurs more favorably for some proteins that are initially unfolded. The p53-Mdm2 complex exemplifies this case because p53 exhibits intrinsic disorder in isolation. Computer simulations at residue level detail will be employed to test the hypothesis that fly-casting is important in the binding of p53 by Mdm2. Because protein binding is costly to simulate—much time is wasted in simulation of diffusion and unproductive encounters—an enhanced sampling approach (weighted ensemble) will be used to efficiently capture such rare events. The particular strength of weighted ensemble is realistic kinetics, which can be utilized to assess the significance of the fly-casting hypothesis.

71

Genetic modification of *Asaia borogensis* using mariner transposition

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Malaria is a debilitating disease and a socio-economic threat to many countries in Sub-Saharan Africa. Increased resistance of mosquito vectors to pesticides and of the *Plasmodium* parasite to anti-malarial drugs decrease the effectiveness of current forms of malaria control. A new strategy to combat malaria is by means of genetically engineering symbiotic microbes of the malaria vector *Anopheles gambiae* to express proteins that inhibit malaria parasite development. *Asaia borogensis* is a bacterial resident of the mosquito midgut, which is also the location of crucial life stages of the malaria parasite. We attempted to create transgenic strains of *Asaia* using *Himar1* mariner transposable elements. During incubation, pSC189 encoding Kanamycin resistance and GFP expression was transferred from *E. coli* SM10 λ pir to *Asaia* by conjugation. Only *Asaia* with inserted transposons were able to grow on selective media. Results of GFP expression and genomic location of insertions into the *Asaia* chromosome will be discussed.

70

Characterization of novel small RNAs in prostate cancer

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Small non-protein-coding RNAs such as microRNAs (miRNAs) function as tumor suppressors and oncogenes. Given that miRNAs suppress gene expression at a post-transcriptional level by binding to specific sites of target messenger RNAs (mRNAs), we investigated whether novel small RNAs obtained from a prostate cancer cell line could bind to mRNAs. We performed a transcriptome-wide screening of all mRNAs to test whether there is any binding site enrichment for novel small RNAs in these mRNAs. Control experiments were performed using randomly selected genomic regions that mimic the length distribution of the small RNAs.

72

Simple Bioinventory System for Multidisciplinary Research Laboratory

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In a multidisciplinary research lab with researchers working in tandem to create and modify genetic material, it is imperative to integrate all the available document resources to consolidate information. In order to facilitate cooperation between researchers, a simple and user-friendly data-mining program must be structured that can be accessed and appended by all researchers. Using Microsoft OneNote, a “notebook” for the lab can be created containing separate sections for data that include tables of inventory to hold information on the lab’s biomaterial resources. For unique resources produced in the lab, files with sequencing and protocol must be included and searchable to allow the user to find all relevant information. The goal is for a user to access information even if the substance or location is unknown. Such a bioinventory provides an effective mechanism for collaboration among busy researchers thus having a positive effect on the research projects within the laboratory.

73

Transcription Factor and microRNA Target Gene Enrichment in Decoupled Partitions of Gene Expression Data

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Abstract: High-dimensional gene expression array data can be partitioned into gene clusters based on similarity of expression across samples or time points. Members of a cluster are more likely to share common regulators. A new technique called the Partition Decoupling Method identifies clusters at multiple levels, even smaller or weaker clusters that may be obscured in a single layer analysis. We explore the possibility that distinct types of genetic regulation will govern the clustering pattern found in different layers of gene expression data. Specifically, we contrast two independent forms of regulation: transcription factors, which promote or suppress transcription, and microRNAs, which act post-transcription by modifying mRNAs. This discovery would yield a more accurate method for identifying likely targets of a specific type of regulatory factor.

75

Using BioNetGen to Model Simplified DNA Processes

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The software BioNetGen allows for one to model molecular interactions by defining rules that specify what types of molecules can bind and change state. Flexibility is gained by allowing the rules to describe a class of interactions that may occur. Using BioNetGen we can model a simplified version of the DNA replication process. This demonstrates that simple operations on DNA are easily accomplished in BioNetGen and shows that modeling other processes involving DNA is feasible. For example, it would be possible to extend the model to include the effects of histone deacetylation on the transcription process—histone deacetylase molecules can bind to nucleotides and then switch them to states that inhibit transcription.

74

DNA Primase of Cluster A1 Phages: An Unusual Gene Arrangement

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Bacteriophages, viruses that infect bacteria, are often viewed as the largest untapped genetic resource with an estimated 10^{31} phage particles worldwide and an average of around 100 genes per phage. During the lytic cycle, some bacteriophages replicate their dsDNA genomes in large quantities, and many components of the bacterial DNA replication machinery are encoded by bacteriophage, including DNA polymerases, helicases, and primases. The Mycobacteriophage Cluster A DNA primase is unusual because it appears to be encoded by two substantially overlapping genes found in different translational frames rather than by one open reading frame. Through cloning and expressing the Cluster A DNA primase, we hope to elucidate the nature of the translation of the DNA primase and resolve this bioinformatic inconsistency.

76

Electronic Structure Calculations for the Quaternary Diamond-Like Semiconductor $\text{Li}_2\text{MnSnS}_4$ using Density Functional Theory

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First principle calculations were used to calculate the electronic structure of $\text{Li}_2\text{MnSnS}_4$, CuAlS_2 , and TiC using the WIEN2K package for materials science. WIEN2K utilizes the full potential linearized augmented plane wave method (LAPW) for calculating crystal properties. These types of calculations are potentially useful, because many physical properties of a material can be predicted based upon analysis of its electronic structure. CuAlS_2 and TiC are known materials and were selected as example compounds to validate the method of calculating the electronic structure for semiconductors with WIEN2K. $\text{Li}_2\text{MnSnS}_4$ is a quaternary diamond-like semiconductor (DLS), which is of interest due to its potential nonlinear optical properties, specifically, second harmonic generation. The band structure, density of states, and electron density was calculated for TiC , CuAlS_2 , and $\text{Li}_2\text{MnSnS}_4$. The results from the electronic structure calculations, which can be used to understand experimental results, will be discussed in this poster.

77

Testing Novel Perfluorocarbon Nanoemulsions for COX-2 Inhibition in Immune Cells

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Tumor progression is supported, in part, by inflammatory processes. Celecoxib, a nonsteroidal anti-inflammatory drug (NSAID), has shown anti-cancer activity in several clinical and preclinical studies. The purpose of this project was to evaluate the toxicity and efficacy of perfluorocarbon (PFC) nanoemulsions carrying an anti-inflammatory drug, celecoxib. Nanoemulsions composed of drug, PFC, hydrocarbon oil, near infrared (NIR) dye and surfactants were prepared using sonication and microfluidization. Dynamic light scattering (DLS) was used to assess particle size and stability. *In vitro* toxicity of the nanoemulsions was assessed in fetal skin derived dendritic cells with a MTS cell proliferation assay. Cellular uptake of the nanoemulsions was quantified using ^{19}F NMR and Odyssey® infrared imager. The anti-inflammatory activity of celecoxib nanoemulsion was determined by measuring prostaglandin byproducts using a PGE₂ EIA kit. Toxicity of the nanoemulsions was highly dependent on the type of hydrocarbon oil used.

79

Effect of age at initial RSV infection on lung macrophage phenotype

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Respiratory syncytial virus (RSV) is the leading cause of acute lower respiratory tract infections in children worldwide, yet there is no vaccine and no effective treatment. While adult rodent models have been instrumental in understanding numerous mechanisms of the host immune response to RSV disease, many aspects of the immature infant immune system cannot be recapitulated in adult animal models. An infant mouse model of primary RSV infection is critical for determining the role of immature alveolar macrophages in RSV disease. We compared the phenotypic immune responses of lung macrophages among 2 to 4 day-old and 7 day-old neonatal mice to determine the effect of age following primary RSV infection. Using a novel infant mouse model of RSV infection, we determined that age at initial infection has a significant effect on lung macrophage phenotype.

78

Characterizing the Structure of the G-quadruplex within CHRNA4

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Four planar guanine nucleotides found in some RNA sequences can fold into G quadruplex structures composed of stacked tetrads. Such structures are very stable due to the Hoogsteen-hydrogen bonding between the guanines within each tetrad and to the presence of potassium ions. Cholinergic Receptor Nicotinic Alpha 4 (CHRNA4) encodes for the $\alpha 4$ subunit of the larger protein, neuronal nicotinic acetylcholine receptor (nAChR), found in nerve cells. The mutated CHRNA4 results in disorders such as autosomal dominant nocturnal frontal lobe epilepsy (ADNFLE) and nicotine dependence. Based on its sequence, it is possible that the CHRNA4 messenger RNA will form a G quadruplex structure. The objective of this study is to use different biophysical methods to determine if indeed this mRNA adopts a G quadruplex structure, and to characterize it.

80

Exploring Speech in Russian Fairy Tales

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Fairy tales are distinctive in that they have no specific author and reflect the beliefs and cultural practices of the community in which they were created. Because of their simultaneous ability to reflect a culture and perpetuate its values, the study of the messages that fairy tales contain lends itself to an examination of gender roles. The primary goal of my research is to determine the connections between speech, which functions as an indication of agency, and gender in Russian fairy tales. I hope to discover how these connections differ from those found in other fairy tale traditions. As part of my research I am examining the use of direct and indirect speech and studying the verbs of speaking associated with different character types. In order to collect this data from a large number of tales, my project employs a variety of computing tools to collect and display information.

81

Lipocalin 2 mediates host survival response to *Klebsiella pneumonia* infection by modulating macrophage polarization.

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The recent exponential increase in antibiotic resistance compels researchers to explore alternatives to antibiotic therapy. A better understanding of antimicrobial proteins and their role in our immune system can lead to a novel way to combat pathogens. Lung injury in the pneumonia model between wild type and *Lcn2* knockout mice were assessed to study the antimicrobial protein lipocalin 2. Survival tests and rectal temperatures revealed a significant difference between wild type and knockout in their ability to fight pathogens. Lipocalin 2 is known to fight pathogens by actively inhibiting bacteria's iron intake. Further investigation via histology, bronchoalveolar lavage, western blot, and real time PCR led us to discover that macrophages in knockout mice were wrongly polarized. Based on these data, we believe that lipocalin 2 is not only responsible for preventing bacterial growth, but also involved in macrophage differentiation.

83

Image-based Texture Analysis Algorithms for Picking Cryo-EM Particles

Watkins, Breana, Burger, Virginia and Chennubhotla, Chakra S., Department of Computational and Systems Biology University of Pittsburgh School of Medicine

Three-dimensional reconstruction of particles picked from Cryo-EM images has dramatically enhanced our current understanding of molecular and macro-molecular structures. However, the method's usefulness is inhibited by the tediousness and inefficiency of the particle picking step, which is generally performed manually and can require millions of particle selections over many months. We hypothesize that the problem of particle picking is similar to recognizing textures in noisy images. To this end, we design orientation-sensitive texture recognition algorithms for picking Cryo-EM particles and demonstrate that the effectiveness of the semi-automatic process on a curated database of Cryo-EM images.

82

A Robotic Wheelchair Arm to Assist with Transfers

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One of the main causes of injury among wheelchair-users and caretakers is from strain due to transfers. Shoulder and elbow joint pain, as well as lower back pain are common problems among these groups of people. Lifts have been found to greatly reduce injury among healthcare workers. This project is to develop a robotic arm that is attached to a power wheelchair to assist with user transfers. There is not currently a wheelchair commercially available that assists with transfers. A transformation matrix is developed for the arm in order to communicate the required positions to the robot.

84

Thyroid Hormone Receptors in the Avian Yolk Sac

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Thyroid hormone (TH) functions by binding to thyroid hormone receptors (TR), which in *Gallus gallus* include TR α , TR β 0, and TR β 2. We detected the presence of TR α RNA in yolk sac membrane, brain, eye, heart, and liver from 15 day chicken embryos by RT-PCR. *In situ* hybridization was established using Xbra in gastrulating *Xenopus laevis* embryos with specific sense and antisense probes. I performed PCR for Xbra sequence, ligated the DNA amplicon into a vector, transformed bacteria, performed PCR for the sequence within the vector, and digested with enzymes to create the probes. I created 200 and 1000 base pair probes for chicken TR α and TR β 0, respectively, and designed primers to create a larger, 892 base pair probe for TR α . *In situ* hybridization will be used to determine the specific locations of TR α , TR β 0, and TR β 2 RNAs in the yolk sac membrane, linking TH with yolk sac regression.

85**The Characterization of Mycobacteriophage LittleE major capsid gene and protein**

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Bacteriophages are viruses that infect bacterial hosts. They are the most common and diverse organisms on Earth, and collectively comprise the single largest pool of genetic information. dsDNA tailed bacteriophage capsids are comprised primarily of many copies of the major capsid protein. The major capsid protein structure, as determined by x-ray crystallography and cryo electron microscopy is conserved among known dsDNA tailed viruses despite as lack of protein sequence similarity. Comparative genomics reveals that the major capsid gene in Mycobacteriophage LittleE has been disrupted by a substantial insertion, which is likely a self-splicing intron: the first such identified in the mycobacteriophages. To characterize the nature of this insertion into the major capsid protein gene of LittleE, we examined the major capsid protein using SDS-PAGE, and determined the N-terminal sequence through electroblotting and Edman degradation. A single band of approximately 43kDA that began DLDRNGG was observed, supporting the conclusion that the major capsid protein is made from a fusion of the two major capsid protein gene products with some N-terminal cleavage due to the use of a Delta-domain during capsid assembly. Isolation of mRNA from LittleE infected cells, RT-PCR and cloning will be performed to determine if the major capsid protein fusion is created through the splicing of an intron in the major capsid gene transcript.

87**The Effect of Various Substituted TREN based ligands for use in Atom Transfer Radical Addition (ATRA)**

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The Atom Transfer Radical Addition (ATRA) reaction is a fundamental organic reaction that adds a polyalkyl halide across a double bond thus creating a new carbon-carbon. It was determined that this reaction could be catalyzed by various transition metals including copper, nickel, and ruthenium. The addition of a reducing agent continuously allows for the reduction of the metal thus increasing the yields of the reaction and "greening" the process. The activity of the metal, which is bound to a nitrogen based ligand, is thought to be directly related to the electronic properties of the ligand. It is hypothesized that the more electron donating the ligand, the more reducing Cu(I) species. This project investigates the activity of various TREN based electron withdrawing/donating ligands in ATRA. Characterization techniques such as X-ray Diffraction, ^1H & ^{13}C NMR, IR, CV, and UV-vis will be used.

86**Analysis of Soil in Allegheny County by PXRD**

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Soil is a common material and therefore is often found at crime scenes. Soil analysis is an important part of forensic science; being able to determine the composition of soil sample from a crime scene and trace it back to specific areas or persons would be useful. Powder X-ray Diffraction was used in this research to analyze prepared soil samples taken from various regions of Allegheny County and determine the inorganic crystalline structures present. The spectra obtained from these samples were run through a database in order to determine the composition of the soil and a method of statistical analysis is currently being made to quantitatively determine if there is a significant difference between spectra. The results have been determined by qualitatively analyzing the peaks for visible differences.

88**Controlling Surface Properties of Metal Oxide Nanoparticles**

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The physical and chemical properties of metal oxide nanoparticles can be tailored by the attachment of organic acids. These acids may allow for control of characteristics, such as increased photoreceptive and sensor abilities. For the first time, zinc oxide nanoparticles were modified using organic acids with carboxylic, phosphonic, and sulfonic functional groups. The modified zinc oxide nanoparticles were characterized using infrared spectroscopy (IR), solid-state nuclear magnetic resonance spectroscopy (SS-NMR), powder X-ray diffraction (PXRD), and stability tests (solvent rinsed, pH, time) were performed to confirm the molecules were strongly bounded on the surface. The band gap was calculated for the modified nanoparticles by UV-Vis absorption.

89

Calorimetric Characterization of an Interactive Mixture of Cefuroxime and Calcium Phosphate in Water

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To thermodynamically determine the interaction of hydrophobic cefuroxime (Lower heat of wetting) and hydrophilic calcium phosphate (Higher heat of wetting) with water both as separate powders and as an interactive, binary mixture, an isoperibol calorimeter was used to measure heats of immersion of powder samples. A high-shear mixer was used to adsorb cefuroxime to calcium phosphate. Physical properties were characterized using BET surface area analysis, sieve analysis, helium pycnometry, and determination of the bulk/tap densities. If the particles separate upon immersion, the observed heat of immersion should be equal or greater than the sum of the values measured for the two separate powders. If the hydrophobic cefuroxime remains on the surface of the calcium phosphate, the observed heat would be less. Therefore, comparisons are being made between the heats of immersion of the separate powders and their mixtures to determine how interactive mixing affects their interactions with water.

91

The Effect of Breast Cancer Treatment on Employment

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An estimated 192,370 women were diagnosed with breast cancer in the US in 2009 and 40,170 died of the disease. Adjuvant therapy, given after surgery and comprised of hormonal therapy with or without chemotherapy, reduces recurrence and overall mortality in postmenopausal women with breast cancer. Mortality rates have decreased from 1990-2006 by 3.2% per year among women younger than 50. The decline in breast cancer mortality has been attributed to the improvement in breast cancer treatment and early detection. However, recent studies corroborate the notion that adverse effects of breast cancer treatment not only affect the personal life of breast cancer survivors, but also the productivity and work experiences of those who return to work. The current literature review seeks to examine the issues faced by breast cancer survivors who return to work and identify possible strategies and supports that may assist in addressing obstacles to employment success.

90

Measuring Turbulent Shear in a Three Dimensional System

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When water flows in a pipe, its speed varies from almost zero at the wall to its maximum at the center of the pipe, and this difference in flow speed is referred to as *shear*. Shear has a number of practical consequences, such as affecting the steadiness of an airplane's flight. Measuring it provides much information about a particular fluid flow. If a flow is turbulent, the shear jumps around over time at one specific location. In this experiment, an array of spinning nozzles introduces turbulence in a large tank filled with water. The mean shear rate is measured near a wall of the tank using a method called photon correlation spectroscopy. This involves a laser, aimed through the tank. The water in the tank is filled with small particles that scatter the laser beam. A photodetector's signal enables one to determine the shear.

92

Problems with Current Continental Approaches to the Philosophy of Science

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Recent proposals for a hermeneutic philosophy of science capable of explaining the paradoxes of quantum mechanics were critiqued due to their inability to justify the existence of theoretical concepts in the life-world. These concepts were shown to be necessary by reviewing the hermeneutic circle—which is the key component in continental models of scientific inquiry—and how this circle requires theoretical entities if it is going to allow human experience to be temporally continuous. It was argued that without this continuity phenomenological approaches would be unable to accurately reflect reality. If phenomenology is to be used for describing natural science it must be done using an ontology that reflects the essential role of theoretical entities in human experience.

93

Automating Refinement of Multiple Sequence Alignments

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Multiple Sequence alignments provide a map of the evolution of a particular gene or protein family. It also provides good guidance for experiments by indicating important residues in the gene or protein family. Good multiple sequence alignments still require human intervention in their construction with the best current methods being less than 70% accurate by residue. To distinguish among different methods, we have devised a method that imposes extensive local pattern information on the results of various global multiple sequence alignment programs. This is similar to the widely used consistency analysis which is at the core of several of the best performing multiple sequence alignment programs. We will show results of applying this procedure to several families of proteins.

95

Distinctive Features of Universal Stress Proteins

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Many bacteria contribute to the contagion of food borne illnesses in the United States. Therefore, there is a need to understand the intrinsic features that enable bacteria pathogens to survive a variety of food processing conditions. Genes encoding for the universal stress protein (USP) domain are known to provide a variety of pathogenic bacteria with the ability to adapt to changing growth and host conditions. The objective of this study is to analyze a variety of genomes that encode for USP genes in order to understand the unique features associated with USPs. Many analysis techniques were used including Multiple Sequence Analysis and Phylogenetic Comparison. This study has yielded the need for further analysis of the proteins.

94

Parallelizing Sellers Algorithm

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Assembling DNA reads in Next-Gen Sequencing is a crucial step to successfully retrieve a genome, where the goal is to merge and align from hundreds to thousands of fragments of a DNA sequence and be able to reconstruct the original sequence, based on a reference genome. Several algorithms have been devised for such operation, but in order to accelerate the computation many resort to heuristics based approaches which can then impact the confidence of the resulting DNA sequence. In 1979, Peter H. Sellers published an algorithm which is specially designed for finding alignments of small sequences in a much larger one. We present a new parallel implementation for this algorithm, which is aimed to address sequence alignments done in the assembling process of Next-Gen Sequencing methods.

96

Experimental Analysis of the Human Serotonin Transporter

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The serotonin transporter (SERT) regulates the levels and distribution of serotonin throughout the nervous system. Serotonin, 5-hydroxytryptamine (5-HT), is considered an excitatory neurotransmitter and is chiefly responsible for many physiological and psychological functions (i.e., cardiovascular function, mood control, and sexual behavior). Current research is focused on discovering the links between serotonin and various disorders such as depression and addiction. As inhibition of SERT leads to elevated serotonin levels, SERT has been found to be the target for many inhibitory substances such as cocaine and anti-depressants. Utilizing methodologies such as click chemistry and mass spectrometry, SERT was experimentally analyzed to identify its putative binding sites and overall structure. In addition, photo-crosslinking was employed to label antagonists and map the binding sites of SERT. Further understanding of SERT may enhance current pharmaceutical approaches for the treatment of serotonin-linked disorders and provide an overall greater understanding of these specific drug-transporter interactions.

97**Surface Modifications of Anodes in Li-ion Batteries**

Nathan Esperon, Dr. Prashant Kumta
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 University of Pittsburgh

The creation of more effective anodes in lithium ion batteries will be important for the development of future energy storage technology. My current work allows me to prepare electrode materials to be used in experimental electrochemical cells, including the use of electroless deposition of copper on a silicon-carbon composite.

99**Combating Blindness with Convenient and Comfortable Glaucoma Treatments**

Sydney Cope, Dr. Steven R. Little
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 Northwestern University

Due to the many issues associated with the current methods for glaucoma drug delivery, such as low patient compliance rates, the invasive nature of some techniques, and the concern of systemic toxicity, we are investigating more convenient and comfortable delivery methods. We are developing a controlled-release delivery system, brimonidine tartrate encapsulated in poly(lactic-co-glycolic acid) microparticles. An *in vivo* study is currently underway to analyze the efficacy and safety of this delivery method. We are also investigating the feasibility of an ocular insert which would utilize the microparticle delivery method and serve as a non-invasive and convenient form of glaucoma treatment.

98**Defining the Role of Peptide Charge on Release Kinetics from PLGA Microspheres**

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 City College of New York

Polymer microspheres are usually employed to release agents in a controlled (and sometimes targeted) manner. Release is dictated by degradation and erosion of the polymer matrix, leading to pathways for diffusion.

An existing model for predicting controlled release from degradable polymer microspheres (developed by Rothstein et al.) predicts controlled release extremely well using a variety of degradable polymers and drugs.

However, this model currently assumes no polymer-drug interactions which has been seen to impact the release of some drugs including highly charged agents.

Accordingly, this NSF-sponsored research intends to explore the effect of peptide charge on polymer interactions and, consequently, controlled release. Ultimately, this work could be used to extend the current predictive model construct to better predict release of drugs that experience both electrostatic and (possibly) hydrophobic interactions with the polymer matrix.

100**Tailoring the Release of Growth Factors from Thermally Responsive Hydrogel**

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Heart failure, commonly caused by coronary artery disease and myocardial infarction, is a widespread, debilitating condition. Due to increased intraventricular pressure and myocardial wall stress, the ventricular wall thins over time after infarction, leading to the need for a transplant or ventricular assist device. Injectable biomaterials could possibly reduce the stress on the ventricular wall by providing mechanical support. A polymer of N-isopropylacrylamide, 2-hydroxyethyl methacrylate, and methacrylate-poly lactide (Poly(NIPAAm-co-HEMA-co-MAPLA) is an injectable, thermoresponsive hydrogel that solidifies upon reaching body temperature. Growth factors may also be incorporated into the hydrogel in order to increase therapeutic effects on surrounding tissue. Basic fibroblast growth factor (bFGF) is important for neovascularization and insulin-like growth factor 1 (IGF-1) is important for cardiomyocyte growth and survival. To extend release *in vivo*, the growth factors may be added directly to the hydrogel, or encapsulated in poly(lactic-co-glycolic acid) (PLGA) microspheres. By altering molecular weight of the hydrogel or particle pore size, the release profile of the growth factor is may be subsequently altered.

101**Benzene- and Naphthalene-based CO₂ Gelators**

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Specific naphthalene and benzene based organoregulators have been shown in the past to form “gels” in various organic liquids. These “gels” are opaque dispersions of very fine solid organoregulator fibers in these organic liquids. This unique property creates possible applications for these compounds as thickening agents which will enhance the viscosity of dense CO₂ with possible applications in enhanced crude oil recovery. Multiple variations of naphthalene with 2,3-substituted oxy-alkane tail groups, ranging from 4-20 carbons in length were synthesized and one such benzene-based compound was studied. These compounds form fibers in supercritical CO₂, and viscosity studies were performed to determine if the best candidates among these enhanced the viscosity of dense CO₂

103**Transport of Particles in Nanoporous Materials:
Effect of Framework Flexibility**

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We used molecular dynamics simulations to study gas transport in carbon nanotubes (CNTs). We compared a CNT model with rigid bonds to one with flexible bonds described by the reactive empirical bond order (REBO) potential. Using these models, we analyzed particle diffusivity and the properties of a nanoporous membrane.

102**Rate-Based Separation in Collisional Particle Flows**

Samantha Schmidt, Dr. Joseph J. McCarthy
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Separation of particles is extremely important in a number of industries. Rate-based separation processes hold promise as both more environmentally friendly as well as less energy intensive when compared to conventional particle separations methods such as vibrating screens. This approach is based on differences in the kinetic properties of the components of a mixture. This rate-based separation example involves the study of the dynamics of particles traveling through an array of asymmetric obstacles, sometimes referred to as a “galton board.” This particular method uses a modified version of the traditional “galton board.” Both simulations and experiments have been used to enhance understanding of this device. Dissipative collisions (both with the particles themselves and with the obstacles) give rise to a lateral diffusive motion of particles and the differences in diffusion lengths will lead to separation of the particles. The extent of separation depends on the different distances traveled by the two types of particles and hence is directly proportional to the time taken to traverse the length of the board, a feature that distinguishes this approach from other traditional and novel separation techniques

104**Amine-Silica Nanosorbents for CO₂ Capture**

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Growing evidence suggests that anthropogenic emissions of carbon dioxide (CO₂), an acidic “greenhouse gas,” contributes significantly to global warming and ocean acidification. Developing efficient methods to capture CO₂ from anthropogenic sources is hence a key aspect of sustainable technology development. Multiple methods exist for carbon capture, though none provide a cost-effective solution. Complex amines supported on silica exhibit excellent sorption capacities and stability. Particularly amine groups grafted onto nanostructured silica show great promise as CO₂ sorbents, albeit at increased synthesis complexity. In this research, a very simple synthesis procedure which yields surprisingly efficient nanosorbents is demonstrated. Tetraethylenepentamine (TEPA), a liquid amine with high CO₂ sorption properties, was impregnated onto supporting silica nanoparticles. These liquid amine-solid silica nanoparticles were investigated and the impact of preparation conditions, operating temperature, and sonication time were determined.

106**Pharmacokinetic Modeling of the Oral Anti-Cancer Agent 5-Fluoro-2'-Deoxycytidine and its Interaction with 3,4,5,6-Tetrahyrdouridine**

Nataliya Machalaba, Dr. Robert S. Parker
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City College of New York

Cancer is a group of diseases that result from an imbalance between cell proliferation and programmed cell death. 5-fluoro-2'-deoxycytidine (FdCyd) blocks DNA methyltransferase activity, which is an enzyme that cells need in order to divide. *In vivo*, FdCyd is quickly metabolized by cytidine deaminase into unwanted and toxic 5-fluoro-2'-deoxyuridine, 5-fluorouracil, and 5-fluorouridine. 3,4,5,6-tetrahyrdouridine (THU), a cytidine deaminase inhibitor, is administered to slow FdCyd metabolism. A five-compartment model best fits the behavior of orally administered THU; a compartmental model of FdCyd and its metabolites is also described. The rate of FdCyd elimination is directly and non-linearly affected by the concentration of THU in the bloodstream. This study defines a set of ordinary differential equations (ODEs) that capture the behavior of FdCyd concentration in the bloodstream in the presence and absence of THU for the purposes of designing combination chemotherapy regimens.

105**Model-Based Regulation of Glucose in Critical Care**

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University of Pittsburgh

The project goal is to develop a model predictive controller (MPC) to allow for tight glucose control without hypoglycemia. In order to for the MPC to handle different patient dynamics and remain effective as a patient recovers, parameters in the model need to be adjusted. For this purpose we embed a moving horizon estimation (MHE) routine within the MPC algorithm. A state-space model predictive controller (SSMPC) with MHE was built in MATLAB (© 2011, The MathWorks, Natick, MA). The program was tested against a 2-input, 2-output continuously stirred tank reactor (CSTR) system with first-order reaction occurring in each CSTR. The controller tracked multiple setpoints and was able to reject unmeasured disturbances. Furthermore, the MHE was able to adjust parameter values to follow changes in system dynamics.