Duquesne University
Undergraduate Research Program

2014 Summer Research Symposium

Sponsored by

The Bayer School of Natural and Environmental Sciences

Keynote Address:

Yoosuf Picard, Ph.D.
Assistant Research Professor of Material Sciences and Engineering
Department of Material Sciences and Engineering
Carnegie Mellon University

"Energetic Beams for Micro and Nanoscale Science – My Undergraduate Research to Present"

Friday, July 25, 2014
9:00 a.m. – 4:00 p.m.
Bayer Learning Center &
Mellon Hall of Science
Duquesne University

Welcome to the
2014 Summer Undergraduate Research Symposium!

It is a pleasure and privilege to welcome you to today's ***17th Annual Summer Undergraduate Research Symposium*** at Duquesne University. Each year the number of student participants and 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 should reassure all of us of the superb caliber of the scientific research and training that occurs on a daily basis in our colleges, universities and research centers. Today's presentations reinforce our conviction and confidence that we are preparing an emerging cadre of future scientific leaders who will possess the creativity, motivation, and intellect to meet and solve the challenges that our society faces. On behalf of the faculty, students, and staff of the Bayer School and Duquesne University, I am pleased to offer my sincerest congratulations to each of the student researchers participating in today's symposium and to convey our best wishes for continued success in your academic and professional careers!

Sincerely,

Philip Reeder,
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

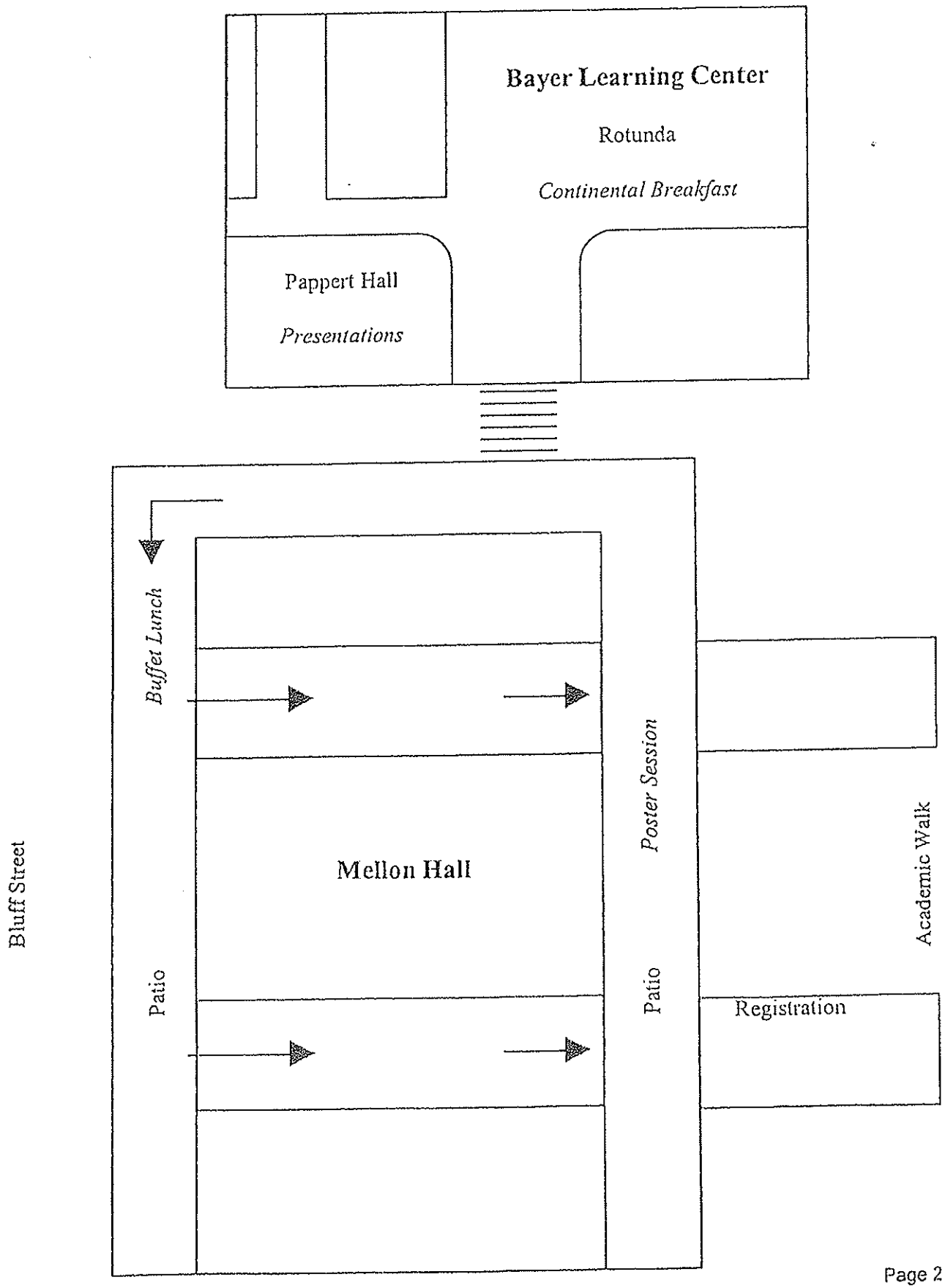
Contents:

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.

Area Map


Bayer Learning Center
Rotunda
Continental Breakfast
Pappert Hall
Presentations
Buffet Lunch
Mellon Hall
Poster Session
Patio
Patio
Registration
Bluff Street
Academic Walk

Plenary Session Schedule
Pappert Lecture Hall
Bayer Learning Center

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10 a.m.	Welcome, Dr. Philip Reeder, Dean, Bayer School of Natural and Environmental Sciences, Duquesne University
10:10 a.m.	Keynote Address, Dr. Yoosuf Picard Assistant Research Professor of Material Sciences and Engineering Department of Material Sciences and Engineering ***"Energetic Beams for Micro and Nanoscale Science – My Undergraduate Research to Present"***

11:00 AM Student Presentations

Sarah Kochanek	**Intramolecular charge-assisted hydrogen bond strength in pseudo-chair carboxyphosphate** Department of Chemistry and Biochemistry, Duquesne University
Allison Williams	**The Messenger RNA p250GAP G-Quadruplex Secondary Structure Biophysical Classification and RGG box Domain/ISO1 Interaction** Department of Chemistry and Biochemistry, Duquesne University
Joseph Robinson	**Genomic Analysis to Detect Convergent Adaptation to Marine and Subterranean Environments** Department of Computational and Systems Biology, University of Pittsburgh

11:45 AM Short Break

Julie Gillis	**Saturated absorption laser spectroscopy of potassium-39 vapor** Department of Physics, Duquesne University
Daniel Fucich	**Development of *Streptomyces coelicolor* for Vaccine Delivery** Department of Biological Sciences, Duquesne University
Katherine Driscoll	**Examination of the role of Rad4 β-hairpin 3 in DNA damage recognition** Department of Computational and Systems Biology, University of Pittsburgh
Janja Mirtic	**Nanoemulsions as new drug delivery strategy for resveratrol and it's analogs** Mylan School of Pharmacy, Duquesne University
Session Moderator	Theordore A. Corcovilos, Ph.D.; Assistant Professor, Department of Physics, Duquesne University

About Dr. Yoosuf Picard:

Biography

Professor Picard obtained a B.S. in Mechanical Engineering from Louisiana Tech University in 2001 and a Ph.D. in Materials Science and Engineering from the University of Michigan in 2006. During his graduate career, he was a Microsystems Engineering and Science Applications Fellow at Sandia National Laboratories where he researched focused ion beam applications as well as pulsed laser ignition phenomenon in energetic thin films. Following his doctoral research on materials modifications by femtosecond lasers, he was a postdoctoral research associate at the U.S. Naval Research Lab (NRL), where he conducted electron microscopy studies of GaN devices, SiC thin films, and metal-oxide nanowires. He was subsequently hired as a staff scientist at NRL to carry out electron microscopy studies of metal alloy surfaces and magnetic metal-oxide thin films. He joined the faculty at Carnegie Mellon University in 2009.

Research Interests

Transmission electron microscopy, scanning electron microscopy, electron channeling contrast imaging, electron backscatter diffraction, dislocation analysis in semiconducting materials and devices, structural analysis in nanoscale materials, atomic scale imaging/analysis of interfaces.

Web

Dr. Picard's faculty page: http://www.materials.cmu.edu/people/picard.html

Dr. Picard's group page: http://neon.materials.cmu.edu/yoosuf/index.html

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OP - Oral Presentation

1

Interactive Functional Near Infrared Spectroscopy

MacGillivray, Caroline
Department of Psychiatry
University of Pittsburgh

Functional Near-Infrared Spectroscopy (fNIRS) is a relatively new technique in the neuro-imaging field that utilizes near-infrared light to detect hemoglobin levels in the outer centimeter of the cortex. fNIRS is extremely useful because it is non-invasive, cost-efficient, and portable but the complete extent of its neuro-imaging capabilities are unknown. This study proposes the use of fNIRS to observe synchronization of neural systems involved in social interaction. To test this hypothesis, pairs of subjects completed a puzzle task called Tangrams both individually and together while their brain activity was recorded with fNIRS. Data analyses indicated increased correlation in pre-frontal cortex activation when individuals completed a puzzle together as opposed to separately. This method of using fNIRS to observe brain activity correlations between individuals is the first step in a novel research program examining brain interactions between pairs engaged in conflict and those presenting with psychiatric disorders.

2

Reduction of Infectious Biofilms on the Native Oxide Surface of Titanium

Bruneel, Nicole; Gawalt, Ellen S.; Reger, Nina A.
Department of Chemistry and Biochemistry
Duquesne University

Titanium is a key biomedical material used for surgical implants, due to its biocompatibility, high strength, low density, corrosion resistance, and non-toxicity to the host. However, titanium implants can be infected in Staphylococcus aureus and Pseudomonas aeruginosa biofilms. Biofilms formed by microbial colonies can be resistant to antimicrobial treatments. Nitric oxide can be a biofilm dispersant by inducing nitrosative and oxidative stress on the bacteria, transitioning sessile biofilm cells to free swimming planktonic cells, which are more susceptible to antimicrobial treatments. It is hypothesized that the oxidative surface of titanium can be modified with 16-phosphonohexadecanoic acid self-assembled monolayers that can be functionalized with a nitric oxide tail group to release nitric oxide in physiological conditions. Diffuse Reflectance Infrared Fourier Transform spectroscopy and contact angle measurements were used to analyze the change in the organization of the monolayer on the surface. These substrates will then be modified for nitric oxide release.

3

Formulation and characterization of binary solid dispersions made using two excipients, Vitamin E (TPGS) as stabilizer and PVPva as polymer

Silvestros, Maria; Buckner, Ira; DeBoyace, Kevin; Wildfong, Peter
Pharmaceutics Department
Duquesne University

Solid dispersions are formulated to enhance (poorly water-soluble) drug profiles. In attempt to form a completely amorphous solid dispersion of drug, polymer, and surfactant, we will improve dissolution of [drug] in the body in the cases where physical instability is not observed. Drug re-crystallization (instability) is notably the reason for non-commercialized products of this nature and the inspiration for this research. In this work, PVPva (polymer) and TPGS – D-alpha-tocopheryl polyethylene glycol 1000 succinate – Vitamin E were incorporated in a binary solid dispersion using melt quench and ice quench techniques and later characterized using Digital Scanning Calorimetry, Hot Stage Microscopy, and Powder X-Ray Diffraction. We did this in order to determine whether we can create a stable amorphous mixture and to determine whether or not we can prevent re-crystallization of the amorphous mixture. With success, we hope to enhance oral bioavailability of drugs in the body upon dissolution.

4

Peptide Sequencing using Gas-phase Peptide Carbocations

Plaviak, Alexandra; Van Stipdonk, Michael J.
Department of Chemistry and Biochemistry
Duquesne University

Tandem mass spectrometry (MS^n) and collision induced dissociation (CID) are among the most important tools used to identify peptides and proteins in proteomics. Fragmentation of gas-phase, protonated peptides creates product ions that reveal amino acid sequence. Recently we found that conversion of peptides to N-terminal imines (as Schiff bases) enhances the sequence information revealed by the MS^n approach. More remarkably, we found that dissociation of Ag^+ cationized versions of these peptide-imines creates never-before seen $(M-H)^+$ ions (essentially peptide carbocations) by loss of AgH. The MS^n fragmentation of these ions provides important sequence information as well. In this presentation, the preparation of the peptide-imines will be described, as well as the generation of the carbocations and their CID behavior. Of particular importance is the comparison of the fragmentation of the carbocations to protonated peptide imines and to protonated peptides that lack the imine group.

5

Cooperative protein binding as mediated through RNA secondary structure

Hanisch, Natalie[1]; Widom, Michael[2]
1 Department of Mathematics, University of Nebraska at Kearney
2 Department of Physics, Carnegie Mellon University

RNA-protein interactions play a key role in gene silencing at the RNA level. MicroRNA (miRNA) are short non-coding RNA (21-23nt) used in a mechanism involving RNA-Induced Silencing Complex (RISC) to mediate gene expression and silencing. Previous evidence suggests RNA-protein cooperativity mediated through the RNA molecule as a mechanism for gene silencing. We use computational models that examine the free energy relationships of many RNA-protein binding situations. To aid our research we are using Vienna RNA, a software collection for determining statistical properties of RNA folding. With these models we can determine whether RNA-protein cooperativity is a common mechanism in the gene silencing functions of RISC, and under what conditions. While it is expected that we will find cooperative relationships in certain conditions, no definitive results have been determined yet. Demonstrating the existence of cooperativity relationships regarding RNA-protein interactions will further our understanding of how RISC gene-silencing is efficiently achieved.

6

^{15}N isotopic substitution of the cytochrome bc1 Rieske Iron-Sulfur Cluster distinguishes the protonation states of histidine side chain ligands

Jagger, Benjamin R.; Wheeler, Ralph A.
Department of Chemistry and Biochemistry
Duquesne University

The Rieske iron-sulfur cluster (2Fe-2S) is a catalytic subunit of the mitochondrial cytochrome bc1 complex critical in ATP synthesis. The cluster is proposed to act as both an electron and proton acceptor for the mobile electron carrier ubiquinol. Thus the mechanism of proton coupled electron transfer in the complex is dependent on the protonation states of the histidine ligands to one of the 2Fe-2S cluster's iron atoms. The paramagnetic irons of the cluster make pKa determination by NMR spectroscopy problematic. We suggest a novel approach to identify the protonation states through IR spectroscopy. Broken symmetry geometry optimizations and a frequency analysis were performed for the different protonation states of the imidazole side chains of the histidine ligands. Qualitatively different ^{15}N isotopic frequency shifts present a possible approach for the experimental determination of the protonation states of the ligands in the oxidized forms of the cluster by using difference IR spectroscopy.

7

Understanding Antigen Discrimination in T-cells using a Rule-based Model

Kingsbury, Lyle; Faeder, James
Department of Computational and Systems Biology
University of Pittsburgh

Discrimination between cognate and innocuous self-peptides by T-cells represents a significant challenge for the adaptive immune system. The mechanisms controlling the extreme sensitivity of T-cell receptors (TCR) are not completely understood, but cooperative binding between pMHC molecules on the presenting cell and the CD8 co-receptor, as well as CD8 and TCR clustering, are suggested to be important factors. Here, we have developed a rule-based computational model using BioNetGen to evaluate the roles of cooperative enhancement, receptor clustering, and pMHC density on the efficiency of antigen discrimination. We show that the search efficiency of the T-cell to locate cognate pMHC is highly sensitive to cooperative enhancement by CD8, but not TCR. This confirms previous findings about CD8-dependent cooperative binding between pMHC molecules, and highlights the potential importance of CD8 clustering as part of the mechanism controlling antigen discrimination in T-cells.

8

Validation of Waterborne Hormone Assays in Mountain Dusky Salamanders

Magyan, Andrew; Thomas, Jess; Woodley, Sarah.
Biology Department
Duquesne University

Waterborne hormone assays are a non-invasive method of testing hormone concentrations in aquatic species. Hormones are extracted from holding water and measured with an EIA. To validate the waterborne assays, hormone levels in the water must parallel those in the plasma, there must be no background hormonal activity in the water, there must be parallelism between diluted samples and standards, and the recovery rates of hormone must be greater than 80%. I worked to validate a waterborne testosterone assay for use in mountain dusky salamanders (*Desmognathus ochrophaeus*). As part of the validation, salamanders were castrated and given a testosterone implant or blank implant to confirm that higher concentrations of testosterone in the animals could be detected with the waterborne assays. My progress in performing and validating waterborne hormone assays will be presented at the symposium.

9

Pharmacological Intervention of EPAC1-Radixin Complex for Targeted Disruption of cAMP Signaling Pathway

Pederson, Eric*; Altschuler, Daniel†; Camacho, Carlos*
Computational & Systems Biology*, Pharmacology & Chemical Biology†
University of Pittsburgh

The cAMP signaling pathway is involved in many cellular processes including cell proliferation in cancer. However, due to the ubiquitous nature of the pathway, finding a useful target for modulating cAMP has proven difficult due to the risk of side effects. Recently, it has been shown that EPAC1-mediated activation of Rap1 (synergistically with PKA) transduce cAMP-mediated cell proliferation with radixin (ERM protein near the cell membrane) as the integration node. EPAC1 contains an N-terminal peptide that binds to radixin, causing the transduction to occur. The goal is to characterize the EPAC1-radixin interaction using experimental data and molecular dynamics simulations and develop small molecules to target and inhibit the interaction while minimally affecting the binding interactions of the several other peptides that are known to bind to radixin. Using pharmacophore-based drug design, small molecules are virtually screened for selective antagonist behavior.

10

BigData with Hadoop, Spark, and ML

Liu, Angela M.
Carnegie Mellon University, Information Systems / Human Computer Interactions
XSEDE Research Internship @ Pittsburgh Supercomputing

The Pittsburgh Supercomputing Center (PSC) provides technology resources that support high-performance computing, massive data storage, and more. This project focuses on utilizing server logs generated about by the PSC's Archiver, a high-capacity disk storage collection. Said logs are being collected in several different areas – this project aims to bring together a selection of logs into a Hadoop cluster for further analysis via Spark. Spark provides methods for working with files on the Hadoop Distributed File System (HDFS) by creating Resilient Distributed Datasets (RDD) which can be operated on in parallel. By using RDDs, Spark can cleanly apply machine learning algorithms. K-means clustering algorithm will be used on the cleaned dataset. With this combination of technologies, this project aims to summarize log data in order to allow more close monitoring and aims to discover possible connections between variables such as CPU, disk IO, file writes, reads, and more.

11

DNA Quantification and Amplification of Rape Kits from 2001

Erlanson, Kiersten; Ludvico, Lisa
Department of Biological Sciences
Duquesne University

The statute of limitations for rape prosecution has increased dramatically and in the case of minors offenders can be tried until the victim has reached 50 years of age. Consequently, rape backlogs can number in the tens of thousands. Two areas in forensic DNA that have allowed for successful prosecution are improvement in extraction techniques and the sensitivity of genotyping. Six female rape kits, dating to 2001, were obtained from the Allegheny County Evidence Depository. The focus of this study is to ascertain the quantity and quality of male DNA from these rape kits. Differential extraction was employed followed by quantification via ABI 7500 and ultimately genotyped using Penta E primers. Amplification of male DNA has been successful in one out of the four rape kits analyzed thus far.

12

Halidophilicity Studies of Copper Complexes with TPEN and TPEN* Ligands in Atom Transfer Radical Addition (ATRA)

Gorse, Erin; Kaur, Aman; Pintauer, Tomislav; Pros, Gabrielle
Department of Chemistry
Duquesne University

Multidentate ligands TPEN (N,N,N',N'-tetrakis(2-pyridylmethyl)ethane-1,2-diamine) and TPEN* (methyl groups in 3, 5 and methoxy on 4 positions of pyridine rings) were evaluated in copper catalyzed ATRA reactions. It was found that these copper complexes performed poorly in methanol, which was the solvent of choice for structurally similar TPMA (tris[(2-pyridyl)methyl]amine). The inefficient catalysis was attribted to the low halidophicity of these complexes in protic solvents, a key step in the reaction mechanism of ATRA. Interestingly, the halidophilicity of both TPEN and TPEN* dramatically increased when the polar aprotic acetone was used as a solvent from a K_x for TPEN * of 11.87 ± 1.55 in pure methanol to 15631 ± 4017 in acetone. The pattern of halide anion dissociation was also seen in the halidophilicity trials performed on TPEN, and was illustrated using the two ligands in the copper-catalyzed ATRA of octene.

13

Constraining the Inflationary Potential with Cosmological Perturbation Measurements

Brawley, Sean
Department of Physics and Astronomy
University of Pittsburgh

Inflationary theory asserts that the universe underwent a period of accelerated expansion 10^{-35} seconds after the Big Bang that continued for at least 10^{-33} seconds; during which its size expanded by a factor of at least 10^{23}. This period of cosmic inflation generates density and gravitational (scalar and tensor) perturbations due to quantum irregularities, required to be present by Heisenberg's Uncertainty Principle, that expand past the Hubble radius and begin to behave classically. Both types of created perturbations obey a power-law power spectrum over a broad range of wavelengths. The amplitude of long-wavelength tensor perturbations can be resolved from precision B-mode polarization measurements of the CMB. Smaller wavelength perturbations, originating later in the inflationary era, should also be detectable via a space-based interferometer. We are determining how well a combination of measurements at these scales can constrain the potential driving inflation: probing physics at uncharted energy scales of 10^{16} GeV.

14

Synthesis of 2,4-Diamino-5-methyl-6-substituted Thieno[2,3-*d*]pyrimidines Designed as Potential Antifolates Against Opportunistic Infections

Letzkus, Olivia; Choudhary, Shruti; Gangjee, Aleem
Mylan School of Pharmacy
Graduate School of Pharmaceutical Sciences
Duquesne University

Pneumocystis pneumonia (Pcp) increases the chance of serious complications in patients with compromised immune system, such as patients with acquired immunodeficiency syndrome (AIDS). This form of pneumonia is a fungal infection of the lungs caused by *Pneumocystis jirovecii* (*Pj*). Dihydrofolate reductase (DHFR) is an essential enzyme that converts dihyrofolate to tetrahydrofolate, a co-factor that is necessary for making thymidylate, purines and certain amino acids. Currently approved treatments for Pcp, such as a combination of trimethoprim - sulfamethoxazole or trimetrexate, suffer from poor patient compliance and non-selectivity. The thieno[2,3-*d*]pyrimidine analogues reported here were designed with the goal of increasing both the selectivity and potency against *Pj*DHFR. These compounds were synthesized with various thioaryl substituents at the C-6 position on the bicyclic thieno[2,3-*d*]pyrimidine scaffold.

15

Isolation of Cyanobacterial Secondary Metabolites with Activity at the 5-HT_7 Receptor

Work, Cody R.; Ahmed, Kh. Tanvir; Tidgewell, Kevin J.
Mylan School of Pharmacy
Duquesne University

Cyanobacterial natural products have been the subject of research interest due to their anti-cancer and anti-fungal activities. The goal of this research is the isolation of secondary metabolites from a cyanobacterial collection made in Las Perlas, Panama. The collection was extracted using a 2:1 DCM:MeOH mixture, separated by column chromatography, and fractions were screened for activity at G-protein coupled receptors (GPCR) using the Psychoactive Drug Screen Program assay. DUQ-0002-I was shown to have affinity for the 5-HT_7 receptor (71.2 % inhibition of binding) in a radioligand binding assay. The 5-HT_7 receptor is a GPCR that plays an important role in memory, and may have implications for treatment of Alzheimer's disease, as well as providing relief for both pain and depression. Using HPLC, pure compounds from the DUQ-0002-I fraction were isolated. Results to date on characterization using NMR and mass spectrometry will be presented.

16

Characterization of Steroid Sulfatase in *Mus musculus*

Hornak, Joseph; Selcer, Kyle W.
Department of Biological Sciences
Duquesne University

Inactive sulfated steroid hormones can be activated upon the removal of the sulfate group. Steroid sulfatase (STS) is the enzyme responsible for this conversion. This study investigated the tissue distribution of STS in the laboratory mouse, *Mus musculus*. Homogenates prepared from various tissues exhibited widely different STS activities, which were analyzed by ^{3}H-E_1S conversion assay. Among the tissues, STS activity was highest in liver and testes. STS activity was time- and temperature-dependent in liver microsomes. Known STS inhibitors decreased activity, indicating that conversion represents authentic STS. STS kinetics of liver microsomes were analyzed using a Lineweaver-Burk plot, which indicated a higher K_m value for E_1S than that reported for human placental STS. Because STS plays an important role in regulating estrogen levels, characterization of this enzyme in the widely used mouse model can provide insight into its overall function, as well as its role in hormone-dependent cancers and osteoporosis.

17

Application of Copper Catalyzed Atom Transfer Radical Addition (ATRA) for the Synthesis of Highly Functional Nitrogen Containing Monoadducts

Martin, Jesse Paul; Gonzales, John; Pintauer, Tomislav; Pros, Gabrielle
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Duquesne University

Atom transfer radical addition (ATRA) is a technique for the formation of C-C and C-X (X = halide, pseudohalide) bonds by the addition of alkyl halide to the double bond of an alkene. In this reaction, catalyst regeneration technique has been utilized to drastically decrease the amount of metal catalyst required, making the process more efficient and environmentally friendly. Reducing agents such as ascorbic acid help to facilitate the reaction by means of catalyst regeneration. Nitrogen containing monomers have never been utilized for such organic transformation. However, contrary to ATRA with common alkenes such as α-olefins and acrylates, the synthesis of monoadduct with nitrogen containing monomers can be challenging due to unfavorable side reactions. Apart from the usual undesirable polymerization, other side reactions include diadduct, tertiary ammonium salts, and hydrolyzed monomer product formation. Another challenge arises with the alkene coordination to the copper centers, which significantly decreases the catalytic activity.

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Design, Synthesis, and Characterization of Vanadium (IV) Complexes of Dithiolene and Dithione Ligands

Ratvasky, Stephen; Basu, Partha; Mogesa, Benjamin
Department of Chemistry and Biochemistry
Duquesne University

Redox-active dithiolene ligands can exhibit multiple well-defined charged states, but their coordination chemistry is primarily focused on the ligand in the reduced state. In this study, we examined both the fully oxidized dithiolene ligand (dithione) and reduced ligand. N,N'-diisopropylpiperazine-2,3-dithione ($^{i}Pr_2Dt^0$) was chosen as the primary ligand in order to represent the desired fully oxidized character while maleonitriledithiolate (mnt^{2-}) was chosen to represent the reduced state. The coordination chemistry of this system with group 5 transition metal vanadium was investigated. Vanadium coordination complexes are known for their catalytic and, in the case of vanadyl acetylacetonate ($VO(acac)_2$), anti-diabetic potential. The V^{IV} vanadyl ion (VO^{2+}) was the primary vanadium form of interest in this study. Metal complexes were characterized using ^{1}H and ^{13}C NMR, FT-IR Spectroscopy, and UV-Vis Spectroscopy.

19

Saturated absorption laser spectroscopy of potassium-39 vapor

Gillis, Julie M.; Brooke, Robert W.A.; Corcovilos, Theodore A.; Zaccagnini, Christopher A.
Department of Physics
Duquesne University

Saturated absorption spectroscopy is an effective and reliable technique that is used frequently in atomic and optical physics in order to precisely measure the hyperfine energy structure of atoms, such as the alkali metals that are used in laser-cooling experiments. We present an effective optical design to measure the D_2-line of potassium-39 at 766.700 921 nm (near infrared) that can be used to frequency-lock our laser diode with 6 MHz (~10 ppb) accuracy. Counter-propagating laser beams are passed through an atomic vapor cell of ^{39}K to obtain sub-Doppler resolution peaks of the excited atoms. The design consists of several optical components including the introduction of an anamorphic prism pair to optimize the beam shape and a set of telescoping lenses for magnification and collimation of the beam.

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Laser Ablation Inductively Coupled Plasma for the Quantitative Analysis of Inorganic Elements in Dried Blood Spots

Sheffield, Sarah; Kingston, H.M. "Skip"; Miller, Logan
Department of Chemistry and Biochemistry
Duquesne University

The process of attaining blood samples has been an invasive process, however dried blood spots (DBS) require a less invasive sampling technique and utilize a smaller volume of patient blood. Inorganic elements found in blood play important roles in human body functions. For example, the ratio between copper and zinc is an indication of the immune system and can be used to physically diagnose autistic patients. Laser ablation (LA) was performed on DBS using an excimer laser connected to an inductively coupled plasma mass spectrometer. DBS cards were previously spiked with naturally abundant or enriched stable isotopes of copper, zinc, iron, manganese, cobalt, and nickel. Isotope Dilution Mass Spectrometry (IDMS) was utilized to quantify, construct, and validate the method. Calibration curves are inherently challenging when using LA because of the variable efficiencies of the ablation. IDMS allows direct mathematical quantification without the use of calibration curves.

21

The Effect of Weak Base on [Cu(Me_6TREN)Cl]Cl Catalyzed ATRA in the Presence of Ascorbic Acid as a Reducing Agent

Wasson, Megan; Kaur, Aman; Pintauer, Tomislav; Pros, Gabrielle
Department of Chemistry and Biochemistry
Duquesne University

Copper catalyzed atom transfer radical addition (ATRA) is used for C-C bond formation by the addition of alkyl halides to various alkenes. Based on electrochemical and mechanistic studies, copper complexes with Me_6TREN (tris(2-dimethylaminoethy)amine ligand were found to be ~10 times more active than TPMA (tris(2-pyridylmethyl)amine). However, catalytic studies on ATRA with different alkenes and alkyl halides showed the opposite trend. The low activity was attributed to the protonation of Me_6TREN ligand in the presence of the reducing agent, ascorbic acid. In this study, different weak bases (triethylamine, piperidine, 1-methylpiperidine, N,N-dimethylaniline, and pyridine) were employed to inhibit the degradation of the ligand and restore the catalytic activity. These amines were used in different stoichiometry ratios relative to ascorbic acid during ATRA on various alkenes with CCl_4 catalyzed by [Cu(Me_6TREN)Cl]Cl. In this study, we found that the 5:1 ratio of amine to ascorbic acid was the most effective.

22

Implementing a Smith-Waterman Mapping Program using MPI

Ortiz García, Armando J.[1]; Marrero, Kevin[1]; Ropelewski, Alexander J.[2]; Seguel, Jaime[1]; Van der Meer, Pieter[1]
[1] Department of Computer Engineering, University of Puerto Rico, Mayagüez
[2] Pittsburgh Supercomputing Center

Sequencing reads from Roche 454 and Life Technologies ION Torrent Next-Generation Sequencers are subject to insertion/deletion errors rather than substitution errors. The impact of the error profile means that mapping programs designed for substitution errors, such as BWA and Bowtie, are much less effective at mapping data produced by these sequencers. We have implemented a novel Parallel Algorithm for Local Mapping Assembly (PALMA) that uses the Smith-Waterman algorithm and a modification of Hirschberg's divide-and-conquer technique, employing the Message Passing Interface (MPI). By applying these techniques, a large sequence such as a genome can be split to allow for a parallel distributed-memory search with a short sequence, such as a read, while incorporating an insertion/deletion model into the mapping procedure. The novel distribution method used by the algorithm improves speed over conventional distribution by minimizing the amount of inner processor communication needed, reducing overall program runtime.

23

Opto-Mechanical Systems for use in an Atomic Physics Lab

Zaccagnini, Christopher A.; Brooke, Robert W.A.; Corcovilos, Theodore A.; Gillis, Julie M.
Department of Physics
Duquesne University

We present two designs for opto-mechanical systems for use in the atomic physics labs at Duquesne University. The first, an extended cavity diode laser (ECDL) uses optical feedback to stabilize a laser diode. A diffraction grating and the back facet of the diode form a Fabry-Perot cavity of 10 cm length and free spectral range of 1.5 GHz. This is expected to narrow the emission spectrum of the laser to less than 1 MHz, sufficient to resolve the atomic spectrum of alkali atoms such as potassium. The ECDL requires optimal mechanical and thermal stability to eliminate noise from the laser. The second system, a wavelength meter, is used to measure the wavelength of a laser. This system includes a Michelson interferometer with a moving cart between two mirrors designed to compare an unknown laser wavelength to a known one (e.g. a HeNe laser at 633 nm).

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Electronic Systems in an Atomic Physics Lab

Brooke, Robert W.A.; Corcovilos, Theodore A.; Gillis, Julie M.; Zaccagnini, Christopher, A.
Department of Physics
Duquesne University

We design and build three major circuits for the use in atomic physics experiments. The first is a photodetector circuit which converts light intensity into an electrical voltage, based on a FPS100 photodiode. Reverse biasing the diode linearizes its response and decreases its response time. The transimpedance gain is set by a resistor, generating a voltage which can be read by an oscilloscope. The second circuit is a digital temperature controller for a vapor spectroscopy cell. A calibrated temperature-dependent resistor is measured using an unbalanced Wheatstone Bridge providing temperature resolution of < 0.01°C over the range 10–80°C. PID feedback is provided by software on an embedded Arduino microprocessor, which drives a resistive heater using pulsed width modulation, controlling the temperature. The third circuit is a high-precision, low-noise current driver for laser diodes. The laser current driver provides DC currents of up to 200 mA with expected noise < 10nA/√Hz.

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Bioinformatics Characterization of Fungal Allergen Proteins.

Borrás-Pacheco, Tania[1]; Nicholas, Hugh[2]; Vázquez-Quiñones, Luis[3]
[1]School of Science and Technology, Universidad Del Este, Carolina, Puerto Rico
[2]Pittsburgh Supercomputing Center, Carnegie Mellon University
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Systemic inhalation of fungal spores and mycelia fragments can induce allergic respiratory diseases. The allergenic component of fungi contains molecules that might trigger type I hypersensitivity reaction mediated by Immunoglobulin E (IgE). *Alternaria alternata* is considered one of the most potent producers of fungal allergens causing upper respiratory tract infections and asthma in immuno-compromised patients. However, the biological functions of many of these allergenic proteins are unknown. The major allergen produced by *A. alternata* is ALTA1; bioinformatics analysis of amino acid conservation of ALTA1 holds potential to understand its allergenic properties. The objectives of this study focus on studying the protein structure around conserved amino acids to understand its allergic/immunological relevance. The results of this preliminary study could lead to insights in understanding the allergic reaction in humans.

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Bioinformatics Characterization of CRTAM to Create a Nano-Biosensor for Prostate Cancer Detection

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Prostate cancer affects about 97% of men in the U.S. population. The American Cancer Society estimates that in 2014 there will be about 233,000 new cases and about 29,480 men will die of prostate cancer. Current screening methods for prostate cancer could lead to under- and overtreatment in patients. There is a need for a diagnostic method that is precise, consistent, and quick. CRTAM (cytotoxic and regulatory T-cell molecule) is a biomarker gene found in aggressive prostate cancer which interacts with Necl-2 and provokes cytotoxicity by the Natural Killer Cells to destroy tumor cells. Using bioinformatics techniques, two exclusive DNA regions in CRTAM have been predicted to be appropriate sequences for a potential nano-biosensor for prostate cancer detection. Additionally, five conserved regions in the CRTAM protein sequence also holds promise for a potential nano-biosensor.

27

Using Carboxylic and Phosphonic Acid Head Groups to Form Mixed Self-Assembled Monolayers

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Titanium and its alloys are commonly used synthetic implant materials. Self-assembled monolayers can be used to increase applicability of these biomaterials and control interfacial properties. The aim of this study is to form monolayers using two different head groups. Self-assembled monolayers of octadecylcarboxylic acid, octadecylphosphonic acid, and a mixture of both were covalently bound to the surface of titanium and Ti-Al6-V4 metal substrates. The results of this study should indicate which acid head group preferably binds to metal surfaces. Diffuse reflectance infrared Fourier transform spectroscopy and contact angle analysis were used to determine the presence, binding, and wettability of self-assembled monolayers on the metal surfaces. Infrared spectra revealed that phosphonic acid head groups were more stable on metal surfaces than carboxylic acid head groups.

28

Synthesis and Characterization of Quaternary Diamond-Like Semiconductors

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The class of diamond-like semiconductors (DLSs)with the general formula I2-II-IV-VI4 is attractive for applications in nonlinear optics, solid state electrolytes, and photovoltaics. These materials exhibit compositional flexibility ,where various elements can be employed to tune the physical properties. Accessing these DLSs as nanophases can further impact properties, for example band gap. Most thin film solar cell materials are made from nanoparticle precursors. The synthesis and characterization of novel quaternary DLSs nanparticles is targeted in this project. The materials are structurally characterized using X-ray powder diffraction (XRPD), morphology and elemental analysis are carried out using scanning electron microscopy coupled with energy dispersive spectroscopy and band gaps' are assessed using UV-Vis-NIR spectroscopy.

29

Reassignment of Instruction Sets Using Digital Evolution

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Evolving computer programs have instructions that are typically encoded by symbols or commands that do not change their meaning in terms of their corresponding machine functions. Here we explore the before-and-after scenarios for how instruction sets may be reassigned using digital evolution experiments. We made adjustments to the digital evolution software AVIDA to implement two new basic steps. First, we configured AVIDA to support multiple forms of an instruction that have different symbolic encodings but the same machine function. Second, we substituted all copies of one of the redundant symbolic encodings in an evolved organism to correspond to a different machine function and examined the results. Our workflow enables us to evaluate different scenarios where substitutions of redundant symbolic encodings impact fitness. There exists a broader implication for how this digital evolution experiment may relate to codon degeneracy in biological systems.

30

Connecting structure to function in "ferritin-like 3 unit pores" of multiple DNA Binding Proteins in Starved Cells

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Abstract: DNA-binding proteins from starved cells (Dps) are prokaryotic dodecameric proteins that store iron as well as prevent free radical generation. Aqueous cytotoxic Fe2+ enters these proteins through 3-unit pores and become oxidized to Fe3+, which is crystallized to an inert form within the internal cavity. Adaptive Poisson Boltzmann and Poisson Nernst Planck solvers were applied to the Dps from Escherichia coli, Thermosynechococcus elongates, Helicobacter pylori, Listeria innocua, and Mycobacterium smegmatis to compute the approximate current of Fe2+ both in and out of the proteins. It was found that although the pores of these 5 Dps are largely homologous, slight structural differences give rise to highly variable Fe2+ current. Fe2+ flux is believed to be adapted to the specific environments that these organisms are subjected. Cells in high stress environments would benefit from rapid Fe2+ uptake to combat the production of reactive oxygen species.

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Tablet Density Analysis with Terahertz

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Tablet density plays an important role in drug release, with high density leading to an inefficiently low dissolution rate. Terahertz time-domain spectroscopy offers the capability to monitor tablet density online. The goal of this study was to develop a density model with Terahertz which is insensitive to chemical variation and robust against tableting parameters, including compression speed, compression force, and weight. Tablets comprised of acetaminophen, lactose monohydrate, micro-crystalline cellulose, potato starch, and magnesium stearate were produced according to a full factorial experimental design involving four chemical ratio levels, five compression force levels, and two compression speed levels. Tablets were made on an Instron single-punch tablet press and scanned using a Terahertz TAS7500, property of Advantest Corporation. The Terahertz time-domain spectra for all tablets were associated with their reference densities, calculated using mass and dimensions of each tablet. Multivariate techniques (partial least squares) were then used to create a density model.

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Enzymatic Investigation of Induced Macromolecular Crowding on Ferredoxin and Ferredoxin-NADP+ Reductase Complexes

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Macromolecular crowding is the phenomenon in which biomolecular properties are altered due to high concentrations of macromolecules in an environment. In order to test the effects of macromolecular crowding on biological redox reactions, the proteins ferredoxin (Fdx), and ferredoxin-$NADP^+$ reductase (FNR), were purified from *Spinacea oleracea*. Extraction was implemented through tissue homogenization and sonication followed by a series of chromatographic steps. Utilizing NADPH as a reductant, FNR is capable of reducing cytochrome c through the intermediacy of Fdx, or reducing the dye dichlorophenolindophenol (DCIP) directly. Fdx-dependent cytochrome c reduction was measured using NADPH, cytochrome *c*, Fdx and FNR; whereas Fdx-independent DCIP reduction activity was measured with NADPH, FNR, and DCIP. To investigate the effects of macromolecular crowding on electron transfer rates, the polymers Ficoll and Dextran were utilized as model macromolecular crowding species and were used at concentrations ranging from 2% to 8%. Results of these studies will be presented.

33

Mossbauer Studies of Molybdenum Oxide-hematite Nanoparticles

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High energy ball-milling is the process in which elemental blends are milled to stimulate high energy collisions among balls thus achieving different types of reaction by diffusion at atomic and nanocrystalline levels. I synthesized twenty sets of nanoparticle systems containing molybdenum oxide and hematite mixed oxides: $xMoO_3$-$(1-x)\alpha$-Fe_2O_3 with x=.1,.3,.5,.7. I used ball-milling, mechanochemical activation, and obtained samples for 2, 4, 8, and 12 hours milling times. I recorded transmission Mossbauer spectra using a ^{57}Co gamma-ray source and an MS-1200 constant acceleration spectrometer. I obtained useful information by non-linear least square fitting of the Mossbauer spectra. The observation of several sextets indicated various nearest neighbors of the ^{57}Fe probe. The occurrence of doublets indicated mutual substitutions between Mo and Fe atoms thus was able to probe the formation of solid solutions at the nanoscale.

34

Species Identification of an Unknown Marine Cyanobacterium

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Cyanobacteria are photosynthetic prokaryotes found in diverse terrestrial and aquatic habitats. In previous studies, compounds produced by marine cyanobacteria have been shown to have pharmacological activity. Using the National Institute of Mental Health Psychoactive Drug Screening Program (PDSP), an unknown species of cyanobacteria collected from Isla Mina in the Las Perlas Archipelago produced compounds with an affinity for the peripheral benzodiazepine receptor (PBR). PBR agonists have shown anticonvulsive, antispasmodic, and anxiolytic effects. The goal of the present study was to determine the species of cyanobacteria that produced these compounds. DNA from the cyanobacteria was isolated and the 16S rRNA gene was cloned into a TOPO vector. The plasmids were sent to be sequenced using Sanger Sequencing. Sequencing this gene allows for the identification of cyanobacteria through phylogenetic comparison to known 16S rRNA cyanobacterial sequences.

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Sulfonylisonitrile from Methyl Sulfinates

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Sulfonylmethyl isonitriles are bifunctional compounds containing isonitrile and sulfonyl groups. Isonitrile and sulfonyl groups are electron-withdrawing groups that facilitate deprotonation of the methylene carbon. Previously, sulfonylmethyl isonitriles were prepared via dehydration of the corresponding formamides, which were synthesized from sulfinate salts. Dr. Lujan-Montelongo devised a new method of synthesizing sulfonylmethyl formamides using sulfinic esters instead of sulfinate salts. Sulfinic esters are more stable than sulfinate salts, and are readily prepared from thiols or disulfides by oxidation with N-bromosuccinimide (NBS) in a CH_2Cl_2/methanol mixture. The procedure does not require heating or a nitrogen atmosphere, and goes to a completion within 15 minutes to 1 hour. Sulfinic esters react with an iminium ion under the influence of microwave heating (3 hours at 100 ˚C) or thermal heating (2-3 hours at 90 ˚C) to form sulfonyl formamides; subsequent dehydration affords desirable sulfonyl isonitriles.

36

Towards flexible, organic small-molecule piezomaterials: device fabrication with 2-methyl-4-nitroaniline

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We have explored aspects of 2-methyl-4-nitroaniline (MNA) as a piezoelectric material. Melt-processing and poling has produced films with piezoelectric response similar to single crystals. Devices on flexible substrates such as Pyralux have also been produced. As MNA is the first small molecule that has been applied to piezoelectric power conversion, it provides a model system for processing methods not available to conventional ceramic, polymer, or nanowire piezomaterials. For example, appropriate surface functionalization is known to crystallographically orient nucleation and growth of polar materials. This could allow production of bulk piezomaterials without the need for poling. Aided by computational work, insight can also be transferred to similar small-molecule systems such as 2-chloro-4-nitroaniline.

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Intramolecular charge-assisted hydrogen bond strength in pseudo-chair carboxyphosphate

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Dianionic and monoanionic carboxyphosphate is predicted to exist in a novel conformation known as pseudo-chair, stabilized by an intramolecular charge-assisted hydrogen bond (CAHB). Separate additive and subtractive correction schemes to the open-closed method are used to estimate the strength of the CAHB. Truhlar's Minnesota M06-2X functional with Dunning's aug-cc-pVTZ basis set is utilized for all computations. Straightforward application of the open-closed method predicts CAHB strengths of 14.5 kcal/mol for the monoanion and 12.0 kcal/mol for the dianion. In our additive correction scheme, reveals that differential van der Waals contributions between the pseudo-chair (closed) and open conformations of carboxyphosphate are essential in determining accurate CAHB strength. Knowledge of an accurate CAHB strength provides deeper insight into the pseudo-chair conformation of carboxyphosphate, offers a partial explanation of its instability in the aqueous phase, and leads to an improved mechanistic understanding regarding how carboxyphosphate is stabilized and used in ATP-dependent carboxylases.

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Visualizing multi-model data with graphical models to identify disease pathways

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Graphical models can be used to transcend traditional notions of distinct pathways, by representing probabilistic dependence relationships among interacting components on a global scale. However, biological data are frequently high-dimensional and the combinatorics make comprehensive independence tests computationally costly; in fact, searching for the optimal graph is a known NP-hard problem. Instead, we used a Mixed Graphical Model algorithm (MGM) that learns subnetworks at significantly reduced computational time. All algorithms are limited by the number of variables they can process, so we searched known gene subnetworks from PARADIGM, and identified those whose connections are statistically supported by melanoma data obtained from TCGA, based on their MGM learned structures. These pathways were further examined by including other relevant components (miRNAs, methylation, clinical outcomes). This method could identify omics variables that are important for clinical facilitation of metastatic melanoma, and serve as a tool for biomarker selection along with personalized patient treatment.

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Synthesis and characterization of dithione ligands for metal chelation

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Coordination complexes of 1,2-dithiolenes are important molecules as they exhibit distinguishing spectroscopic and structural properties. These molecules may be important in developing new materials as well as mimics for certain biological metal centers. This project will involve synthesis of 1,2-dithiolene ligands and their purification. The reaction scheme involves a two step process where an amine is condensed with diethyl oxalate forming a diketone, which then will be sulfurized using Lawesson's reagent. The target compounds are separated using column chromatography and will be characterized by IR and ^{1}H NMR spectroscopy. The coordination chemistry of this ligand will be explored.

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Photoacoustic burn depth study of phantom tissue

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No accurate, noninvasive imaging option is available to assess burn injury. Photoacoustics offers a solution to the dilemma by allowing doctors to scan entire burn sites without penetration of the tissue. An Nd:YAG laser was directed at layered skin phantoms. Three layers of 100, 200, and 300 μm thick gels each had different layer absorbances due to dye concentration, just as layers of human skin have different absorption coefficients that correlate to their depth within the tissue. The laser created photoacoustic waves, sensed by a transducer and displayed on an oscilloscope. The photoacoustic waves were fit with an exponential model to reconstruct the sample layers. The results show that photoacoustic wave analysis accurately displays the absorbance and depth of layered tissue phantoms, suggesting a prospective option for burn diagnostics.

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The Detection of Organic Components Found in Gunshot Residue by Use of LC-QQQ-MS to Assess Home Reloaded Ammunition

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In addition to the rise of gun violence in the past decade, gun sales broke records and ammunition shortages have plagued the country. Because these recent ammunition shortages have driven sportsman and shooting enthusiasts alike to reload their own ammunition, gunshot residue (GSR) resulting from home-reloaded ammunition may become prominent physical evidence in firearm related crimes. An optimized method was developed for liquid chromatography with triple quadrupole mass spectrometry (LC-QQQ-MS) to examine the common organic components of GSR which results from both home-reloaded and factory-manufactured ammunition. Through the optimization of LC-QQQ-MS parameters, the seven most common organic components of GSR were successfully separated and detected. The developed method provided R^2 values of (>) .999 for the seven organic components' calibration curves and limits of detection and quantitation were determined. After GSR from both factory-manufactured and home-reloaded ammunition was extracted, differentiation between the two types of ammunition was achieved.

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Applications of Graph Analytics with Big Data

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Graphs are mathematical models that represent relationships between a collection of entities. In fields such as physics, chemistry, computer science, and even linguistics, graph-theoretic methods are used to solve problems that would be too complicated to tackle using other methods. In the world of Big Data, graph analytics is key to understanding the structure of substantial amounts of data, in addition to revealing the data's underlying patterns and relationships. The focus of my research will be on graph applications in the realm of Big Data using essential tools such as RDF and SPARQL. I will be working closely with the Pittsburgh Supercomputing Center's (PSC) Sherlock system, a graph analytics appliance from YarcData which enables rapid large-scale graph analytics, and Neo4j, a leading graph database that allows for high-speed graph queries. My research will include performance comparisons between Sherlock and Neo4j on Blacklight, a high-performance compute resource at the PSC.

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Essential Lewis acid catalysis in the synthesis of copper (II) cyanomethides

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Cyanomethide complexes were recently synthesized and characterized. However, fundamental chemistry does not support the synthesis of copper (II) cyanomethides from copper hydroxide complexes and acetonitrile. Copper hydroxide complexes are good bases ($pK_a \approx 15$) but are not strong enough to react with acetonitrile, a weak acid ($pK_a \approx 25$). Lewis acid coordination with acetonitrile is proposed to enhance acidity and promote the reaction. We have used Truhlar's M06-L density functional with Dunning's cc-pVDZ basis set to find that the copper complexes are C_1 symmetric, consistent with single X-ray crystallography. Optimized structures allow for thermodynamic evaluation and influence of a Lewis acid on the reaction energetics. Our results show that copper hydroxide complexes do not react directly with acetonitrile but rather with acetonitrile coordinated to a second Lewis acid copper atom. Essentially, Lewis acid copper coordination to acetonitrile explains the formation and stability of copper (II) cyanomethides.

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Effects of Viscosity and Macromolecular Crowding on the Diffusion-Controlled Rate Constant of Ferredoxin NADP$^+$ Reductase

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The rate at which many reactions occur is controlled by the ability of one particle to diffuse to another. One such reaction is between ferredoxin NADP$^+$ reductase and its substrate, a key mechanism in the overall process of photosynthesis. Experiments simulating the intracellular environment often neglect to include the high concentration of macromolecules within the cytosol of the cell. The presence of these macromolecules causes a crowding effect impacting the rate at which reactions occur within the cell. Utilizing the methods of Brownian dynamics, simulations were run to calculate the reaction rate of the ferredoxin NADP$^+$ reductase enzyme binding with a corresponding substrate under standard conditions as well as conditions including macromolecular crowding. The resulting data indicated that the diffusion-controlled rate of the reaction was reduced when introduced to crowded conditions. The results indicate a greater understanding of the interactions occurring using a realistic model of the intracellular environment.

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High-Temperature Solid-State and Lithium Polysulfide Flux Synthesis of Quaternary Lithium-Containing Diamond-Like Semiconductors

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Diamond-like semiconductors (DLSs) have applications in photovoltaics and nonlinear optics (NLO). The majority of benchmark IR-NLO materials are DLSs, which have been researched extensively because of their second harmonic generation properties originating from their noncentrosymmetric crystal structures. Silver and copper containing ternary and quaternary DLSs dominate the list of benchmark materials; however, they suffer from low laser damage thresholds. Quaternary lithium-containing DLSs with a general formula of I2-II-IV-VI4 are not as prevalent in literature due to the difficulty in synthesizing them in phase-pure form; however, the replacement of silver or copper on the I-site in these compounds broadens the possibilities for high power NLO applications due to the widening of the band gap and the correspondingly higher laser damage threshold that is expected to follow. X-ray powder diffraction and scanning electron microscopy coupled with energy dispersive spectroscopy were utilized to characterize the synthesized materials.

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Investigating substituent effects on the fragmentation spectra of protonated peptides modified to create N-terminal imines

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Tandem mass spectrometry (MS^n) and collision induced dissociation (CID) are among the most important tools used to identify peptides and proteins in proteomics. Fragmentation of gas-phase, protonated peptides creates product ions that reveal amino acid sequence. Recently we found that conversion of peptides to N-terminal imines (as Schiff bases) enhances the sequence information revealed by the MS^n approach. Further investigation of substituent effects on the fragmentation spectra through the interchange of the aldehyde/ketone reactant in the modification step may reveal even more important sequence information. It is the goal of this research to prepare peptide-imines in the gas phase, investigate the influence of substituents on product ion distributions and assess improvements to MS^n sequencing gained by the modification.

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Testing for Antibiotic and Biocide resistance in Bacteria Isolated from Fracking Impoundment and Produced water from Marcellus Shale

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The produced water from the hydraulic fracking of the Marcellus Shale contains various microbes that can survive its high total dissolved solid concentration (TDS) with elevated salinity and organic content. In this study, strains of bacteria enriched from impoundments used to store produced water and produced water from wells, were isolated and characterized using media formulated with high TDS. Streak plating on solid medium was used to isolate pure cultures and their morphology was determined by light microscopy. Antibiotic and biocide resistance tests for the bacterial strains were done on solid medium utilizing Sensi-Discs and various concentrations of glutaraldehyde. Previously isolated strains LP-1 and SWPA-1, and new enrichments were resistant to Ampicillin, but sensitive to Nalidixic Acid, Erythromycin, and Polymyxin. Glutaraldehyde was an effective microbicide.

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Virtual Screening and Modeling of Phosphoglycerate Mutase 1

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Phosphoglycerate Mutase 1 (PGAM1) is a glycolytic protein upregulated in many types of cancer cells. In a phenomenon called the Warburg Effect, cancer cells have a higher rate of glycolysis than healthy cells. Altering PGAM1 activity can change cancer cell proliferation and thus is an important pharmacological target for cancer suppression. A small molecule, MJE3, inhibits PGAM1 activity and decreases cancer cell proliferation. Since MJE3 covalently binds to PGAM1, it is not a feasible drug to temporarily decrease PGAM1 activity. A binding model of MJE3 to PGAM1 was created using Molecular Dynamic simulations and protein-ligand dockings. Key binding characteristics were used to form pharmacophore models to perform virtual screenings of purchasable compounds for potential new drug targets of MJE3 inhibition.

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Assessing the Thermal Oxidative Stability of Ultra Low Sulfur Diesel using SMORS Methodology

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Fuel oxidative instability is defined as formation of deposits and gums that block filters, small injection ports and lacquer engines surfaces. Thermal Oxidative instability can occur during storage and/or while in use in engines. Fuel produced from animal fats, vegetable oil, and crude oil undergoes autoxidation in the presence of atmospheric oxygen. To measure the Thermal Oxidative stability, Soluble Macromolecular Oxidative Reactive Species, better known as SMORS methodology was used to examine the thermal oxidative stability of commercial Ultra Low Sulfur Diesel (ULSD).SMORS are derived using a separatory funnel and a Rotary Evaporation System (ROTOVAP) that evaporates the methyl which essentially makes the SMORS. SMORS methodology was used to quantitate the extent of diesel fuel oxidation.

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Nanoemulsions as new drug delivery strategy for resveratrol and it's analogs

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Resveratrol is a natural compound with anticancer and anti-inflammatory effects. Its pharmaceutical use is limited by poor solubility and rapid metabolism. Two strategies that may be employed to increase the bioavailability are: use of metabolically-stable analogs and formulations that enhance drug solubility. Combining these approaches, we prepared nanoemulsions loaded either with resveratrol or resveratrol trimethylether. Nanoemulsions also carry perfluorocarbons (for ^{19}F MRI) and NIR dyes (for optical imaging) for *in vivo* studies. Quality assessment was performed using dynamic light scattering. The average droplet size was 140 nm and zeta potential was -10 mV. Nanoemulsions were stable under storage and cell culture conditions. Drug loading was 90% for resveratrol and 80% for the analog. Nanoemulsion exposure did not show any reduction in cellular viability. Nanoemulsion uptake in macrophages was confirmed by confocal microscopy and NIR fluorescence measurements. In conclusion, presented nanoemulsions are promising novel drug carriers for resveratrol and its analogs.

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Absolute Binding Free Energy Calculations Bovine Pancreas Beta-Trypsin in Complex with Benzamidine

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Knowing the binding free energy between a protein and a small molecule is an important quantity in the drug discovery process. CHARMM-GUI *Ligand Binder* allows users to calculate the absolute binding free energy of a small molecule bound to a protein using the free energy perturbation/molecular dynamics (FEP/MD) techniques. The CHARMM-GUI will be used to calculate the binding free energy between the protein trypsin and two substrates, benzamidine and para-fluorobenzamidine. This protein substrate system is used to validate the CHARMM-GUI interface.

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Sparse Representation of Image Data for Image Compression

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Fourier and Wavelet bases have been used to sparsely represent image data in applications such as the JPEG and JPEG 2000 compression algorithms. However, learned dictionaries using e.g. the K-SVD algorithm of Elad et al. allows for further specialization, leading to more powerful sparse image representations. We analyzed the compression capabilities of the K-SVD algorithm in comparison to other non-learning algorithms including the Discrete Cosine Transform and the Fourier transform.

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ATRA Reactions of Alkenes with Novel Catalyst Cu(BPPMA-Me_2)Br]Br

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Copper catalyzed atom transfer radical addition (ATRA) is a fundamental way to form carbon-carbon bond through the addition of alkyl halides to the double bond of an alkene. Through catalyst regenration, different reducing agents such as ascorbic acid and 2,2'-azobisisobutyronitrile (AIBN) were used along with the catalyst and significantly decreased the amount of copper complex required for ATRA reaction. Due to this, the processes became more efficient, cost effective and environmentally safe. The copper catalyst [Cu(TPMA)X]X (X= Br^- or Cl^-) (tris(2-pyridylmethyl)amine=TPMA) was used in ATRA reactions with various alkenes before. In the pursuit of finding a more active catalyst, which can make the reaction more efficient, a novel catalyst [Cu(BPPMA-Me_2)Br]Br (BPPMA-Me_2= *N*,*N'*-bisc-3,5-dimethyl-pyrazolmethyl)-*N*-(pyridin-2-ylmethyl)methamine) was employed on alkenes (1-octene, 1-hexene, styrene, methyl methacrylate, and methyl acrylate) using polyhalogenated alkanes. The catalyst did react promisingly with 1-octene and other similar alkenes but it was not as effective for more active alkenes.

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Experession, Transfection Optimization, and Production of Major Hominoid Semen Coagulation Proteins

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The semenogelin proteins (SEMG1 and SEMG2) are the major factors responsible for the coagulation of semen in multiple primate species. Differences in gene lengths coupled with rapid evolution may be responsible for variations in semen physiology among humans, chimpanzees, and gorillas, which may reflect mating behavior differences. In order to thoroughly study these proteins, I will overexpress and purify recombinant SEMG1 and SEMG2 in a mammalian cell culture system. Initially, I cloned the coding sequences of these genes, as well as that of the green flourescent protein (GFP) into two expression plasmids, pSG5 and pFLAG-CMV, with restriction digestion, ligation, and transformation into *E. coli* cells. I grew and maintained the 293T human cell line in culture, in order to optimize transfection conditions using the easily visualized GFP, by comparing different protocols. After completing optimizations, I will transfect the SEMG1 and SEMG2 constructs to produce recombinant proteins in this cell line.

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The Fusion of Exposure Bracketed Pairs

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In low lighting conditions it is difficult to capture images with high detail and true color information. Images captured with short exposure times will have sharp detail but also retain noise and lack true color. On the other hand, images captured with long exposure times will retain true color information but lack sharp detail particularly due to nonlinear motion. This problem can be addressed by fusing exposure bracketed sets of images with the goal of maintaining detail, true color, and not enhancing artifacts or noise. The proposed method is based on a variational approach by Bertalmio and Levine and has potential applications to video enhancement, colorization, and high dynamic range imaging.

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Determination and Characterization of G-quadruplex Structures in Various Messenger Ribonucleic Acids

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Guanine-rich sequences of RNA have the ability to fold into a G quadruplex structure. It has been demonstrated that the presence of a G quadruplex in the 5'- untranslated region (UTR) of the mRNA has the ability to regulate its translation. Correlations between the structural properties of the G quadruplex and translation regulation activity still remain unclear. Therefore, the G quadruplex structures of each mRNA must be characterized. Various techniques such as circular dichroism (CD) spectroscopy, UV spectroscopy thermal denaturation, nuclear magnetic resonance (NMR) spectroscopy, and native polyacrylamide gel electrophoresis (PAGE) can be used to characterize the structural properties of each G quadruplex. The purpose of this study was to use these biophysical methods to determine whether a G quadruplex structure forms in several neuronal mRNAs, such as SMNDC1, CHRNA4, LRP1, and Drebrin mRNAs.

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Development of Indazole Type-III MEK5 inhibitors

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MAPK (mitogen activated protein kinase) signaling pathways are complex yet important kinase cascades. The singular parallel event is the phosphorylation of an ERK by its MEK. MEK5's only substrate is ERK5. The MEK5 signaling pathway allows cells to survive oxidative stress and is significantly up-regulated in squamous cell carcinoma, prostate, and most importantly in early and triple-negative breast cancers. Prior medicinal chemistry addressing MEK1 inhibitors by others has mapped out a unique "type III" binding domain resulting in Mekinist, a first in class MEK1 type III inhibitor. We will present the development of novel indazole compounds designed as MEK5 type III (or allosteric pocket) inhibitors. Design, synthesis, and testing of these compounds will be presented. In addition to this indazole compound, other 7-membered and 5-membered ring compounds are currently being synthesized each exploring possible MEK5 type III inhibitor activity with unique structures to explore multiple scaffolds.

58

The impact of substituent size and electronegativity on the band gap of TiO_2 polymorphs

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The electronic structure of TiO_2 has been extensively studied through a variety of experimental and computational methods. Its properties range from thin film photovoltaic cells to optics. TiO_2 provides an excellent model to study computationally due to the wealth of experimental data and its inexpensive computational cost. Our hypothesis is that larger crystal radii of substituent atoms decrease the band gap of crystalline TiO_2. Atoms of different crystal radii were selected for substitution into three polymorphic forms of TiO_2, which are rutile, anatase, and brookite. Our computational approach utilizes the linearized-augmented plane-wave approach of density functional theory in the WIEN2k computational software, and includes the incorporation of the modified Becke-Johnson potential, to determine the band gap and density of states for each case. Initial results showed that sulfur substitution in a 2x2x2 rutile supercell resulted in a slight decrease in the band gap.

59

Effect of population variance in speed on *E. coli* thermotaxis in a shallow gradient

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Thermotaxis is essential for the survival of *E. coli*. Yet, only recently has research on thermotaxis in shallow gradients been done. We know that speed modulation is important to this process, but we do not know much about the influence of population variability. In our current work, we explore the impact of within-population variance in speed on an E. coli colony's ability to respond to these shallow thermal gradients. We simulate the motion of a population of bacteria in a narrow channel where the medium exhibits a shallow thermal gradient along one dimension. We then change the variance of the speed distribution and compare the results. We find that the variance influences the population's response to the gradient. Since this variance may result from genetically controllable molecular noise, this research could have implications for the importance of tuned molecular noise in intracellular systems.

60

Substrate Transport and Conformational Change of the Monoamine Transporters

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Neuronal cells communicate through the use of neurotransmitters. Neurotransmitter concentrations are modulated through the use of transporter proteins. Monoamine transporters (MATs) are proteins that reuptake monoamine neurotransmitter back into the presynaptic neuron. The translocation of monoamine involves an open-outward (OO) to open-inward (OI) conformational change of the MAT. What is not well understood is the reverse conformational change of the MAT from OI to OO. We hypothesize that a potassium ion (K^+) is needed to drive the reverse conformational change. Using molecular dynamics, we simulated a dual lipid bilayer system including a MAT in its halo form in one bilayer and a MAT in its apo form, open to the intracellular space, in the other bilayer. Two systems are currently running, each one containing a separate MAT. In one system, K^+ is seen entering the apo form of the protein. Results will be further discussed in this poster.

61

Title: The ssNMR peak matching of geometry optimized organic crystals

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Anisotropic shielding tensors and solid-state nuclear magnetic resonance (ssNMR) chemical shifts are highly sensitive to atomic positions. The ^{29}Si ssNMR spectrum of triphenylsilanol contains 8 unique peaks unassigned to the inequivalent Si sites in the triphenylsilanol crystal. Since shielding and shifts are highly sensitive to small changes in crystal structure, the organic crystals have been geometry optimized using the molecular mechanics module FORCITE. Shielding tensors can be calculated using density functional theory, and chemical shifts can be calculated from shielding values using a least squares fit. Here, the chemical shielding tensors have been calculated using the Perdew-Burke-Ernzerhof generalized gradient approximation functional and a plane wave basis set to peak match the triphenylsilanol spectrum. This process has been applied to 1,4-dimethoxybenzene, a compound with known ^{13}C chemical shift assignment and crystal structure to show agreement between computational and experimental approaches. We report chemical structures and shift assignments for 1,4-dimethoxybenzene and triphenylsilanol.

62

Stress: Friend or Foe? The Effects of Corticosterone on Infection Intensity

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Worldwide amphibian declines have been linked to *Batrachochytrium dendrobatidis* (*Bd*), an often-lethal fungal pathogen. Environmental stressors may increase amphibian susceptibility to *Bd*. We hypothesized that exposure to the stress hormone, corticosterone (CORT), would increase *Bd* infection in red-legged salamanders. Subjects were treated with either CORT or oil for 9 days prior to inoculation with *Bd* zoospores or vehicle. We analyzed skin swabs collected 1-2 weeks post-inoculation to assess infection. DNA from *Bd* zoospores was extracted from swabs and quantified via qPCR. *Bd*-exposed animals had increased zoospore equivalents compared to the vehicle controls. Results showed a nonsignificant trend (p=0.066) for subjects treated with *Bd*+CORT to have a higher infection load than those treated with *Bd*+vehicle. However, there were no significant differences in disease symptoms between *Bd* inoculated animals treated with CORT versus oil vehicle. Therefore, increased stress conditions may not fully predict disease susceptibility and mortality.

63

Development of Spore Associated Protein Fusions in *Streptomyces coelicolor* spores

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Endospores from unicellular bacteria have been used for vaccine production, probiotics, and as biosensors while exospores from filamentous bacteria have not been thoroughly investigated. SapC is a spore-associated protein of the filamentous sporulating soil bacterium *Streptomyces coelicolor.* Although it is associated with the *S. coelicolor* spore, SapC is not predicted to be a secreted protein. A goal of this project was to fuse the gene encoding SapC to the gene encoding the B subunit of the heat labile toxin of *Escherichia coli* (LTB) to determine if this fusion protein can be expressed and incorporated on the spore surface. Another goal was to make C-terminal truncations of SapC fused to LTB to locate the secretion signal of SapC. SapC-LTB expression and localization was characterized by SDS-PAGE and Western Blot analyses. This could lead to a viable method for oral vaccine production.

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Development of *Streptomyces coelicolor* for Vaccine Delivery

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One type of vaccine production has traditionally been explored using endospores from unicellular bacteria. However, similar use of exospores from filamentous bacteria such as *Streptomyces coelicolor* has not been investigated thoroughly. SapE and SapD, spore associated proteins, are believed to be associated on the outside of *S. coelicolor* spores. This project focused on fusing the gene encoding the β subunit of the heat liable toxin (LTB) of *E. coli* to the *sapE* and *sapD* genes in order to express and incorporate the LTB antigen on the spore surface. The SapE-LTB and SapD-LTB encoding fusion genes were inserted into the *S. coelicolor* chromosome in order to express LTB on the spore coat. Recombinant spores have been characterized using SDS-PAGE and western blot techniques. Because of the durability and longevity of spores and their associated proteins, antigens expressed on exospores could potentially result in an oral vaccine with extended shelf life.

65

Tribological properties of monolayers and mixed monolayers of octadecylcarboxylic acid and octacosanoic acid on α-aluminum oxide surfaces

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A self-assembled monolayer (SAM) is a spontaneous adsorption of amphiphilic organic molecules on a solid inorganic surface. Highly ordered monolayers may be formed when the head groups of adsorbing molecules strongly bind with surfaces of metals and metal oxides; therefore, SAMs have been used to modify surface properties including friction, lubricity, and hydrophobicity. In this study, SAMs of octadecylcarboxylic acids (ODCA) and octacosanoic acids (OCA), and mixed SAMs of each were produced on the [0001] basal surface of α-aluminum oxide. Five samples, including 100%, 50%-50%, and 25%-75% ODCA and OCA, were prepared using solution deposition, sonicated in methanol to reduce multilayers, and characterized using diffuse reflectance infrared Fourier transform spectroscopy (DRIFT), water contact angles, and atomic force microscopy (AFM). DRIFT revealed that highly ordered SAMs of all carboxylic acids were formed while the interfacial friction was measured by AFM. Water contact angles evaluated surface properties following modification of the surface.

66

Examination of the role of Rad4 β-hairpin 3 in DNA damage recognition

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Nucleotide excision repair (NER) corrects various types of DNA damage, including bulky chemical adducts and UV-induced photoproducts. Damage recognition, spearheaded by Rad4-Rad23 in budding yeast, serves as the earliest step of NER. The β-hairpin 3 on Rad4 has been hypothesized to insert itself in double-stranded DNA when it detects a lesion, thus triggering the rest of the NER pathway. Through fluorescence anisotropy, we have shown that wildtype Rad4 binds to damaged DNA with a K_d of 20.67 nM, while mutants also bind with comparable affinity (K_d of 24.3 nM for deleted β-hairpin 3 and K_d of 12.83 nM for deleted domain 3). Atomic force microscopy was used to measure the bend angles for undamaged and damaged DNA substrates. Undamaged DNA was found to have a 32.29° bend angle, while substrates damaged with cyclobutane pyrimidine dimers or fluorescein were found to have bend angles of 20.77° and 4.191° respectively.

67

Bladder pain-induced changes in central amygdala gene expression

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The central nucleus of the amygdala (CeA) is a brain region involved in modulating both pain and emotion. Interestingly, activation of the right CeA, but not the left, has been observed in a variety of pain conditions, including noxious bladder distension. To more fully understand the molecular mechanisms responsible for the observed lateralization, we used quantitative real-time polymerase chain reaction (qPCR) to evaluate gene expression in the left and right CeA following noxious bladder distension in female mice. Gene expression was assessed in sham animals, animals that underwent bladder distension, and animals that underwent bladder sensitization prior to distension. Specifically, we investigated changes in c-Fos, metabotropic glutamate receptor 5 (mGluR5), and arrestin domain-containing protein 4 (Arrdc4) mRNA levels.

68

The Impacts of Acidification on Macroinvertebrates in Two Pennsylvania Streams

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Acid mine drainage is known to have a harmful impact taxonomic diversity of acid intolerant macroinvertebrates by affecting their niches. Benthic macroinvertebrates are aquatic insects that spend their nymph stage in the stream and emerge to breed, and their diversity and abundance influences the success of other terrestrial and aquatic organisms that prey upon them. At the Carnegie Museum of Natural History's Powdermill Nature Reserve in Rector, Pennsylvania an acidified stream (Laurel Run) and a circumneutral stream (Powdermill Run) were studied for the abundance and diversity of their macroinvertebrates. Data on abundance and diversity was collected by using sticky traps at three time points between late spring and early summer. With a taxonomic key, the organisms collected were identified to the family level. I expect these results to improve our understanding of acid mine drainage and its negative impact on taxonomic diversity in an aquatic ecosystem.

69

Synthesis and Characterization of $Cu_2ZnGeVI_4$ (VI = Se, Te) Quaternary Diamond-like Semiconductors

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The crystal structures of several quaternary diamond-like semiconductors (DLSs) with the general formula of I_2-II-IV-VI_4 have been reported in the literature; however, these materials have not been completely characterized. Information regarding applications of these materials are acquired from systematic and thorough assessment of the physicochemical properties. Quaternary DLSs with this formula have potential applications in photovoltaics, thermoelectrics and nonlinear optics. Single-phase samples of these compounds were prepared by high-temperature solid-state synthesis. The crystal structures were then investigated using X-ray powder diffraction and compared with configurations found in the literature. Optical diffuse reflectance UV-Vis-NIR spectroscopy was used to estimate the band gap of the semiconductors. Morphological and compositional characterization was performed using a scanning electron microscope with an energy dispersive spectrometer. Elemental mapping was performed to evaluate the homogeneity of the samples. Multiple synthesis techniques and heating profiles were explored to determine the conditions necessary to prepare phase-pure materials.

70

Niche Partitioning between Acadian Flycatchers and Red-Eyed Vireos.

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Acadian Flycatchers *(Empidonax virescens)* and Red-Eyed Vireos *(Vireo olivaceus)* are songbirds that co-inhabit the riparian zone of deciduous forests during breeding season, preying on invertebrates by aerial hawking or gleaning from leaves, respectively. Competition occurs when two species try to utilize the same resources. One way to avoid competition is to utilizing different resources, known as resource partitioning. We studied whether the two species partition niches based on nest locations. Nests of the two species along Powdermill Run located at Carnegie Museum of Natural History's Powdermill Nature Reserve field station near Rector, Pennsylvania were measured using metrics designed to address questions regarding differences in nesting behavior such as nest position, height, surrounding vegetation, and tree species. Differences in these metrics would be evidence for niche partitioning, but no differences may suggest other means of partitioning, such as prey or foraging behavior.

71

The study of the Notch-Delta signaling pathway in *Manduca sexta*

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Cell differentiation is a vital part of the developing embryo in order for the organism to develop diverse cellular systems to survive. The Notch-Delta signaling pathway involves transmembrane proteins that regulate cell fate determination in many cell types. During *Drosophila* muscle development, Notch-Delta interactions regulate the determination of muscle founder cell fates. The Notch signaling pathway is also highly conserved among metazoan animals. This research investigates the role of Notch-Delta signaling during *Manduca sexta* embryogenesis, as well as during later development stages during the larvae and pupae stages. We predict that Notch-Delta signaling will be detected during *M. sexta* muscle development in the embryo. The levels of expression during differing stages can be an important indicator of the role that Notch plays during different types of muscle development. Understanding the role of Notch-Delta signaling during *M. sexta* muscle development will help elucidate the evolution of muscle patterning in insects.

72

Studying hedgehog gene expression in *Manduca sexta*

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In insects, developing muscles require signals from motor neurons for proper accumulation and proliferation of muscle precursors. Originally identified in *Drosophila* and present in all bilaterians, the Hedgehog (Hh) signaling pathway may regulate the accumulation and proliferation of embryonic and postembryonic muscle precursors. The Hh receptor complex contains Patched and Smoothened proteins. By accessing a database of expressed sequence tags from *Manduca sexta* (http://agripestbase.org/manduca/?q=home), we have identified and sequenced Hedgehog, Patched, and Smoothened genes within *Manduca sexta*. We will characterize their expression patterns of these genes during development. We expect to find that the Hh pathway within *Manduca sexta* embryos is highly conserved in all stages of development. However, we expect to find differences in the level of Hh expression in different muscles depending on the type, location, and stage of development of the muscle. This will provide evolutionary insight in the divergence of muscle development.

73

Purification and Effects of Macromolecular Crowding on Kinetic Activity of Ferredoxin and Ferredoxin:NADP$^+$ Reductase

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Macromolecular crowding is a phenomenon in which high concentrations of macromolecules, such as proteins, crowd the intracellular matrix. This crowding alters protein interactions and associated biochemical functions. The proteins ferredoxin (Fdx) and ferredoxin-NADP+ reductase (FNR) from *Spinacea Oleracea* were used in this study. During photosynthesis, these proteins act to transfer electrons from photosystem I to NADP$^+$. We utilized the reverse reaction, modeling the ability of this system to reduce cytochrome *c* using NADPH. After testing various methods from the literature, purification of ferredoxin and FNR was accomplished with a modified method using Toyopearl HW-65 gel filtration and DEAE cellulose ion-exchange columns, taking advantage of Toyopearl's ability to function as a hydrophobic matrix at high ionic strength. Kinetic experiments were conducted using dicholorophenolindophenol (DCIP) (ferredoxin-independent) or cytochrome *c* (ferredoxin-dependent) as electron acceptors. Kinetic assays will be presented that examine the effects of varying macromolecular crowing agent concentrations on electron transfer rates.

74

Solvation Effects in Bimolecular Diels Alder Cycloaddition of Cyclopentadiene: A Tool for Benchmarking Expected Errors in More Sophisticated Diels Alder Reactions

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The bimolecular Diels Alder cycloaddition of cyclopentadiene occurs with minimal charge separation and dispersion, thus follows a non-ionic gas-phase mechanism when in solution. The challenge for theory and computation is to compute the gas-phase parameters accurately, and differentiate the subtle effects of solvent upon computed activation energies in cycloadditions. Second-order Moller-Plesset theory (MP2) and Truhlar's M06-2X density functional with Dunning's cc-pV[D,T,Q]Z correlation consistent basis sets, and AM1, PM3, PM6, and PDDG semiempirical methods have been used with two different solvent schemes. The Gaussian09 and TeraChem programs were used. Semiempirical methods greatly overestimate, and DFT and MP2 are within 15% of the experimental activation energies. Tomasi's polarizable continuum model was used to estimate solvation effects and compared to an all-atom explicit-solvent approach. The effect of solvation is generally accounted for in the implicit solvation scheme. The preliminary results for the explicit solvent approach will be discussed.

75

Biophysical Analysis Of *CDK5R2* DNA Secondary Structures

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In addition to the classic DNA double helix structure, certain guanine rich DNA sequences can form secondary structures known as G-quadruplexes, and their complementary cytosine rich strand can form i-motif structures. G-quadruplexes can be formed by the stacking of multiple G-quartets which are formed by the Hoogsteen base pairing of several guanine residues. The i-motif structures are formed by the stacking of cytosine-cytosine base pairs and are stabilized at low pH values. The *CDK5R2* DNA contains multiple guanine and cytosine base pairs and has the capability to form both a G-quadruplex and an i-motif secondary structure. To characterize the different secondary structures of these DNA strands, many biophysical techniques were utilized including circular dichroism spectroscopy, ^{1}H nuclear magnetic resonance spectroscopy, UV spectroscopy, and native polyacrylamide gel electrophoresis (PAGE).

76

Chronic Variable Stress: A Model of Mouse Depression and Anxiety

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Chronic variable stress is a paradigm in which mice are exposed to environmental stressors during their active cycle (7 PM – 7 AM). The stressors in this experiment include light/dark cycle reversal, tilted cage, wet cage, small cage, and white noise. The idea is that these stressors are uncontrollable and unpredictable. Results are highly difficult to replicate due to laboratory differences, not to mention the use of C57BL/6 mice, the most emotionally resilient strain of mice. Our efforts include attempting to make a model for depression/anxiety in a group of mice in as little time as possible (10 and 15 Day durations). To analyze depression and anxiety caused by stressors, we will look at their behavior in the Sucrose Preference Test, Light Dark Preference Test, Open Field Test, Elevated Zero Maze Test, and Tail Suspension Test.

77

Pharmacophore Development Aimed at Inhibiting the Spi-1/DNA: C/EBPβ Interaction

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The Spi-1/PU.1 and the C/EBPβ transcription factors cooperate *via* a critical protein-protein interaction at the promoter of the human *IL1B* gene, coding for Interleukin β (IL-1β), a macrophage cytokine that mediates acute inflammatory responses, but can also lead to chronic disease when highly expressed. IL-1β-dependent inflammation may be prevented through the discovery of a small molecule that can bind to a pocket formed in the DNA major groove in the vicinity of Arginine 232 in Spi-1/PU.1, a recognition site for C/EBPβ interaction. We used MMTSB tools for structure preparation and solvation of the Spi-1/DNA complex, as well as NAMD 2.9 to conduct molecular dynamics (MD) simulations in order to generate a stable complex. The stable complex will be used to generate a pharmacophore that will be used to screen a library of small molecules using MOE. The results of this project provide a basis for developing an effective anti-inflammatory therapeutic.

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Electronic Structure Calculations of Li_2-II-IV-VI_4 Diamond-like Semiconductors

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Diamond-like semiconductors (DLSs) are compounds whose structures are derived from either the cubic or hexagonal form of a diamond. DLSs are versatile and have many potential technological applications. Several DLSs are commercially available in photovoltaics and nonlinear optic applications. DLSs are also of interest for their potential use in thermoelectric materials. Through the use of the WIEN2k computational software package, the electronic structures of various quaternary DLSs were determined, most notably density of states (DOS) and band structure. This program utilizes the full-potential linearized augmented plane wave (FP-LAPW) method of density functional theory (DFT) to perform electronic structure calculations on extended solids, such as DLSs. It has been hypothesized that a change in the tetravalent metal of the compound will affect the band gap accordingly. This is due to a rationale surrounding the impact of crystal radius and orbital overlap on the valence/conduction band of extended solids.

79

Analysis of Sex-Based Differences in a Mouse Model of Stress-Induced Analgesia

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Stress is known to enhance pain under chronic conditions, while acute periods of stress can suppress pain. Stress-induced analgesia (SIA) occurs when somebody experiences pain suppression during a stressful event. This phenomenon has been well documented in humans, particularly in soldiers and professional athletes. Recent studies have drawn attention to the presence of sex differences in animal research, including pain. Here, we investigated sex-based differences in a mouse model of SIA. Male and female mice were restrained to induce stress before receiving a formalin paw injection, a common inflammatory pain model. Behavioral assays were used to assess mechanical spontaneous behavior and mechanical hypersensitivity. On the molecular level, the signaling molecule extracellular signal-regulated kinase 1/2 (ERK1/2) was analyzed in the central nucleus of the amygdala (CeA) in the brain. The CeA is known to integrate information about stress and pain and ERK1/2 is phosphorylated (i.e. activated) three hours after formalin injection.

80

Genomic Analysis to Detect Convergent Adaptation to Marine and Subterranean Environments

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All organisms are the product of a large range of selective pressures determined by their environments. We have created a platform to analyze 58 mammalian genomes to identify genes that experienced shifts in selective pressure during adaptation to a specific environment. We have applied the platform to identify candidate genes that show altered evolutionary rates in response to marine and subterranean environments. In agreement with our predictions, these candidates were significantly enriched in for function in visual perception in subterranean mammals and epidermal development and muscle physiology in marine mammals. Interestingly, we found additional enrichments of immune genes in subterranean mammals and olfactory genes in marine mammals, suggesting other adaptations and changes to genetic pathways associated with these environmental shifts. Future efforts will characterize the presence of positive selection among these candidate genes and apply our platform to a wider array of environmental changes and species.

81

A Biochemical Analysis of Cyclin-Dependent Kinase 5 Regulatory Subunit 2 mRNA G-quadruplex Structures and Their Role in the Pathogenesis of Fragile X Syndrome

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In silico energy modeling has shown that guanine-rich regions of certain nucleic acids are capable of forming secondary structures known as G-quadruplexes. These structures are often subject to unique protein binding and therefore encourage gene regulation throughout both transcription of DNA and translation of messenger RNA. Such regulation implicates G-quadruplex-containing nucleic acids as probable components in the pathogenesis of genetic disease. We have selected a guanine-rich portion of the mouse cyclin-dependent kinase 5 regulatory subunit 2 (*CDK5R2*) mRNA 3' untranslated region for the study of regulatory G-quadruplexes. Circular dichroism spectroscopy, ^{1}H-nuclear magnetic resonance spectroscopy, UV spectroscopy, and polyacrylamide gel electrophoresis (PAGE) were utilized to confirm the presence of and characterize G-quadruplex structures in the selected sequence. Additionally, PAGE binding assays were used to illustrate the binding of fragile X mental retardation protein, which plays a major role in the development of the genetic disorder fragile X syndrome, to *CDK5R2* mRNA.

82

Influence of Competitive, Attractive, Ground State, Complex Interactions on the Stereochemical Outcome of Diels-Alder Reactions of Enals Catalyzed by Group 13 Chiral Lewis Acids

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Group 13 chiral Lewis acids (X = B, Al, Ga) complexed with substituted enal dieneophiles have been used in asymmetric Diels Alder reactions; however, the factors that influence stereochemical control are not yet well understood mechanistically. One factor, a "formyl hydrogen bond" between a boron Lewis acid and the formyl hydrogen of an enal, has been proposed to contribute to selectivity through the formation of a rigid bidentate complex. A new factor, a novel competing interaction between the enal vinylic alpha-hydrogen and a boron Lewis acid is now also proposed. Second-order Moller-Plesset theory and M06-2X density functional with Dunning basis sets, and semiempirical methods have been used to study these two bidentate complexes. The new, previously unconsidered, interaction and factor is found to compete with the formyl hydrogen bond in the ground state complex depending upon the ring size and strain inherent in the chiral Lewis acid enal complex.

83

The Investigation of the Presence of Organic GSR on SEM Stubs

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Various extraction methods (100% methanol; 50% acetone/50% water (v/v); 100% acetonitrile; 75% isopropanol/ 25% water (v/v); and 50% acetone/50% acetonitrile (v/v)) were tested to determine the ideal method for extraction of organic gunshot residue (GSR) from scanning electron microscope (SEM) stubs. The ideal method was based upon the percent recovery of the seven standards investigated (Akardite II Solid, Ethyl Centralite, Methyl Centralite, and Single Based Gun Surveillance, which has four components of its own which include diphenylamine(DPA), N-nitrosodiphenylamine(N-NO-DPA), 4-nitrodiphenylamine (4-NO_2-DPA), and 2-nitrodiphenylamine (2-NO_2-DPA). These standards were quantified by the Liquid Chromatography/ Mass Spectrometry (LC-MS/MS).

84

Stability of Self-Assembled Monolayers of Organic Acids on Cobalt

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Self-assembled monolayers (SAMs) are molecular assemblies formed spontaneously on metal oxide surfaces by adsorption. The head groups of the adsorbing molecules strongly bind to the metallic surface. This project is focused on determining the feasibility and conditions for forming self-assembled monolayers of phosphonic acid on cobalt oxide. Samples were prepared using solution deposition. The concentration for the solution was 0.017 g of ODPA. The total time of deposition for success was 1 hour. The surfaces were analyzed with infrared spectroscopy, which indicated that the monolayers formed. To make sure that the monolayers were stable, the cobalt coupons went through a rinse in THF, HCl, or NaOH and were then sonicated. The hydrophobicity of the SAM-modified surface was determined by using contact angle measurement.

85

Organic Synthesis of Novel SSRI Analogues

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The serotonin transporter protein (SERT), a member of the neurotransmitter sodium symporter family (NSS), functions as a homeostatic regulator via reuptake of serotonin from the synaptic cleft into the presynaptic cell. The inhibition of SERT function is of primary interest in the treatment of depression and anxiety disorders. There is no documented high-resolution crystal structure of SERT to date. As such, the crystalline structure of the bacterial homolog of SERT, LeuT, was utilized in the development of a protein-based pharmacophore. Virtual screening (VS) of a small molecule structural library using this generated SERT computational model yielded a novel selective serotonin reuptake inhibitor (SSRI) candidate ligand, SM11. Novel synthesis schemes for SM11 analogs are developed in order to yield high purity compounds. Analog binding affinity is then evaluated via competitive membrane binding assays. Results of the binding assay are used to elucidate the drug binding site.

86

Optimization of a Mixed Resolution Monte Carlo (MRMC) Model of Estrogen Receptor Alpha (ER-α)

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Molecular docking, a method that predicts the orientation of a molecule and its target, can computationally screen thousands of drug candidates. One of the current challenges in docking is the inclusion of the natural flexibility of receptors in a computationally affordable way. A mixed resolution Monte Carlo model of estrogen receptor alpha, which combines all-atomistic detail in the ligand binding domain with coarse-grained efficiency in the scaffold, has been developed as a test case for the flexible receptor problem. “Successful” docking is recorded when the ligand returns to the crystal pose after having been randomly rotated. Optimal run time, types of trial moves, and trial move schedule were determined, using estradiol as the ligand and a root mean squared deviation cutoff of 1.5 A for successful runs. The final energy of the system, self-similarity, and cluster size were explored as potential predictors for key ligand poses.

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Ab initio dynamics of the unfolding and decarboxylation of carboxyphosphate in aqueous solution

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Carboxyphosphate is a key intermediate in de novo purine and pyrimidine biosynthesis. Inhibiting this pathway is a novel idea that could lead to the creation of new antifungal and antimicrobial agents. The extremely short half-life of carboxyphosphate makes it difficult to study experimentally. The decarboxylation mechanism is currently unknown, but it is hypothesized to begin with all conformations funneling to the pseudo-chair monoanion conformation; the pseudo-chair will then unfold to the linear conformation and the C-O bridge bond will elongate yielding CO_2 and P_i. Ab initio dynamics simulations were performed, using the TeraChem program, on the pseudo-chair monoanion and dianion with the B3LYP/6-31G(d) functional. Carboxyphosphate was placed in a sphere of ~100 waters with spherical boundary conditions. The simulations have run for 40 ps; conformational changes of carboxyphosphate have been observed. These simulations were also performed using TIP3P for the waters. These results were compared back to those of the QM simulations.

88

Analysis of Crz1-mediated gene regulation in response to inhibition of sphingolipid biosynthesis.

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In *Saccharomyces cerevisiae,* the Crz1 transcription factor is involved in the regulation of calcium ion homeostasis. Results from our laboratory have also linked activation of Crz1 to altered sphingolipid biosynthesis. To confirm this linkage and to identify genes involved in the process, we employed a plasmid with a promoter region containing Crz1 binding sites is linked to *LacZ.* A wild type strain bearing the plasmid was treated with the drug myriocin, which inhibits sphingolipid biosynthesis. The resulting increase in β-galactosidase activity confirmed that disruption of sphingolipid biosynthesis activates Crz1. To identify other genes that are involved in the process, we are employing yeast strains bearing single gene deletion mutations and comparing those results to the wild type strain. We are testing strains harboring deletions in genes involved in calcium metabolism (*MID1, CCH1,* and *YVC1*) and phosphatidylcholine biosynthesis (*OPI3* and *CHO2*). These results will further our understanding of Crz1-mediated gene expression.

89

Quantum Models of Methylphosphonate Adsorption onto the Rutile (110) Surface

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Modification and functionalization of TiO_2 surfaces by adsorption of phosphonic acids is of great interest in view of its applications in biomaterials and corrosion protection. Indeed, experimental studies indicate strong and stable P-O-Ti bond formation during adsorption of phosphonic acid on TiO_2 surfaces. However, the mode and strength of adsorption continues to be debated. We have investigated the adsorption modes and bonding strength between the rutile (110) surface and methylphosphonate using quantum chemistry with periodic boundary conditions. The Crystal09 quantum software package was used with the Perdew-Burke-Erzerhof-0 functional and the STO-3G basis set. The surface free energy and structure, ligand binding energy and structure, and vibrational spectrum were computed. The computations indicate tridentate bonding between the rutile (110) surface and methylphosphonate, which is consistent with experimental data from FTIR spectroscopy. Understanding the mode and strength of adsorption can lead to a new generation of biomaterials that could withstand corrosion and prevent biological rejection.

90

Quantum Modeling of Alkyl Carboxylic Acids Adsorbed to α-Al_2O_3(0001) Surface

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Department of Chemistry, Slippery Rock University

Sapphire is a crystalline form of aluminum oxide (Al_2O_3) and due to its remarkable hardness; it is used for highly durable bearings in precise electronic and optical instruments. Coatings to minimize frictional drag forces are necessary, yet a framework that describes the control of frictional force through surface modification has not been reported. In our collaboration, the adsorption of acetic acid and its derivatives on the (0001) surface of α-Al_2O_3 has been studied using *ab initio* quantum calculations in CRYSTAL09. Two-dimensional slab models that were periodic in the xy plane were developed using density functional theory, specifically the Perdew-Burke-Erzerhof functional, and Pople basis functions. Our surface energy and ligand adsorption energy are consistent with experimental data. The preliminary data indicates that even and odd alkyl chain lengths of carboxylic acids adsorbed on a α-Al_2O_3(0001) surface produce a differential in tail packing resulting in differences in terminal carbon density that ultimately produces measurable changes in frictional drag forces.

91

Molecular Dynamics Modeling of Noncanonical Structures of RNA

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In neurological disorders ALS and FTLD,the formation of noncanonical RNA structures from truncated transcipts of DNA have been identified as a significant factor in malfunctioning neuronal cells. Prior research has investigated the primary structures related to the progression of these disorders, but better understanding of these findings require atomistic detail. I have explored using computational tools to model the potential structures' interactions within their native environment. From these built structures, I used metadynamics-assisted molecular dynamics for data analysis to evaluate the free energy surface of these conformations to explore some of their attributes. This will help to determine possible role of the G-quadruplex conformation, which has been shown to heavily influence progressive neuronal death, in being more active in docking interactions and in its rate of proliferation.

92

Self-Diffusion Activation Energies of 1-methyl-3-pentylimidazolium chloride using Compensated Arrhenius Equation with Molecular Dynamics

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If ionic conductivities can be increased, ionic liquids could replace volatile electrolytes currently used in lithium ion batteries. Molecular Dynamics simulations have been performed to investigate the structure and dynamics of 1-methyl-3-pentylimidazolium chloride at different temperatures. The dynamics of the system were characterized by defining the mean squared displacement (MSD) from the dynamics trajectories. Diffusion coefficients were determined using the Einstein equation for diffusion over a distance and compared to published experimental values. A compensated Arrhenius formalism that scales out the temperature dependence of the dielectric constant in the exponential prefactor was then used to determine the activation energy for diffusion.

93

The Kalman Filter Applied to Glucose Levels in Critically Ill Patients

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[3]: The CRISMA (Clinical Research, Investigation, and Systems Modeling of Acute Illness) Laboratory, Department of Critical Care Medicine, University of Pittsburgh

Many critically ill patients suffer from fluctuating blood glucose levels, leading to hypoglycemia and/or hyperglycemia which can worsen health outcomes for these patients. Targeted Glycemic Control (TGC) can help to improve such outcomes. A critical challenge in controlling blood glucose is the reliability of subcutaneous sensor measurements. Continuous Glucose Monitors (CGM) yield noisy and potentially biased measurements. 24 patients underwent simultaneous measurement using two CGMs, and the raw signals were processed using original and adaptive Kalman filters to fuse the CGM data into a single, smoothed glucose measurement. Kalman filter effectiveness was tested by analyzing the residuals between the filtered glucose measurements and more accurate, but less frequent, fingerstick measurements. The Kalman filters improve signal accuracy and could be used to drive a TGC algorithm.

94

Self-Diffusion Activation Energy for 1-Methyl-3-Pentylimidazolium Tetrafluoroborate with Compensated Arrhenius Equation from Molecular Dynamics Simulation

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Ionic liquids are potential replacements for polymer electrolytes currently used in lithium ion batteries. Increasing their ionic conductivities by reducing activation energies for diffusion would make ionic liquids viable battery materials. Recent theory has addressed the temperature dependence of organic liquid electrolytes by suggesting that the non-Arrhenius behavior exhibited by their conductivities is due to a temperature dependent prefactor. This has led to the proposal that ion transport in organic liquid electrolytes is governed by a single activated process. This research applies the compensated Arrhenius equation to diffusion of the ionic liquid 1-methyl-3-pentylimidazolium tetrafluoroborate ([MPIM+][BF4]). Diffusion coefficients of [MPIM+][BF4-] are calculated by means of the Einstein equation for diffusion over a distance using mean squared displacements vs. time obtained from molecular dynamics simulations. The calculated diffusion coefficients calculated at several different temperatures are compared to experimental values and used to calculate the activation energy for diffusion.

95

The Messenger RNA p250GAP G-Quadruplex Secondary Structure Biophysical Classification and RGG box Domain/ISO1 Interaction

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The gene that encodes for p250GAP is found on chromosome 11 and encodes a protein belonging to the RhoGAP family which affects the plasticity of neurons, specifically in the brain. It is hypothesized that mRNA p250GAP interacts with the Fragile X Mental Retardation Protein (FMRP), a protein linked to Fragile X Syndrome, the most common form of inherited mental impairment. FMRP uses its arginine-glycine-glycine (RGG) box to interact within its mRNA targets, named a G-quadruplex. To confirm first the presence of a G-quadruplex in p250GAP mRNA, a series of biophysical techniques were employed including 1H NMR spectroscopy, CD spectroscopy, UV spectroscopy, and native PAGE gels. Following these experiments, fluorescence spectroscopy and native PAGE were used to quantify the interactions of p250GAP mRNA G-quadruplex with the RGG box domain and full length FMRP.

96

Road Salt Effect on Stream Chloride Levels

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The chloride concentration throughout the Pine Creek Watershed is far above the EPA recommended standard and as a result aquatic life in the system is being stressed. It is twice as high as neighboring watersheds and it is not known why. The goal of my project is to determine whether these high concentrations are due to road salt. I tested at 9 sites on Pine Creek from its headwaters to its outflow into the Allegheny River. Chloride concentration consistently increased by over 50% at all test sites and as much as 300% at some sites after snowfall occurred and salt was added to the roads. This indicates that road salt contributes to the high levels of chloride. This data is being extended to include stream flow data and impervious surface analysis which will assist in further confirming that road salt is a factor in raised chloride concentrations.

97

Porosity Improvements in Electrospun Synthetic Vascular Grafts using Porogens and Surfactants

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Electrospun scaffolds are promising for vascular grafts due to their easy implantation and regenerative abilities. However, the low porosity of electrospun materials limits cell infiltration and tissue development. We hypothesized that using solid porogens and surfactants in spinning solutions would increase porosity by increasing the space between fibers. We sought to improve porosity by suspending salt crystals in the spinning solution and later leaching them out of the graft to create pores. SEM micrographs revealed that salt particles were spun into the graft, but salt also reduced fiber collection efficiency. We then used sodium dodecyl sulfate (SDS) and ammonium lauryl sulfate (ALS) to decrease fiber surface resistance enabling fibers to discharge rapidly and reducing close packing due to electrostatic attraction. Although the salt porogens proved impractical, ALS appears to increase porosity without compromising spinning efficiency. We are currently assessing porosity of the ALS grafts through SEM and gravimetric analysis.

98

Segregation in a rotating drum mixer: density segregation and segregation of non-spherical particles

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Segregation is one of the most important problems in the processing of granular materials. Segregation occurs when particles have different mechanical, physical or chemical properties; some examples of typical properties that may differ in industrial settings include density, size, shape and cohesion. The case of particles with different shape is very common in industry, but is not well studied. In this poster we experimentally study a prototypical example of shape-based segregation using particles that are a mixture of spherical and cylindrical shapes. Additionally, we computationally examine the impact of cohesion on segregation. We study cohesion that is base don the attraction between particles that is caused by a small amount of liquid binder at the contact spots. Specifically, we study the impact of cohesion on density segregation of particles using the Discrete Element Modeling (DEM). Comparisons of our computational results to a newly proposed model will be presented.

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First principles modeling of radium in calcite and barite for fracking wastewater remediation

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University of Pittsburgh

Natural gas extraction by hydraulic fracturing (fracking) can release naturally occurring radioactive materials (NORMs) from underground via fracking wastewater. A potential remediation method is to absorb the NORMs into a mineral solid which can then be safely disposed, but the mechanisms by which NORM absorption occurs is not presently understood. As a starting point to understand these mechanisms, we carried out first principles quantum mechanics studies to predict how radium binds within two candidate wastewater remediation materials, calcite and barite. Structural details from state of the art Kohn-Sham density functional theory calculations are reported as well as progress placing Ra interstitially in the bulk materials. This work lays the foundation for future studies on radionuclide absorption into minerals.

100

Solar Energy Harvesting

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Swanson Engineering
University of Pittsburgh

The topic of our research is solar-electricity and solar-fuel conversion using surface plasmons. One approach for greater efficiency is to enhance the light absorption of new types of plasmonic particles. To effectively apply surface plasmons to DSSCs, it is essential to explore the physical interactions among surface plasmons, solar light modulation, and carrier/exciton generation in the nanostructured films. The optical resonances and the near electromagnetic field response can be tuned by changing the dimension of the core and shell components. The incorporation of plasmonic particles consisting of metallic nanoshells enlarges the optical cross-section of dye sensitizers coated onto the photoelectrode and increases the energy conversion efficiency of DSSCs. The enhanced photon-electron conversion is attributed to tunable surface plasmons of the nanoshell.

101

Fabrication and Characterization of Multicomponent Particle-based Crystals

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Colloidal crystals are arrays of organized particles used in fields such as catalysis, photonics and optical sensing due to their potential for higher surface area to volume ratios, small inner-pore sizes and surface patterning. These crystals are typically composed of particles on the nano- and submicron-scales and formed from single or multi-sized particle populations. Most research regarding fabrication of multicomponent colloidal crystals has been executed with nanoparticles; however, for biomedical applications, increasing mass transport due to a larger (micron-scale) pore structure may prove advantageous. However, micron-sized particles are challenging to organize on a three-dimensional level. To produce these multicomponent crystals we have developed a unique fabrication method introducing ultrasonic energy to the particles, allowing them to self-assemble into a crystalline configuration. With this composite material we hypothesize we will be able to create an ordered porous material and study its mechanical properties for biomedical applications.

102

Computational Modeling of Filtration Fundamentals

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In the chemical industry today, filtration can play an important role, from clarifying a material to removing unwanted by-products. Knowing exactly how to filter a product and how to do it consistently can be an art that takes many trial and error attempts to perfect. This work aims to develop a computational model that combines the fluid flow dynamics of the Lattice Boltzmann Method (LBM) and the particle interaction schemes of the Discrete Element Method (DEM) in order to model filtration in lab-scale equipment. Results that include pressure versus flow as a function of filter cake height for a variety of filter cake geometries will be collected. In order to test the validity of the LBM-DEM method, follow-on work that will compare simulated results to an experimental system that is currently under construction will be conducted.

103

Understanding the Early Stages of Metal Nanoparticle Growth Through Density Functional Theory Calculations

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Metal nanoparticles are unique in their diversity of technological applications, ranging from active catalysts for energy generation to drug delivery carriers in medicine. Since nanoparticles physiochemical properties are directly related to their structural characteristics, our aim is to gain a fundamental understanding of the metal nanoparticle growth mechanisms. Specifically, we use Density Functional Theory calculations to investigate the early stages of Au and Cu metal growth when coordinated with thiolate-groups (capping agents). Solvent effects have also been accounted in our study. Our results demonstrate a thermodynamic preference to the formation of the $Au_4(SCH_3)_4$ and $Cu_4(SCH_3)_4$ species (tetramers) which exhibit high stability. Regarding the bimetallics formation, we show that the metal-thiolate complexes can be will mixed forming bimetallic structures even at these early stages of growth.

104

Fabrication and Optimization of Deep UV Photonic Crystals

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University of Pittsburgh

We are investigating different synthetic conditions of highly charged silica nanospheres which we use to create photonic crystal wavelength selecting devices. These photonic crystals consist of a crystalline colloidal array of small (30-45 nm diameter) silica nanospheres which are highly monodisperse in size and charge. The current goal is to optimize the size and charge of the particles in order to improve the diffraction properties of our photonic crystals i.e. strong diffraction with a narrow bandwidth. These particles were functionalized with strongly acidic groups, resulting in a high negative surface charge. This high charge leads to electrostatic repulsion between nanospheres and self-assembly into face centered cubic photonic crystals which Bragg diffract a narrow wavelength region of UV light.

105

REGENERATING COMPOSITE LAYERS FROM SEVERED NANOROD-FILLED GELS

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University of Pittsburgh

Building upon our previous efforts to design a self-regenerating polymer gel utilizing interfacially-active nanorods, we explore a method to regrow a polymer matrix with embedded nanorods which better resembles the uncut material. When the regenerated gel layer reaches certain heights, we observe that the nanorods localized at the interface break free and consequently diffuse into the regrowing gel. With these nanorods dispersed in the new gel, we form a nanocomposite polymer matrix. In order to compensate for the loss of the interfacial nanorods that served as anchors, we introduce a new cross-linker into the original gel that forms bonds with the active chain ends of the regrowing gel. These covalent bonds bridge the cut gel and regenerated layer, creating a coherent system. The strength of the interface can be tuned by varying system parameters, and a uniform degree of cross-linking throughout the entire gel can be achieved with optimal parameters.

106

Understanding Adsorption on Bimetallic Nanoparticles with Computational Chemistry Theoretical Calculations

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University of Pittsburgh

The interactions of molecules (known as adsorbates) with nanoparticles are key in the performance of nanoparticles in any technological application. One can fine tune the adsorbate-nanoparticle interactions by changing the nanoparticle morphologies, such as, their size, shape and metal composition. In this project, we used Density Functional Theory calculations to investigate the adsorption of CO and CO_2 on Au-based bimetallic nanoparticles as a function of metal composition. The decoration of Au_{13} nanoparticles with other metals can result in surprising differences in adsorption energies. As an example, we observed seven times higher adsorption energy of CO_2 on $Au_{12}Zr$ in comparison to the monometallic Au_{13} cluster. This work provides a fundamental understanding of adsorption on bimetallic nanoparticles and potential guidelines for the efficient capture of the environmentally harmful gases CO and CO_2.

107

Electrospun Nanofibrous Materials as Electrodes in Li-S and Na-Ion Batteries

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With global energy demands on the rise, much research is ongoing into the field of batteries as energy storage devices. Whether it is a handheld device or larger electric vehicles, storage needs are currently met with the lithium-ion battery (LIB) technology. LIB technology is limited in energy density and there is a need to explore new materials' chemistries with greater theoretical specific energies to complete the transition away from fossil fuels. This work investigated several nanofibrous materials as potential electrodes in lithium-sulfur (Li-S) and sodium-ion batteries (SIB). Using electrospinning technique, polymerized nanofibrous mats containing sulfur (for Li-S) and tin (for SIB) were created. Electrospun fibers are preferred due to their high area/mass ratio and the ease of creating conductive composites. Following characterization of the mats by SEM and XRD, the materials were tested for battery cycling stability, areal capacity and rate capability in a two-electrode coin cell.

108

Investigating Effect of Encapsulation on Pancreatic Differentiation of Human Embryonic Stem Cell

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2 Department of Bioengineering
3 McGowan Institute of Regenerative Medicine
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Type 1 Diabetes is an autoimmune disease affecting millions of people worldwide, resulting in the loss of insulin producing beta cells in the pancreas, causing insulin deficiency. There is a critical need for a renewable source of insulin producing cells. Human embryonic stem cells (hESC) have been distinguished by their unique ability to differentiate to any cell type in the body. These pluripotent stem cells can give rise to the endoderm layer and are further matured to insulin producing beta cells. A previous project in our lab showed that the use of calcium alginate encapsulation of hESCs for mature enhanced mature differentiation compared to differentiation on tissue culture plastic. In this work we investigate the effect of commonly used alginate capsule compositions on pancreatic differentiation of hESCs. It is necessary to optimize both pancreatic differentiation with the barrier capacity of alginate capsules for implantation for type 1 diabetes treatment.

109

Quantifying Regional Intratumor Tissue Heterogeneity

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University of Pittsburgh

Prior to comprehensive genetic profiling techniques, cancer-specific tumors were expected to be similar regardless of the patient. Surprisingly, not only were tumors significantly different among patients, but tumor tissue also consisted of chemically diverse cancer cells, known as intratumor heterogeneity (ITH). Furthermore, surviving (potentially metastatic) cancer tissue tends to be significantly different from the pre-existing tissue. Therefore, iterative personalized cancer treatments may effectively combat such an adapting disease. Through genetic testing and in situ imaging of tissue sections via fluorescence-based immunohistochemistry, the spatial distribution of specific biomarkers within a cancer cell can be visually expressed. In this work, the ITH spatial distribution was analyzed via Gaussian mixture models. It is expected that such analysis will reveal regional relationships among biomarker expressions. Essentially, ITH spatial pattern recognition in cancer tissue may aid clinicians' diagnosis and prognosis, and perhaps ease the development of personalized cancer treatments.

110

Rule-Based Modeling of B-Cell Receptor Clustering

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Transmembrane B-Cell Receptors (BCRs) can bind to extracellular antigens with high affinity and specificity, and initiate a signaling cascade leading to an immune response. While the cytoplasmic signaling components of B-Cells have been elucidated, the mechanism by which antigen binding transmits a signal across the plasma membrane is poorly understood. Several studies have shown that antigen induced clustering of BCRs on the plasma membrane is critical for B-Cell activation, suggesting that spatial reorganization is the mode of signal transmission. Experimental evidence has implicated the Cμ4 ectodomain of BCRs in their clustering, but no model has been reported which explains this phenomenon in detail. We have developed a rule-based model to describe how cooperativity between antigen binding BCRs and BCR dimerization at this domain leads to the formation of higher order oligomers. Using Monte Carlo simulations in the MCell software suite, we tested our model and statistically characterized the degree to which cooperativity leads to BCR clustering.

111

Dengue Fever

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Dengue is a mosquito born human disease with an increasing incidence worldwide and has been reported in the southern US. Dengue is usually self-limited, but there is a significant chance of the disease being severe, requiring hospitalizations. Using existing clinical data from Brazil, we create statistical models to predict the probability that a patient will develop severe disease when initially presenting with Dengue. From these models, a score will be constructed to guide clinical decisions before the onset of severe Dengue fever. The data included symptoms, environment information, and family information. As a first step, we created as a first step a logistic regression model to predict whether a patient had a previous episode of dengue. Decreasing age, the presence of a headache and fever significantly increased the likelihood that the current episode was a primary infection. Models examining the likelihood of developing severe dengue are currently under development.

112

Exploring Surface Mediated Polymer Electrolyte and Nanostructured Calcium Phosphate Composite (NanoCaPs) Layers for Non-Viral Gene Delivery

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Surface mediation using multilayer polyelectrolyte assembly (MPA) is a promising approach being developed for gene delivery, but is hindered by low transfection rates. Biodegradable NanoCaPs are efficient at binding and condensing the pDNA, improving transfection. Incorporating NanoCaPs into the MPA fabricated using a cationic polymer and an anionic polymer can also provide controlled release of pDNA creating the potential for nucleic-acid based therapies. In the current work, polyethlenemine (PEI), a cationic polymer and an anionic polymer are used to build up bi-layers on Ti substrate. Fluorescent microscopy was employed to visualize cells transfected with NanoCaPs encapsulating pDNA coding for green fluorescent protein (GFP). In addition, transfection was quantified using flow cytometry. Furthermore, the morphology of the substrates were analyzed using scanning electron microscopy (SEM). Initial results demonstrate that enhanced transfection can be achieved using MPA incorporating NanoCaPs and that the transfection increases with prolonged culture.

113

Spatial and Temporal Patterns of Lung Granulomas during *Mycobacterium tuberculosis* infection in Non-human Primates

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Tuberculosis, due to *Mycobacterium tuberculosis (Mtb)* infection, kills 1.5 million people every year. Lung granulomas, localized areas of Mtb infection, are dynamic and independent from one another and their progression determines infection outcome. Little is known about how granulomas are distributed throughout the lung and how they progress over time. Using serial data from PET CTs of macaques infected with Mtb, we investigated the spatial distribution of granulomas. We assessed the proximity of granulomas to major lung airways, other pre-existing granulomas and positional distribution of the lungs in of each animal during infection. These observations show the disease concentrating itself posteriorly and close to the airways. As the disease progresses, it spreads outwards to every part of the lung. We developed a probability model to predict where new granulomas would form during reactivation after TNF-neutralization. These findings help us better understand how Mtb spreads within the lungs during infection.

114

Validation of a systems model for human bronchial epithelial cells with and without Cystic Fibrosis

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Cystic fibrosis (CF) is an autosomal recessive disorder caused by defects in the CF transmembrane conductance regulator (CFTR) gene, leading to absent/malfunctioning chloride channels on the airway epithelium and upregulation of sodium absorption. We seek to measure liquid and solute transport in a human bronchial epithelial (HBE) cell model in order to support the development of a systems model of airway epithelial physiology. Using a small radiolabeled molecule, DTPA, we can quantify airway surface liquid (ASL) volume changes in CF and non-CF HBEs. Experiments used basolateral ouabain (an inhibitor of sodium absorption) or apical or basolateral mannitol addition to modulate ASL absorption rates. In vitro, apical mannitol addition slows DTPA clearance (while basolateral addition increases clearance) by creating a transepithelial osmotic gradient, determining direction of water absorption. This creates a zero-convection case to determine whether permeability differences exist between CF and non-CF epithelia, augmenting the accuracy of our systems model.

115

Utilizing an Interactive Educational Module to Teach Middle School Students about Diabetes

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[2] Engineering Education Research Center, Swanson School of Engineering, University of Pittsburgh

In the United States, currently 25.6 million individuals have diabetes. Between 1988 and 2008, the number of individuals with diabetes increased by 128%, a trend that could lead to 1 in 3 Americans being diabetic by 2050. Most tellingly, 90-95% of the current diagnoses are for Type II diabetes where the number one risk factor is obesity. This risk factor may be minimized through maintenance of a healthy diet. Utilizing an interactive educational module based upon a diabetes computer model, we propose to show middle school students the impact foods can have on their blood sugar levels. This module will be accompanied by a lesson plan that discusses the risks associated with diabetes, how to read nutrition labels, and the importance of a healthy diet. Through this form of education we seek to help students understand their health better and how they can take an active role to avoid diabetes.

116

Material characterization of ion-doped magnesium phosphate systems

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Tri-magnesium phosphate (TMP) based powders have novel application as bioceramics. In order to more closely mimic the chemical structure of the mineralized bone matrix and improve functionality as a biodegradable and osteoconductive scaffold, TMP powders were doped with calcium and strontium ions via an aqueous, pH controlled precipitation reaction. The resulting powders were then heat treated in order to compare the material properties of both the as synthesized and thermally altered phases. Preliminary analysis using X-ray diffraction spectroscopy (XRD) indicates an amorphous as synthesized phase and a multiphasic structure after thermal treatment for all doped samples, suggesting a nonideal ionic substitution. Further studies including Fourier transform infrared spectroscopy (FTIR), SEM imaging, and thermogravimetric analysis/differential scanning calorimetry (TGA/DSC) were also performed in order to produce a more in depth material characterization. Preliminary cell culture studies assessing metabolic activity and cellular viability were also conducted in order to develop a basis for cytocompatibility.

Colleges and High Schools Represented at the 2014 Summer Undergraduate Research Symposium

Allegheny College
Boardman High School (Ohio)
Carnegie Mellon University
Case Western Reserve University
Chartiers Valley High School
Chatham University
Duquesne University
Franciscan University of Steubenville
Gettysburg College
Grove City College
McKeesport Area High School
Mt. Lebanon High School
North Allegheny High School
North Carolina A&T State University
Northeastern State University (OK)
Pennsylvania State University
Slippery Rock University
Smith College
St. Francis University (PA)
St. Vincent College
Sto-Rox High School
Susquehanna University
Swarthmore College
Syracuse University
Tennessee State University
The College of New Jersey
Universidad Metropolitana, San Juan, Puerto Rico
University of Ljubljana
University of Nebraska at Kearney
University of Pittsburgh
University of Pittsburgh at Johnstown
University of Puerto Rico, Mayaguez
University of South Carolina
University of Texas at Austin
Washington and Jefferson College
Wayne State University
West Mifflin High School
Yale University

Notes