The 2012 Summer Research Symposium

Sponsored by

The Bayer School of Natural and Environmental Sciences

Keynote Address:

S. James Gates, Jr., Ph.D.,
John S. Toll Professor of Physics and Center for String and Particle Theory Director,
University of Maryland
“Uncovering the Codes for Reality”

Friday, July 27, 2012
9:00 a.m. – 4:00 p.m.
Bayer Learning Center & Mellon Hall of Science
Duquesne University
Pittsburgh, PA
Welcome to the 2012 Summer Undergraduate Research Symposium!

It is a pleasure and privilege to welcome you to today’s 15th 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,

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

Schedule:

9:00 AM Registration and Poster Set-Up
Continental Breakfast
Mellon Patio, Academic Walk Side
Rotunda, Bayer Learning Center

10:00 AM Welcome and Keynote Address
Pappert Hall, Bayer Learning Center

11:00 AM Plenary Session (Student Presentations)
Pappert Hall, Bayer Learning Center

1:00 PM Picnic Lunch
Mellon Patio, Bluff Street Side

2 – 4:00 PM Poster Session
Mellon Patio, Academic Walk Side

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Instructions to Authors:

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

Authors presenting talks during the Plenary Session should report to Pappert Hall no later than 9:15 a.m. A tech assistant will be available to download your PowerPoint presentation.
10:00 AM Welcome
David W. Seybert, Ph.D., Dean, Bayer School of Natural and Environmental Sciences, Duquesne University

10:10 AM Keynote Address
S. James Gates, Jr., Ph.D., John S. Toll Professor & Director of Center for String & Particle Theory, Physics Department, University of Maryland
“Uncovering the Codes for Reality”

11:00 AM Student Presentations

Daniel Spagnolo
Computational Assessment of Cardiac Hypertrophy in Zebrafish
Department of Chemical & Petroleum Engineering, University of Pittsburgh

Matthew DeStefano
Interdigital Alkylations: A Study of Stereochemical Control
Department of Chemistry and Biochemistry, Duquesne University

Emily Speranza
Image Analysis of Mitochondria Texture in Response to Shear Stress in HGPS Patients
Department of Chemical Engineering, Carnegie Mellon University

11:45 AM Short Break

Joseph Gault
Design and Implementation of High School Chemistry Labs Utilizing Remote Scanning Electron Microscopy
Department of Chemistry and Biochemistry, Duquesne University

Kate Rodriguez
Surface Functionalization of Zinc Oxide Nanoparticles via the Attachment of Organic Acid Self-Assembled Monolayers
Department of Chemistry, Washington & Jefferson College

W. Ryan Parker
Conformations of PolyQ Peptides Using Metadynamics
Department of Chemistry and Biochemistry, Duquesne University

Jessica Coates
Genomic Analysis of an Emergent Pathogen: Monkeypox (MPX) virus in the Democratic Republic of Congo
Department of Computational Biology, University of Pittsburgh

Session Moderator
Ralph Wheeler, Ph.D.; Professor and Chair, Department of Chemistry and Biochemistry, Duquesne University
About Dr. S. James Gates, Jr.

Sylvester James (Jim) Gates, Jr., is the John S. Toll Professor of Physics at the University of Maryland and director of its Center for String and Particle Theory. Known for his work on supersymmetry, supergravity and superstring theory, Dr. Gates uses mathematical models to explore the elementary particles and fundamental forces of nature.

Before joining the faculty of the University of Maryland in 1984, Dr. Gates held postdoctoral appointments as a Harvard University Society of Fellows Junior Fellow and as a Research Fellow at California Institute of Technology. He currently serves as a member of the Maryland State Board of Education and the U.S. Presidential Council of Advisors on Science and Technology (PCAST).

In 1984, working with M.T. Grisaru, M. Rocek, and W. Siegel, Dr. Gates co-authored *Superspace*, the first comprehensive book on the topic of supersymmetry. He has published more than two hundred papers. Some of his research in physics has led to the creation of surprising new results in the field of mathematics, including complex manifolds, network theory, and representation theory. International aspects of his career includes appointments as a Fellow of the Stellenbosch Institute for Advanced Studies (South Africa), Professor-at-large at the University of Western Australia (Australia), and a Distinguished Research Chair of the Perimeter Institute (Canada), and a Fellow of the Institute of Physics (United Kingdom). He authored the Italian book, *L’arte della fisica*, published in Rome, and popular-level discussion entitled “Symbols of the Power,” published in the British journal *Physics World*. “Symbols of Power” describes research begun in 2004 on Adinkras, a new concept that links computer codes like those used in browsers to the supersymmetric equations of fundamental physics.

During his career, Dr. Gates has received a number of honors for his teaching, including the 1999 College Science Teacher of the Year from the Washington Academy of Sciences, the 2002 Distinguished Scholar-Teacher from the University of Maryland, and the 2003 Klopfsteg Award from the American Association of Physics Teachers. In 2006, the American Association for the Advancement of Science honored him with the Public Understanding of Science Award.

He has been featured extensively in many science documentaries on physics, most notably *The Elegant Universe* in 2003. In 2006, he completed a DVD lecture series titled *Superstring Theory: The DNA of Reality* for The Teaching Company to make the complexities of unification theory comprehensible to lay people. During the 2008 World Science Festival, Dr. Gates narrated a ballet, *The Elegant Universe*, with an online resource presentation of the art forms (called Adinkras) connected to his scientific research. The NOVA/PBS Fall 2011 presentation of the science documentary *The Fabric of the Cosmos* prominently features Dr. Gates.
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1 Zwitterion-Functionalized CNTs for Efficient Desalination
Taylor, Michael G.; Chen, Hang-yan; Johnson, Karl J.
Department of Chemical and Petroleum Engineering
University of Pittsburgh

The lack of availability of clean water for drinking and agriculture in many parts of the world is a growing crisis. Cost-effective and energy-efficient large-scale desalination of seawater is a key technology for addressing water needs for many communities. Carbon nanotubes (CNTs) offer the promise of more energy efficient desalination due to higher water flux resulting from the almost frictionless flow of water through the interior of CNTs. In our study, we have performed non-equilibrium molecular dynamics simulations on multiple saltwater systems passing through a membrane consisting of four single-walled CNTs (~1.5 nm diameter), functionalized with varying numbers of zwitterion groups, embedded between two graphene sheets. When two zwitterions are used to functionalize the CNTs, a near 100% ion rejection rate is observed, regardless of any ion solution we tested, along with high water flow rates. We conclude that zwitterion functionalized nanotubes are good candidates for improved desalination membranes.

3 Evaluation of Machine Learning Algorithms to Support Diagnosis of Lung Cancer Data
Nicholson, David1,2; Langmead, Christopher J.2
Department of Computational Biology
Carnegie Mellon University

Lung cancer is one of the most deadly diseases for both men and women. Early detection, however, dramatically improves outcomes. We hypothesize that techniques from the field of machine learning can aid in the early diagnosis of lung cancer. Thus, the two goals of this research are: (a) to identify biomarkers of lung cancer from a panel of serum analytes; and (b) to evaluate several machine learning algorithms for their ability to produce diagnostic models from the selected biomarkers. To date, we have identified panel of seven informative biomarkers (Cytokeratin 19, sE-Selectin, MIF, Prolactin, SAA, TTR, and Rantes) by calculating their information gain relative to the primary outcome of lung cancer. We are presently evaluating models constructed using several machine learning algorithms (decision trees, random forests, naïve bayes, support vector machines, and logistic regression) in terms of their overall accuracy, sensitivity, specificity, and AUC scores.

2 Genomic Analysis of an Emergent Pathogen: Monkeypox (MPX) virus in the Democratic Republic of Congo
Coates, Jessica1,3; Rogers, Matthew1,2; Ghedin, Elodie1,2
1TECBio REU at Pitt
2Department of Computational and System Biology, University of Pittsburgh School of Medicine
3Spelman College

The monkeypox virus (MPX) is a zoonotic virus largely endemic to the Democratic Republic of the Congo. Following the eradication of smallpox, cases of MPX have increased in individuals without vaccine protection against smallpox. More frequent incidences of the virus could lead to MPX becoming more virulent, occupying the niche left vacant by smallpox and potentially being able to sustain transmission without an animal vector. Primary samples, collected from individuals with confirmed monkeypox infections, were sequenced with the SOLiD (Applied Biosystems) platform; sequence gaps were closed by Sanger sequencing. Following sequencing, full genomes were assembled and analyzed for coding sequence differences, single-nucleotide polymorphisms, and phylogenetic relationships to determine the viral genetic diversity within the geographic region where the samples were collected. The sequence data are also being compared with the epidemiological information available for each of the specimens to determine whether genetic diversity can be associated with different disease outcomes.

4 Alternate Molecular Cloning of NapA from Campylobacter Jejuni: Ligation Troubleshooting
Nassif, Samih1; Stolz, John1; Basu, Partha3
1Department of Chemistry and Biochemistry; 2Department of Biological Sciences.

Campylobacter jejuni is a pathogenic bacterium which utilizes nitrate reduction for growth via a periplasmic nitrate reductase (Nap). The catalytic subunit, NapA, is a molybdenum-containing 4Fe-4S protein. Heterologous expression of NapA has been carried out. However, the presence of a 6x His-tag in the protein can be problematic. Kinetic studies of the recombinant protein reveal a low affinity for nitrate (2.2 mM), compared to native Sulfurospirillum barnesii NapA (0.29 mM). Herein alternate molecular cloning of napA from C. jejuni is presented. The empty vector, pMCSG28, contains a C-terminal TEV cleavable 6x-His Tag with Xba I and Xma I restriction sites close to one another. Problems were encountered during the T4-driven ligation steps, where transformations in 100 ug/ml Ampicillin containing LB agar plates yielded empty vector transformants. To solve this, ligation conditions including temperature, incubation time, amount of ATP and insert:vector molar ratio were tweaked to improve insertion of the gene.
5 Mechanism for alternating access in concentrative nucleoside transporter from Vibrio cholera
Giagreco, Nicholas1,3; Lezon, Timothy1,2
1TECBio REU at Pitt, Department of Computational and Systems Biology, University of Pittsburgh School of Medicine3School of Arts and Sciences, University of Rochester

Secondary Transporters regulate uptake of substrate coupled with ion transport. Crystallization of these proteins in the past decade allowed for investigation into the molecular mechanism of transport. These structural analyses revealed internal symmetries, hypothesized as integral components of their transport domain. Computational analyses of transport proteins yielded alternate conformations, supporting the theory of alternating access mechanism of membrane protein transport. First proposed in the 1960s by Peter Michel, this explains substrate access to each side of the membrane by a series of conformational changes. Experimental evidence conducted alongside these analyses confirms the existence of these alternate conformations in human homologues in vivo. With the recent crystallization of Vibrio cholerae concentrative nucleoside transporter, structural and computational analysis predicting the molecular mechanism of transport can now be conducted using implicit membrane anisotropic network models and the software package ProDy, developed at UPMC, to predict the protein dynamics of transport.

6 A Study of the Presence of Gunshot Residue in Pittsburgh Police Stations
Ali, Leah; Wetzel, Stephanie
Department of Chemistry and Biochemistry Duquesne University

Due to the risk of secondary transfer of gunshot residue (GSR) by police vehicles, stations, or officers prior to GSR sampling, it was necessary to create a baseline for the amount of GSR present at police stations or in police vehicles. Samples taken from the back of a Ross Township police vehicle, jail cell, and interview chair were manually analyzed using scanning electron microscopy-energy-dispersive X-ray (SEM-EDX) techniques for the presence of particles containing at least ten percent by weight antimony, barium, and lead. These particles were classified as unique GSR, while particles containing various combinations of lead, antimony, barium, calcium, and silicon were classified as characteristic. For a sample to be considered as positive for GSR, there must have been at least three unique GSR particles present. Thirty two characteristic and no unique GSR particles were found among the samples analyzed; consequently no samples were considered as positive for GSR.

7 Constraining the Light-to-Mass Ratio of High-Redshift Galaxies Using Satellite Dynamics
Berthoud, Kent
Department of Physics and Astronomy University of Pittsburgh

The visible matter in galaxies is not enough to account for their being gravitationally bound; this deficit is explained through aptly named, non-luminous, dark matter. Using recent data from the DEEP3 Galaxy Redshift Survey, we studied the motions of faint satellite galaxies around more luminous hosts. For these galaxies, observed as they were when the universe was at half its current age, the actual contribution of luminous versus non luminous mass is not very well known. We can better constrain the light-to-mass ratio by relating the dispersion of the satellite galaxies’ line of sight velocities to the mass of the central galaxy’s dark matter. Dark matter halos play an important role in galaxy evolution and better constraints on the dark mass help to elucidate the dark-matter/galaxy relationship.

8 Design and Implementation of High School Chemistry Labs Utilizing Remote Scanning Electron Microscopy
Gault, Joseph H.; Janicki, Emily L.; Rosmus, Kimberly A.; Larry, Nolan R.; Aitken, Jennifer A.
Department of Chemistry and Biochemistry Duquesne University

Three chemistry labs were designed to implement the use of the scanning electron microscope (SEM) in a high school classroom setting. Scanning electron microscopy uses electrons to produce magnified images of samples with a resolution on the order of several nanometers. The SEM at Duquesne University was set up for wireless access through a standard Internet connection. An introductory laboratory using a copper penny serves to introduce students to the microscope and basic techniques of microscopy. A more advanced laboratory on imaging aluminum hydroxide crystals obtained from a standard aluminum can was also designed. Morphological analyses of silvite and halite were the central focus of the final lab. The concepts of the labs include Pennsylvania State Standards, which are highlighted in the respective laboratory manuals.
9  Morphine induces conditioned place preference in mice
George, David C.; Kolber, Benedict J.
Department of Biological Sciences and Chronic Pain
Research Consortium, Duquesne University

The conditioned place preference (CPP) assay is an animal model widely used to examine learning associated with drugs of abuse. In this CPP model, based on Pavlovian conditioning, the opioid morphine (unconditioned stimulus), known for its effective analgesic properties, is continually paired with a specific physical environment (conditioned stimulus). We hypothesized that if mice were treated with morphine (10 mg/kg i.p.) once daily for 3 days and placed in a distinctive box after each injection that a preference for the morphine-associated environment would develop. Supporting this hypothesis we found that mice spent significantly more time in the morphine-paired box compared to a control-paired box (n=20, 1-way ANOVA p=0.0003). The next step in this assay is to test a new drug, Fenobam, an mGluR5 antagonist, for its possible analgesic effects.

Figures:
1. Meta-Analysis Graphs
2. 5 Day Morphine CPP setup.
3. Fenobam Analysis

11 Optimization and Production of C. jejuni Periplasmic Nitrate Reductase A
Adams, Andrew*; Magalon, Axel†; Basu, Partha*
*Department of Biological Sciences, and †Department of Chemistry and Biochemistry, Duquesne University,
Laboratoire de Chimie Bactérienne, Mediterranean Institute of Microbiology, CNRS and Aix-Marseille University,

A molybdenum containing catalytic subunit of periplasmic nitrate reductase (NapA), is hypothesized to be critical to the pathogenic bacterium, Campylobacter jejuni (Cj), in the colonization of the human intestinal tract. The overall objective of the project is to understand the structure-function relationship present in Cj-NapA. To this end, the napA gene, together with the genes for the auxiliary proteins NapL and NapD, have been cloned into plasmid vectors. In order to obtain the gene products proper, the plasmids are inserted into a strain of Escherichia coli. We have been investigating NapA expression as a function of IPTG concentration, and induction time. Once optimized, the NapA will be purified via affinity chromatography, and the quality of the protein will be assessed by SDS-PAGE followed by mass spectrometry. Herein we present the most up to date results of the project.
Multiple sequence alignments are useful for conducting phylogenetic inference and are used as a means to infer the structure and function of a protein in conjunction with previously obtained knowledge. Alignments produced by current multiple sequence alignment methods rarely produce the best model of sequence evolution, requiring hand-editing of alignments to ensure that important biological motifs are aligned. We devised a multiple sequence alignment pipeline which anchors these motifs and builds a multiple sequence alignment around them eliminating the need to hand-adjust alignments around key motifs. This alignment method produces superior alignments than native alignment algorithms.

N-acetyl cysteine protects neuronal cells from proteasome inhibition in a glutathione-independent and Hsp70-dependent manner

N-acetyl cysteine has been shown to benefit Alzheimer’s patients and is currently in clinical trials for Parkinson’s disease. Its protective mechanism of action is thought to be the enhanced synthesis of glutathione. The present study reveals that N-acetyl cysteine can protect neuronal cells from proteasome inhibition in a glutathione-independent manner. Proteasome inhibitors such as MG132 increase protein misfolding, mimicking the proteotoxicity in neurodegenerative diseases. N-acetyl cysteine caused a rise in heat shock protein 70 (Hsp70) levels when co-applied with MG132 but did not affect glutathione in our model. In contrast, inhibition of Hsp70 abolished the protection. N-acetyl cysteine reduced the MG132-induced rise in ubiquitin-conjugated proteins, suggesting that levels of misfolded proteins were considerably reduced. These findings suggest that this versatile compound can also protect cells without raising glutathione but by raising heat shock proteins and support its clinical use against neurodegeneration.

PS-PEO Nanostructures: The Effect of Spreading Solvent

Polystyrene-block-poly(ethylene oxide) (PS-PEO) is an amphiphilic diblock copolymer that phase separates into nanostructures classified as continents, spaghetti, and dots when applied to an air/water interface. The nanostructures formed can be utilized as polymer templates for particle growth and are useful in semiconductor applications. The effects of spreading solvent on the size and density of the PS-PEO nanostructures were analyzed. A polymer series containing constant PEO chain length and variable PEO chain lengths were analyzed at a concentration of 1.0 mg/mL in carbon tetrachloride and 1,2-Dichloroethane using a Langmuir Trough. The nanostructures were transferred as Langmuir-Blodgett films onto a mica substrate at 2.0 mN/m and imaged with an atomic force microscope (AFM). The height, width, and structure density of the nanostructures formed were analyzed for both solvents and compared against each other as well as data previously compiled for the spreading solvents chloroform, 1,1,2,2-tetrachloroethane, and toluene.

PS-PEO Nanostructures: A Look Inside Transfer Ratios and Hysteresis

Polystyrene-block-poly(ethylene oxide) (PS-PEO) is an amphiphilic diblock copolymer that, when applied to an air/water interface, phase separates into nanostructures forming a monolayer. Such features can be imaged by transferring the polymer onto a substrate using the Langmuir-Blodgett technique and an atomic force microscope (AFM). In this study, we investigate a series of polymers containing constant PEO but variable PS content. We specifically examine the effect that surface pressure has on polymer nanostructures. In particular, we investigate the ability of the film to transfer at various pressures by measuring the transfer ratio. We are also measuring the degree of hysteresis in a film and its ability to relax after compression to a certain pressure. Isotherm and atomic force microscopy (AFM) results will be presented. The overall goal is to control and manipulate these nanostructures through better understanding of the parameters that impact their shape, size, and density.
17 Development of Synthetic Precursor to Molybdenum Cofactor
Peterson, Antoinette; Pimkov, Igor; Basu, Partha
Department of Chemistry and Biochemistry
Duquesne University

Molybdenum cofactor deficiency (MCD) is a rare genetic anomaly causing neurological problems and rapid death in patients. Synthesizing molybdenum cofactor may lead to a potential treatment for MCD. The focus of this project is on building a precursor that can form the basic structure of the pyran and dithiolene units of molybdenum cofactor (6-hydroxy-4-(hydroxymethyl)-2-thioxo-4H-[1,3]dithiolato[4,5-c]pyran-7(6H)-one). This presentation will discuss in detail the successful synthesis of 4-phenyl-1,3-dithiolane-2-thione and a three-step synthesis of 4-(2,2-dibromovinyl)-2,2-dimethyl-1,3-dioxolane, both of which are needed to synthesize the aforesaid precursor.

19 Quantitative Modeling Representing Binding of p53-protein interactions and DNA
Hota, Aditi1,3; Faeder, James R.1,2
1TECBio REU at Pitt
2Department of Computational and System Biology, University of Pittsburgh School of Medicine
3School of Engineering and Applied Sciences, Harvard University

p53 is a tumor suppressor protein which functions as a transcription factor of numerous downstream targets that play a role in cell cycle arrest, apoptosis, and senescence. Different p53-protein interactions alter the activity of the p53 transcription factor by either enhancing or inhibiting its ability to bind to DNA. This project aims to model and quantify how the p53-DNA binding event changes upon p53-protein interactions. A simple model relating p53-DNA binding and transcriptional output is modified according to different p53-protein interactions and their effects on transcriptional output. It is expected that protein interactions at particular domains of p53 will have corresponding transcriptional outputs related to the activating or inhibitory effect of the protein interaction. Understanding the degree to which these interactions influence p53 transcriptional output is important since fluctuations in the downstream p53 elements can alter cell cycle processes which could then impact the development and spread of cancer.

20 Determination of Dark Matter Spin at a Lepton Collider
Christensen, Neil D.; Salmon, Daniel J.
Pittsburgh Particle physics, Astrophysics, and Cosmology Center
Department of Physics and Astronomy
University of Pittsburgh

The existence of a new form of electrically neutral (dark) matter has been inferred from various astronomical observations such as anomalous galactic rotation curves, bulk matter flows of galaxies, gravitational lensing, big bang nucleosynthesis, and the cosmic microwave background. Although dark matter has not yet been measured directly, many current particle theory models predict a weakly interacting massive particle (WIMP) with the right properties to fit these observations. If these theoretical models are correct, it is likely that WIMPs will be produced at current and future particle colliders. When this occurs, it will be necessary to investigate the properties of this particle, such as its spin. In this project, we simulate the production of dark matter at a lepton collider and analyze the construction of a new angular distribution which is correlated with the spin of the dark matter particle and will thus be instrumental in determining this property.
21  **Characterization of the Arsenic Oxido/reductase from Alkalilimnicola ehrlichii strain MLHE-1**  
Hunker, Jeffrey L.¹; Kanmanii, Narthana Jeganathar¹;  
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Arsenic, despite its toxicity, can be used by certain microorganisms to support growth. Arsenite (As(III)) oxidation and arsenite (As(V)) reduction can be paired with the appropriate electron acceptor or donor respectively in anaerobic respiration. Alkalilimnicola ehrlichii strain MLHE-1 is a haloalkaliphilic Gammaproteobacterium isolated from Mono Lake, California that has a unique arsenite oxidase, Arx. Although the enzyme is able to operate biochemically in both directions, physiologically it only operates in vivo as an oxidase. We hypothesize that this preferred directionality may be due to the enzyme having a higher affinity for arsenite over arsenate. To determine the specificity for the two arsenic species, the ArxAB complex was extracted from cells grown chemolithoautotrophically with As(III) and nitrate. 1L cultures were harvested and separated into cell membrane and soluble fractions. Highly enriched fractions were prepared using ion exchange chromatography. Enzyme kinetics (Km, vmax) were determined using Methyl Viologen activity assays.

22  **Resonance-Assisted Hydrogen Bonding (RAHB) in Carboxyphosphate**  
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Resonance-assisted hydrogen bonding (RAHB) is a controversial phenomenon that describes flow of charge from conjugated π-electrons to enhance the strength of the intramolecular hydrogen bond. RAHB was investigated as a possible explanation for the unusually high stability (11 kcal/mol) of the pseudo-chair conformation of dianionic carboxyphosphate. Using Truhlar’s Minnesota M06-2X functional and Dunning’s aug-cc-pVnZ (n=D,T,Q,5) basis sets, the NMR shielding constants and chemical shifts for both the hydroxy proton and the phosphorous of carboxyphosphate have been calculated and compared to the analogous values for monohydrogen phosphate. NMR properties were also calculated for calibration systems: twelve phosphorus systems with phosphoric acid used as the reference system. It was found that the difference between the computed H1 chemical shifts of carboxyphosphate (11.3 ± 0.1 ppm) and hydrogen phosphate (1.1 ± 0.3 ppm) was significant (p = 0.002) using a student t-test. RAHB is found to be a valid explanation for the increased stability of dianionic carboxyphosphate.

23  **Determination of protonation states of residues within the cytochrome b6f complex through molecular dynamics simulations**  
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Department of Chemistry and Biochemistry  
Duquesne University  
Photosynthesis is a process used by plants, algae, and some bacteria to convert light energy into useable form. Energy conversion occurs through successive oxidation-reduction reactions in the electron transport chain to generate an electrochemical gradient. Cytochrome b6f is an integral membrane protein located between Photosystem II and Photosystem I in the electron transport chain. Cytochrome b6f transports electrons between the two photosystems through the reduction of plastoquinone to plastoquinol, while simultaneously translocating protons to facilitate the production of ATP. This project utilizes constant pH molecular dynamics simulations to determine if acidic amino acid side chains, will be protonated at physiological pH. Initial calculations of the pKa values in the cytochrome b6 subunit are presented. The protonation data will ultimately be used in conjunction with molecular dynamics simulations to model proton and electron transfer in the complex to better understand the mechanism and possible pathways.

24  **Using norepinephrine transporter (NET) ligands as in silico templates for discovery and design of novel-scaffold NET inhibitors**  
Strong, Benjamin J.; Surratt, Christopher  
Department of Chemistry and Biochemistry; Mylan School of Pharmacy; Duquesne University  
Norepinephrine (NE) is a chemical messenger key to mechanisms involving pain, anxiety and depression. Drugs that inhibit synaptic removal of NE and serotonin (5-HT) by their respective transporter proteins are first-line therapies in addressing depression and anxiety, but carry significant adverse effects due to nonspecific NE and 5-HT actions.. We seek compounds of novel structural backbone (scaffold) that retain synaptic boosting of NE and additionally regulate downstream NE receptors in a way that minimizes side/adverse effects. A norepinephrine transporter (NET) computational model in the molecular modeling software MOE (Molecular Operating Environment) was used for virtual screening of a compound library in predicting new NET ligands. Established NET ligands were docked to the model to achieve a docking score. These scores did not correlate well with experimentally derived binding affinity constants for the compounds, indicating that the MOE scoring function must first be optimized. Once achieved, the virtual NET model should yield novel NET ligands in a fraction of the time required for in vitro pharmacologic discovery.
Predicted structures of aggregates of the human gamma-D crystallin protein found in cataracts
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Human age-onset cataracts are a disease caused by the aggregation of gamma-D crystallin, a structural protein in the lens of the eye. The resulting aggregation causes progressive blindness. The purpose of this research is to determine the causes of these aggregates and their resulting structures. It is hypothesized that a hydrophobic core, five contiguous hydrophobic residues, is critical for the aggregation of gamma-D crystallin. Initial molecular dynamics simulations of small peptides containing a hydrophobic core of gamma-D crystallin were performed to examine possible aggregate structures. Accurate structures of the aggregates will provide a basis for the long-term goal of designing drugs that will inhibit these aggregations to potentially prevent or treat cataracts.

Solvothermal Synthesis of Inorganic-Organic Hybrid Materials with Tetra-Dentate Chelating Ligands
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Solvothermal synthesis is an effective method to produce open framework structures at moderate temperatures. These compounds are of interest due to their electrical, optical, semiconductor properties and reversible storage of small molecules. The synthesis and characterization of the series [M(tren)]2Sn2S6 (M=Mn2+, Fe2+, Co2+, Ni2+, Cu2+, Zn2+ and tren = tris(2-aminoethyl)amine) was completed. [Fe(tren)]2Sn2S6, [Co(tren)]2Sn2S6, and [Zn(tren)]2Sn2S6 were previously characterized. The manganese, nickel and copper analogs were synthesized and then characterized by using single-crystal x-ray diffraction, x-ray powder diffraction, and UV/Vis/NIR band gap measurements. Results from the single crystal x-ray diffraction showed distinct differences in bonding geometry around the transition metal center that translate into different motifs in the extended structure.

N,N'-Bis(3-aminopropyl)-1,2-ethylenediamine is being substituted for tren to make a new series of open framework compounds. This variation of the common triethylenetetramine ligand was used to promote a square planar ligand-metal configuration allowing the creation of long chains.

Atmospheric Pressure-Matrix Assisted Laser Desorption/Ionization-Time of Flight Mass Spectrometry as a Viable Method for Forensic Fiber Analysis
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A study was performed to determine if atmospheric pressure-matrix assisted laser desorption/ionization-time of flight mass spectrometry (AP-MALDI-TOF MS) would be a viable method for fiber analysis. If different carpet fibers could be distinguished based on their additives using AP-MALDI-TOF MS, this method could be a breakthrough in the forensic science community. Fiber extracts were made using two different solvents and analyzed via AP-MALDI-TOF MS to see if carpet additives could appear as unique peaks on the mass spectra. This technique is a promising method for carpet fiber characterization.

The Synthesis and Characterization of Novel I2-II-IV-VI4 Diamond-Like Semiconductors
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Duquesne University

I2-II-IV-VI4 diamond-like semiconductors (DLSs) are interesting for technological applications in photovoltaic solar cells, spintronics and non-linear optics, specifically second harmonic generation. Many quaternary DLSs have not been fully studied due to their challenging syntheses. These structures exhibit tetrahedral coordination that resembles either a cubic or hexagonal diamond lattice. A new lithium-containing DLS has been synthesized using high-temperature solid-state methods. The compound has been characterized using single crystal X-ray diffraction, diffuse reflectance spectroscopy, X-ray powder diffraction, and scanning electron microscopy coupled with energy dispersive spectroscopy. These characterization techniques have been used to solve the Li2-II-IV-VI4 crystal structure in the Pn space group, approximate a band gap, analyze phase-purity, and determine crystallite size, morphology, and composition.
29 Electronic structure calculations of CuInS2 with varying muffin-tin radii.
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Diamond-like semiconductors are normal valence compounds whose structures are derived from diamond, either the cubic or hexagonal form. These materials are of interest for their use in solar cells, non-linear optics, and thermo-electric devices. The properties of diamond-like semiconductors can be calculated using electronic structure methods. One approximation in the electronic structure calculation is the muffin-tin radius. The purpose of this project was to determine if the calculated properties of a chalcopyrite (I-III-VI2) diamond-like semiconductor, such as CuInS2 were dependent on the muffin tin radii (RMT). Various RMT values were selected and the various properties were calculated using density functional theory in WIEN2k. Initial results showed that RMT values had little to no effect on the electron density, the band structure, and the band gap of CuInS2. However, the chosen RMT values did have a significant effect on the local density of states.

31 Characterization of the activity of a γ-modified Peptide Nucleic Acid molecule designed against the IIId domain located within the 5' UTR of the Hepatitis C Viral RNA genome
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Hepatitis C, caused by the hepatitis C virus (HCV), is a life-threatening disease affecting about 170 million people worldwide. The HCV genome is composed of a large open reading frame flanked by conserved 5' and 3' UTRs. The conserved 5' UTR of HCV forms the internal ribosome entry site, which directs viral protein translation. Domain III in the 5' UTR, specifically segment IIId containing the sequence GGG, is critical in anchoring the 40S ribosomal subunit for translation. Our lab has proven that long range RNA-RNA interactions between IIId and 5BSL3.2 (located in the coding region) promote replication. A γ-modified peptide nucleic acid molecule (PNA) has been engineered to target the IIId domain to potentially inhibit both recruitment of the 40S ribosomal subunit and long-range RNA-RNA interactions. Different biochemical and biophysical methods were used to characterize binding of the PNA to the IIId region and to analyze its effect upon HCV translation.

30 Biochemical and Biophysical Characterization of the SMNDC1 mRNA to Fold into the G-quadruplex Secondary Structure
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Specific guanine-rich nucleic acid sequences have the potential to form G-quadruplex secondary structures. These structures form when four guanine residues engage in Hoogsteen base pairs to form a planar G-quartet, and such G-quartets can then stack either inter- or intramolecularly to form the G-quadruplex structure, which is further stabilized by potassium cations. G-quadruplex structures are predicted to regulate translation in the 5'- and 3'-untranslated regions (UTRs) of messenger RNA (mRNA) sequences. We have investigated several human neuronal 5'-UTR mRNA sequences predicted to form the G-quadruplex structure, one of which is the survival motor neuron-related-splicing factor 30 (SMNDC1). Various biochemical and biophysical methods were utilized to verify the formation of the G-quadruplex secondary structure in SMNDC1 mRNA. We also characterized the binding of SMNDC1 mRNA to the fragile X mental retardation protein’s G-quadruplex-binding domain called the arginine-glycine-glycine box.

32 Green and Efficient Synthesis of Copper(I) Cyanide-Based Polymers Under Ambient Reaction Conditions
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Copper(I) cyanide-based coordination polymers have a potential application as zeolitic material and for storing highly explosive hydrogen and methane gas. Conventionally, these polymers are synthesized from highly toxic cyanide precursors via solvothermal and hydrothermal methods, which require harsh reaction conditions such as high temperature and high pressure over prolonged reaction times. A new green and highly efficient method for the synthesis of these polymers under ambient reaction conditions has been reported. In this method, copper(II) amino acid complexes, [CuI(II)(AA)(NN')(X)] (AA=alanine; NN'=1,10-phenanthroline or 2,2'-bipyridine; X=Cl- or Br-), are reduced in the presence of ascorbic acid and 2,2'-Azobis(2-methylpropionitrile) (AIBN) generating copper(I) cyanide-based polymers. Currently, we have been investigating the effect of different concentrations of AIBN, solvents (methanol, propanol, DMSO, and acetonitrile) and amino acids (phenylalanine, glycine, leucine, and proline) on the structure of the resulting polymer.
33 Characterizing the Interactions Between a Mutated Fragile X Mental Retardation Protein and the G Quadruplex mRNA Structure
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Fragile X Syndrome (FXS) is the most common form of inherited mental retardation affecting approximately 1 in 4,000 males and 1 in 8,000 females. FXS is linked to the expansion of cytosine-guanine-guanine trinucleotide repeats in the fragile X mental retardation 1 (fmr1) gene causing hypermethylation of the cytosines, transcriptional silencing of fmr1, and loss of the fragile X mental retardation protein (FMRP). However, one patient phenotypically expressed FXS despite FMRP production. Further studies revealed a frame shift altering guanine-insertion in the fmr1 gene, which affected the major G quadruplex binding site of FMRP called the arginine-glycine-glycine (RGG) box. In this study, we utilized different biochemical and biophysical methods to compare the binding activity and translation regulator function of the newly-discovered, mutated FMRP RGG box binding domain to the G quadruplex forming human Semaphorin 3F mRNA with those of the wild-type FMRP RGG box binding domain.

34 Pain neurons in the central nucleus of the amygdala are primarily inhibitory neurons
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The central nucleus of the amygdala (CeA), which is located in the limbic forebrain of both humans and rodents, is hypothesized to be involved in the long-term adaptation to persistent pain. During persistent pain states extracellular signal-related kinase (ERK) is phosphorylated in the CeA. Here, we simulated a persistent inflammatory state in mice and then detected phosphorylated ERK (pERK) in the CeA. Next, we sought to identify the neurotransmitter status of these pERK neurons. We hypothesized that these neurons were inhibitory neurons, which can be detected by staining for gamma-Aminobutyric acid (GABA). Our staining showed that the CeA is comprised primarily of GABAergic neurons. When both pERK and GABA were stained for, a large amount of overlap was found to exist between the two staining patterns. Overall, these results suggest that the CeA cells associated with persistent pain (i.e. pERK neurons) are GABAergic inhibitory neurons.

35 The Investigation of Copper-Catalyzed Atom Transfer Radical Addition (ATRA) in the Presence of Monohalogenated Alkyl Halides
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Copper (I) regeneration in atom transfer radical addition (ATRA) and cyclization (ATRC) has significantly reduced the amount of catalyst, thus creating a “green” process. This method was first applied in the addiction of polyhalogenated alkyl halides to various alkenes, and was extended utilizing monohalogenated alkyl halides such as bromoacetonitrile (BrACN), 2-bromopropionitrile (2-BrPN), and 2-ethyl bromophenyl acetate (EBrP). The monohalogenated alkyl halides were investigated because a single carbon-halogen bond is more expedient for further organic transformations. In optimizing this process, the best results were achieved when reactions were performed at 80°C in ethanol for 24 hours with tris-2-pyridylmethylamine (TPMA) copper(II) complex in conjunction with ascorbic acid palmitate. Under these conditions, ATRA of BrACN, EBrP, and BrPN to styrene and 1-octene was very efficient producing monoadducts in moderate yields (27-95%).

36 Enhancing the Functions of Anti-VEGF antibodies through clustering on an Injectable Scaffold
Goehring, Thomas R.; Liu, Wen; Meng, Wilson
Duquesne University

The EAK protein scaffold system was found to be a viable platform for attaching Anti-Vascular Endothelial Growth Factor (VEGF) antibodies in the hope of slowing or halting the progression of tumor development in mice. Using SDS-PAGE electrophoresis, properties of the EAK-antibody scaffold were assessed under various temperatures and pH conditions. This was done to better understand the stability of the scaffold system as a whole as well as its components function under tumor physiologic conditions. Mouse studies were also conducted in order to compare the efficacy of the scaffold system to free Anti-VEGF within mouse tumors.
The emergence of new sequencing technologies has led to a deeper understanding of evolution through the use of phylogenetics. One branch of phylogenetics that has blossomed is the study of evolutionary rates of genes. Evolutionary rates of ensembles of genes have been studied in E. coli, yeast species, and others, but not in a mammalian model. We use the phylip package, the paml package, and perl to look at the evolutionary rates of 4853 genes from 19 mammals. Using the Gene Ontology tool, we categorized these genes into several different biological processes and looked for significant accelerations. We found significant acceleration in genes involved in mitosis and cell cycle in mice, in cofactor metabolism in cows, in cellular amino acid metabolism in orangutans, and in genes involved in circulatory system process in chimps. We show that this analysis can yield very beneficial biological insights regarding longterm adaptation of genetic systems.

Hutchinson-Gilford progeria syndrome (HGPS) is a segmented premature aging disease caused by a mutation in a nuclear structural protein used to study advanced cellular aging. Vascular cells, including endothelial cells are disproportionately affected in patients. Previous studies of protein expression in animal models have suggested changes in endothelial mitochondria function. We examine changes in mitochondria, in endothelial cells expressing the HGPS mutant following 0, 5, or 10 dyne/cm2 of shear stress. We utilize different segmentation algorithms to automate the image analysis processes. We then perform customized shape and texture algorithms to monitor mitochondrial textures in response to shear for diseased and control cell lines. We find that cells expressing the HGPS mutant show different amounts and distributions of mitochondria, as well as an altered shear stress responsiveness of mitochondria. Due to the inherent links between mitochondria and the cytoskeleton, differences in disease cell lines indicate aberrant cell mechanics.

Beta-lactamases catalyze the hydrolysis of beta-lactam molecules enabling bacterial resistance to beta-lactam antibiotics. Beta-lactam sensing proteins, BlaR and MecR, contribute to this bacterial resistance by acylating beta-lactams which then transmits a signal through the cell membrane ultimately regulating the production of beta-lactamas and the sensing proteins themselves. The sensor domain has sequence and 3D structure similarity to the class D beta-lactamas (OXAs). In this presentation, we will display our results from molecular phylogenetic and other associated analyses of these sensors that identify residues most likely critical for the maintenance and diversity of structure and function and that distinguish them from Beta-lactamas that complete the hydrolysis catalytic cycle. In addition, the DNA alignment was analyzed to determine signatures of natural selection. This analysis will provide insight into the critical features of this enzyme family and could be beneficial to better understanding how they adapt over time.
41 Predicting Bulk Properties of Butyl-3-methylimidizolium Hexafluorophosphate using Molecular Dynamics Simulation
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Butyl-3-methylimidizolium Hexafluorophosphate [bmim][PF6] is a room temperature ionic liquid. It has been investigated for its application in CO2 sequestration. BMIM’s negligible vapor pressure allows it to be useful in industrial solvent applications and potentially useful as a solvent for electrochemistry. In contrast to its positive characteristics, its high viscosity leads to lowered ionic conductivity. Molecular dynamics simulations will be done to examine the structure of [bmim][PF6] by using the NAMD software. The comparison of viscosity, conductivity, and ionic current values to experimental and calculated literature values will then be done.

42 Modeling Cell Membranes with Dissipative Particle Dynamics
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Dissipative particle dynamics (DPD) is an approach to molecular dynamics that aims to capture complex hydrodynamic behavior. DPD is a computationally efficient method for describing complex systems by utilizing a coarse-grained particles technique. We study cellular membranes, a complex lipid bilayer that can be approximated using a particle-focused approach. This cell membrane is coarse-grained and modeled as a two dimensional surface to make simulations more computationally efficient than a pure molecular dynamics technique. A pore of a specified size is introduced to the membrane in order to measure the shear stress that the membrane can withstand before it ruptures. This makes it possible to capture realistic behavior of cells within intestinal crypts. Given the complexity of the system of interest, and the offset in computational demand provided by DPD, it is possible to simulate realistic physical systems at scale.

43 Utilizing Scanning Electron Microscopy for Use in High School Chemistry Laboratories
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Scanning electron microscopy (SEM) is used to observe the surface morphology of a material and to measure sample features such as crystallite size. Through this project, an experiment was designed that remotely utilizes the SEM in high school chemistry laboratories via internet connection. The purpose of the experiment is to observe the morphologies crystal sizes of basic salt and sugar specimens and then to synthesize crystalline candy of the two. The morphological information recorded by using the SEM is then used to create a hypothesis of which morphological features the crystalline candies would display. The candies are then imaged using the SEM to prove or disprove the hypothesis.

44 Learning Molecular Biological and Biochemical Techniques in Investigating Periplasmic Nitrate Reductase
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Molybdenum containing enzyme, periplasmic nitrate reductase (Nap), plays an important role in the vitality of pathogenic bacterium, Campylobacter jejuni. The catalytic subunit, NapA is being cloned and overexpressed in E.coli. There are many techniques such as cell culture, DNA extraction, purification, and cloning that are involved in the proper overexpression of this important protein. To this end, I have been learning these techniques, and how they apply to the overall goals of the project. In this presentation, I present my experience with the experiments, and results.
Stability of Alkanethiols on Gold
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The stability of thiols on gold is a subject of interest in the fields of chemistry and electronics. This is due to their widespread application in technologies such as bio-sensors and electrodes. Our ongoing work is to develop stable films of various thiol molecules on the surface of gold with different tail groups. 11-mercaptoundecanol, 11-mercaptoundecanoic acid, and mercaptoundecane, were used to form self-assembled monolayers. Solution deposition methods were utilized, and the substrates were analyzed using Diffuse Reflectance Infrared Fourier Transform Spectroscopy, to confirm film deposition and film stability after solvent rinse, as well as Matrix Assisted Laser Desorption/Ionization Time-of-Flight Mass Spectrometry, to determine monolayer versus multilayer film coverage.

Pigment Extraction and Separation using Thin Layer Chromatography
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Thin layer chromatography (TLC) is used to separate organic molecules based on their affinity for a mobile and stationary phase. The stationary phase is made up of a thin layer of silica gel on an aluminum support. As the mobile phase flows through the stationary phase, it carries the components of the sample mixture with it, allowing for separation. Various colored leaves were obtained to compare their specific pigment profiles. To extract the pigment, the leaves were ground using a mortar and pestle with acetone as the extraction solvent. Using TLC, the mobile phase composition and spot volume were optimized to ensure the best separation and the most visible colored spots. A 4:1 petroleum ether: acetone solution was used for the mobile phase with a spot volume of approximately 40µL. Based on the colored elution bands, the specific pigments in each leaf were able to be identified.

Catalyzation of Copper in TMC ATRA/ATRP
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In this study, we set out to examine the structural, electrochemical, and kinetic behavior of eight unique copper complexes that have the predisposition to be used as catalysts in ATRA or ATRP reactions. Complexation reactions were carried out to generate the following; 
[Cu(I)(TREN-B)][Cl], [Cu(I)(TREN-4CB)][Cl], [Cu(I)(TREN-4MB)][Cl], [Cu(I)(TREN-4TFB)][Cl], [Cu(I)(TREN-B)][Cl2], [Cu(II)(TREN-4CB)][Cl2], [Cu(II)(TREN-4MB)][Cl2], and [Cu(II)(TREN-4TFB)][Cl2]. Characterizations were carried out used infrared, NMR, and mass spectroscopy. Solid state and electrochemical characterizations were carried out using x-ray crystallography and cyclic voltammetry respectively. Kinetic studies were conducted using UV/Vis spectrometry with carbon tetrachloride as the alkyl halide and (2,2,6,6-tetramethylpiperidin-1-yl)oxidanyl (TEMPO) as the radical trapping agent. This allowed for the kinetic isolation of the activation process in the ATRP reaction and helped us calculate the activation rate constants (kact) for the respective copper complexes.

Predicting the pKa’s of isolated molecules and molecules in proteins
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The determination of theoretical pKa’s is the main purpose of this research. The pKa’s will be calculated using quantum chemical methods with different thermodynamic cycles. We have selected molecules with found experimental pKa’s to test. While it is relatively easy to find the pKa’s of isolated molecules, molecules in proteins prove to be difficult for experimental scientists. To find the pKa of a molecule when in a protein is only a matter of time. Once the pKa’s of the isolated molecules are able to be accurately calculated, this will be applied to more complex molecules, eventually resulting in the accurate pKa calculations of molecules when in proteins.
49 Prediction of Influenza A virus Hemagglutinin binding sites using dynamics perturbation analysis
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University of Pittsburgh

We determined the amino acid residues responsible for the species specific binding of the Hemagglutinin (HA) protein in the Influenza A virus using dynamic perturbation analysis (DPA). DPA identifies the regions of greatest change in protein conformational distribution by measuring relative entropy of minimal surface perturbations in a normal-modes model. Those regions may theoretically indicate biological activity such as ligand binding in HA proteins. To compute the normal modes, we modeled HA as an isotropic elastic network with springs linking every alpha-carbon between protein residues, using published 3D crystallographically-determined HA structures. Calibrated using known ligand binding sites, the DPA algorithm successfully predicted the primary and secondary binding sites of HA to sialic acid residues of human respiratory epithelial cells, as well as other potential regions of interest. This method can be applied to other proteins of the influenza genome for which drug targets currently do not exist.

50 Structural Basis of the RNA Polymerase II Nucleotide Addition Cycle
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The nucleotide addition cycle (NAC) is the elementary step in transcription by RNA polymerase II (pol II). The NAC consists of multiple sub-processes: selection of a complementary ribonucleotide, catalysis of phosphodiester bond formation, and translocation of the RNA-DNA hybrid. Current models of the NAC are based mainly on interpretations of X-ray crystal structures of pol II transcribing complexes. However, given the dynamic nature of transcription, static structures provide limited insight. Molecular dynamics simulations may offer a more effective means of investigating transitory conformations of the pol II active center that underlie the NAC. Taking this approach, we test the findings of previous studies that have suggested key nucleotide-peptide interactions as the mechanisms responsible for ribonucleotide selection and bond catalysis. Additionally, we aim to uncover short-lived active site transformations that could provide insight into the transcriptional role of magnesium ions and the structural elements involved in hybrid translocation.

51 Molecular Phylogenetic Analysis of Integron-encoded Class A β-lactamases
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The GES (Guiana Extended Spectrum) enzymes comprise an emerging group of integron-encoded class A β-lactamases conferring resistance against penicillin, cephalosporin and carbapenems. Integron associated GES-like determinants can be laterally transferred among clinical strains limiting the availability of treatment options for serious bacterial infections. In order to better predict the effect of evolved mutants and specifically GES-21, a new GES variant recently discovered in wastewater, we initiated a sequence-based bioinformatic study of this enzyme family. In this presentation, we will show our results from molecular phylogenetic and other associated analyses that identify residues and motifs important for the structure and function of these enzymes. In addition, the DNA alignment was analyzed to determine signatures of natural selection. Through this and other biophysical methods, we plan to develop a computational approach to predict that the functional effect of mutations to integron-encoded class A Beta-lactamases retrieved from natural environments.

52 Chemical Immobilization of Bone Morphogenetic Protein 2 on Ceramic Scaffolding Enhances Substrate Bioactivity
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Bone morphogenetic protein 2 (BMP-2) is a member of the TGF-β growth factor family that exhibits multiple functionalities in the process of bone remodeling. As such, surface modification of intrinsically bioactive ceramic scaffolds with BMP-2 could serve to further enhance the osteogenic effects of the scaffolds at a bone defect site. In this study, calcium aluminate (CaAlO) and calcium phosphate (CaP) scaffolds were modified with BMP-2 by direct surface adsorption or chemical immobilization utilizing an organic linker system. To determine the effects of the modified substrates on primary cell growth, human osteoblasts were deposited on each substrate and analyzed at Day 1, 4, and 7 growth points using a Live/Dead Cytotoxicity assay. It was shown that the method of biomolecule attachment as well as scaffold composition influenced cell viability, and that chemically immobilized BMP-2 on CaP scaffolds promoted cell viability to the highest degree.
Surface Coverage Analysis of Self-assembled Monolayers on Zinc Oxide using Inductively-Coupled Plasma Optical Emission Spectrometry

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The growing interest in the modification of nanoparticles for the use in solar cells has heightened the awareness of surface coverage of the particles. The amount of a substrate bonded to the surface of another compound can be tailored to alter the properties of the surface, improving its functionality. Inductively-Coupled Plasma Optical Emission Spectrometry’s inherent sensitivity makes it useful in determining concentration of elements. In this study, zinc oxide nanoparticles were modified by adding self-assembled monolayers of octadecylphosphonic acid (ODPA) to the surface. The bonding of the acid to the surface was confirmed through infrared spectroscopy (IR). Surface coverage was then analyzed using ICP-OES. A theoretical calculation of the ODPA surface coverage on zinc oxide was calculated and compared to the ICP-OES data.

Efficacy of the Drug Delivery of Palmitoylethanolamide (PEA) in Emulsions using Triple Quadrupole Mass Spectroscopy

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Palmitoylethanolamide (PEA) is a fatty amide that has been shown to be effective for significant pain reduction in clinical trials of neuropathic, sciatic, and lower back pain. Interestingly, PEA production naturally increases in cells local to where inflammation. A 5 µM standard of PEA was directly infused using a Harvard Apparatus Syringe pump at 0.1 mL/min into a 6460 Agilent Triple Quadrupole Mass Spectrometer. The parent ion was observed at 300.3 m/z as the [M + H]+ ion. The fragmentation of PEA was observed using collision induced dissociation from 10-50 V. Collision energy of 20 V was used to develop a multiple reaction monitoring method and was used to determine the linear range which was between 10 and 500 nM. The effectiveness of olive oil as a vehicle used for the delivery of PEA as a drug in cell and animal models is under examination.

Effects of ovariectomy and estradiol replacement on behavior in Allegheny Mountain dusky salamanders

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Little is known about the role of estradiol in female amphibian behavior. A better understanding of the normal role of estrogen in amphibians is needed because amphibians are often used as an indicator of environmental estrogens. We hypothesized that estradiol is required for female mating behavior. To test this hypothesis, we surgically ovariectomized female salamanders (Desmognathus ochrophaeus) to reduce circulating estrogen and placed either an estradiol or control implant in the salamander. It was predicted that ovariectomy would reduce, and estradiol implants would restore, normal mating behavior. Salamanders that underwent surgery were significantly less active and ate less than salamanders that did not, suggesting that the surgeries were stressful. Surprisingly, all animals showed high levels of mating, implying that estradiol may not be necessary for mating.
57 Calorimetric Titration Methodology for Studying Drug Interactions
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The purpose of this study was to create a methodology to thermodynamically characterize interactions between a drug and a receptor/incipient. This method may then be applied to characterize specific interactions between drugs of abuse and their receptors. Titration of Tris(hydroxymethyl)aminomethane with 0.1 M HCl in an isoperibol calorimeter was used to develop the method due to the significant and well known heat associated with this reaction (11.35 kcal/mol HCl). This method was also used to test physical interactions several different drugs and excipients. From this method the accuracy, precision, and limit of detection were calculated. Limited interactions were measured in the potential model systems, being below the detection limit in most cases. Nevertheless, a reliable calorimetric titration method has been developed. Based on the detection limit, this method is useful for many reactions with specific heat above the limit of detection.

59 Multi-Environment Support for RAE: An Interactive Web-Based Biomedical Informatics System for Pediatric Orthopedic Patients
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The purpose of the RAE biomedical information system is to facilitate patients’ understanding of potentially serious orthopaedic disorders through an interactive educational experience. The RAE software produces dynamic and personalized presentations containing both disorder-specific and patient-specific information, as well as printable information packets to combat learning attrition and to help the patient stay on track. Our contribution to the project this year involved enhancing the software’s patient-related personalization capabilities in three ways. In order to refine the information packets, the print functionality was expanded, allowing the user to specify forms to print at the start of a presentation. Other enhancements include the addition of a dynamic BMI chart and an interactive activity form. The new BMI chart is generated from the patient’s supplied height and weight values. Finally, an improved activity plan form allows the clinician to dynamically select appropriate physical activities for the child during the current treatment phase.

60 Inhibiting PARP-1: When is Water Important?
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Poly (ADP-ribose) polymerase is an enzyme that facilitates DNA repair at single-strand break sites. Efficient and selective inhibition of this enzyme can aid in chemotherapy treatments; hindering the ability of the cancer cells to survive the incurred DNA damage. Some x-ray crystal structures of PARP-1 have a water molecule bridging the inhibitor and protein, while other crystal structures with a different inhibitor do not. Molecular dynamics simulations and free energy perturbation (FEP) calculations were performed on a system having a bridging water molecule (pdb code: 1efy), as well as a system without a bridging water molecule (pdb code: 2rcw) in order to quantify the importance of this binding pocket water. Initial FEP results indicate the bridging water in the 1efy binding pocket has a free energy value of ~6.054 kcal/mol, while its free energy in apo is just over 9 kcal/mol. The significance to overall binding energy will be discussed.
Mechanisms to restore cardiac force production are of great therapeutic interest because defects in contractility are often the detrimental physiological manifestation of cardiovascular diseases. In order to examine the biophysical bases for acetylation-induced increase in cardiac force production, two groups of skinned cardiac muscle fibers were studied: (1) experimental group treated with relaxing solution containing histone deacetylase (HDAC) inhibitor (trichostatin A, TSA, 200nM) to increase myofilament acetylation and (2) control group treated with relaxing solution (Vehicle). Using a model-based analysis of force data collected from experiments involving step-like length perturbations of each fiber, we quantified the magnitude and kinetic parameters of the dynamic recruitment and distortion processes involved in cardiac force production. Parameter values estimated from the data revealed that the increased force production in myofilament protein acetylated fibers is due to both a larger number of actin-myosin cross-bridges being formed and a greater force being produced by each cross-bridge.

The objective is to data-mine and archive allergen toxic data in a repository and to define chemical characteristics that lead to specific mechanistic routes. A database of 367 chemicals with known skin sensitizing allergen potential was compiled from literature sources. All chemicals were batch processed through Toxtree software using the skin sensitization alerts module. A total of 98 of the 367 chemicals were incorrectly classified, with 53 false negatives and 45 false positives. The incorrectly classified chemicals were analyzed. A new rulebase for groups of chemicals previously incorrectly identified through the current Toxtree program will be proposed. It is hypothesized that the modifications to the software could result in enhanced functionality and a more efficient prediction of allergen potential.

Diamond-like semiconductors (DLSs) are materials whose crystal structures are derived from diamond. These materials are of interest due to their potential use in photovoltaic solar cells, nonlinear optics, and thermoelectric devices. Due to the chemical complexity of quaternary DLSs, not many have been studied thoroughly. However, the compositional flexibility of these materials makes them ideal for physical property tuning. In this study, copper-containing quaternary DLSs were prepared by high-temperature solid-state reactions of the elements. Several samples with varying dopant amounts were analyzed. The band gaps were estimated by using diffuse reflectance UV/Vis/NIR spectroscopy. Scanning electron microscopy was used in order to examine crystallite size and morphology, while elemental mapping and semiquantitative analysis of these samples were performed using energy dispersive spectroscopy. The location of the dopant within the sample was given specific attention. X-ray powder diffraction was used to identify the phase and assess the phase purity of the sample.

Doripenem is a large molecule within the carbapenem class of beta-lactam antibiotics. Molecular dynamics (MD) simulations can reveal critical details of the Michaelis complex between doripenem and beta-lactamase enzymes (that have varying hydrolyzing capabilities). However, MD simulations can be challenging due to the lack of molecular mechanical (MM) force fields parameters for antibiotic molecules and thus have to be developed. In this presentation, we will show our parameterization results within the CHARMM force field parameterization protocol employing ParamIT (sb.nrbsc.org), a MM parameter optimization and data management software program. Because doripenem is a large molecule, several fragments were parameterized and finally pieced together to create the final parameter set. The calculated geometry, vibrational modes, dihedral potential energy scans and interactions with water molecules obtained from the developed MM force field and their agreement with Quantum Chemical calculations will be presented.
A Left-Venticle Coupled Model of the Systemic Circulation with Application to Uterine Artery Doppler Analysis

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The traditional interpretation of an abnormal Uterine Artery Doppler (UAD) scan is that there is a problem in the uteroplacental circulation. However, there is reason to believe that aberrations in uteroplacental circulation are not the sole determinants of abnormal UAD; problems in the systemic circulation can also contribute. It is not feasible to experimentally quantify the relative contributions of the systemic and uterine circulations to an abnormal UAD under in vivo conditions, so a mathematical modeling-based approach is ideally suited for this purpose. Using the existing validated models of the left ventricle (LV) and systemic arterial circulation (SAC), I have implemented a coupled LV-SAC system model that is able to accurately reproduce pressure and flow waveforms at various cardiovascular sites. I am presently modifying this coupled model to include the uteroplacental circulation. This final coupled model will enable a level of analysis sophisticated enough to rigorously explore the stated question.

PS-PEO Nanostructures: The Effect of Adding Small “Plasticizers”

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Polystyrene-b-poly(ethylene oxide) (PS-PEO) is an amphiphilic diblock copolymer that phase separates to form patterned nanostructures which are classified as continents, spaghetti, dots, and mesh. These characteristic features can be imaged from Langmuir-Blodgett films under an atomic force microscope (AFM) and the nanostructures examined for pattern, height, width, and structure density. The assembly of these polymers was found to be affected by the addition of small molecules, serving as “plasticizers.” Two series of polymer and small molecule compositions were studied, looking at mixtures of a 216,000 PS-PEO (7.4\% PEO) and either 3-pentadecylophenol (PDP) or 4’-pentyl-4-biphenylcarbonitrile (5CB) in various ratios. In addition to film imaging, isotherm plots of mean molecular area versus surface pressure were obtained as well. This study should provide an enhanced understanding of the PS-PEO interactions at the air/water interface and thus allow for increased control over the nanostructures formed.

Computational Assessment of Cardiac Hypertrophy in Zebrafish

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It is well known that zebrafish are excellent in vivo models for human heart studies, due to the physiological similarity between human and zebrafish hearts and the transparency of zebrafish embryos which promotes bioimaging techniques. Consequently, the zebrafish heart model can be used in drug trials to assess the risk of cardiac hypertrophy as a side effect for commercial drugs. In this study, we describe a high throughput routine for calculating the force of contractility of a zebrafish heart from videos of live embryos. We administered various drugs to zebrafish embryos, and used video data to calculate optical flow which quantifies heart displacement. Then, we applied an inverse harmonic oscillation scheme to estimate the force of contractility of the zebrafish heart, which is used to evaluate the risk that each drug possesses for cardiac hypertrophy in humans. Minimal human intervention is needed to implement our routine for large-scale drug trials.

Quick-SNA5PS: An Online Server for Detecting Signatures of Natural Selection

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We will present our online service, Quick-SNAP5 (Quick Detection of Signatures of Natural Selection through Analysis of Amino Acid Alignments Annotated on Protein Structures). A user can upload an amino acid multiple sequence alignment with Uniprot or GenBank Translation identifiers along with a phylogenetic tree in Nexus format and the program retrieves the DNA sequences (along with extensive error checking) and performs a codon-delimited DNA alignment. From the DNA alignment, the user can select various options and perform analysis on synonymous and non-synonymous substitution rates to detect signatures of natural selection with the HYPHY program. The program returns the results of this analysis along with residues undergoing positive and negative (purifying) selection annotated on the multiple sequence alignment display in Jalview. Finally, scripts are generated to visualize the locations of these residues on protein structures using VMD. This interface is available as a module to the HarvestSeq resource (sb.nrbsc.org).
In this study, we set out to examine structural, electrochemical and, kinetic behavior of eight unique copper complexes that have the predisposition to be used as catalysts in ATRA or ATRP reactions. The tetradequate ligand tris-(2aminoethyl)amine (TREN), was synthesized and modified to incorporate electron-donating or electron-withdrawing functional groups (H, Cl, CH₃, CF₃) in the phenyl ring’s para position. Complexation reactions generated four copper(I) and four copper(II) complexes as follows: [Cu(TREN-B)][Cl], [Cu(TREN-4CB)][Cl], [Cu(TREN-4MeB)][Cl], [Cu(TREN-4TFB)][Cl], [Cu(TREN-B)][Cl₂], [Cu(TREN-4CB)][Cl₂], [Cu(TREN-4MeB)][Cl₂], and [Cu(TREN-4TFB)][Cl₂]. Subsequent characterizations were performed using infrared, NMR, and mass spectrometry. Solid state and electrochemical characterizations were executed using x-ray crystallography and cyclic voltammetry respectively. Kinetic studies were conducted using UV/Vis spectrometry with carbon-tetrachloride, the alkyl halide, and (2,2,6,6-tetramethylpiperidin-1-yl)oxidanyl (TEMPO) the radical trapping agent. This allowed for kinetic isolation of the activation process in the ATRP reaction and provided the parameters needed to calculate the activation rate constants (k_{act}) for each copper complex.

Breast cancer is the most common type of cancer amongst women worldwide but is easily treated if detected early enough, typically through imaging. As such, screening mammography is very prevalent and correct diagnosis is imperative. For this retrospective study, 8 radiologists read 120 mammography cases and we used the eye movement data derived from their readings to extract image patches which captured the radiologists’ attention. 59 of the cases contained cancer in a known location while the other 61 cases contained no cancer. Using this data set, we identified which patches contained a cancer and built an innovative classifier of breast cancer image patches. In particular, we normalized the dataset for contrast changes, use principal component analysis (PCA) and show that the PCA based methodology of analyzing image regions derived by eye movement studies leads to an effective classifier for early detection of cancer in mammogram images.

We used the transfer matrix method to optimize two anti-reflective coatings by finding the thickness of each that resulted in the lowest intensity of reflected light. The first is a silicon dioxide coating on a diamond-like carbon (DLC) substrate, which then has single layer graphene suspended over it. The graphene’s motion is detected by measuring the interference between light reflected off itself and that reflected off the substrate. The other anti-reflective coating is a Hyflon coating on a quartz lens used in the same experiment. We used a monochromator to experimentally verify the optimal thicknesses predicted by the transfer matrix method. It was necessary to upgrade this instrument to communicate with a PC via an Arduino microcontroller and several new Python modules such that specific commands could be sent to the monochromator and data could be returned.

Density functional theory and ab initio calculations on CP have identified a single, unique dianionic pseudo-chair conformation (PC) stabilized by a strong intermolecular hydrogen bond. It has been proposed that the intramolecular hydrogen bond in PC is strengthened by a phenomenon called resonance-assisted hydrogen binding (RAHB). Natural bond orbital (NBO) and natural resonance theory (NRT) calculations on CP suggest the existence of RAHB in PC. In order to validate and better understand the RAHB in PC, NBO and NRT calculations have been carried out on two classes of structural analogues of the carboxyphosphate. First class of the analogues was obtained by substituting the bridging oxygen of PC. The second class of analogues was obtained by substituting the hydrogen bond acceptor oxygen on the carboxy side. Results suggest that the resonance effects in carboxylate alone strengthen the intramolecular hydrogen bond. Finally, effects of the substitutions on bond orders, bond lengths, charges and intermolecular hydrogen bond are discussed.
Conformations of PolyQ peptides using Metadynamics
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Huntington's & Alzheimer's disease are consequences of a conformational structure change that allows proteins to aggregate as insoluble masses in cerebral blood vessels. Current literature states that proteins with long polyglutamine (polyQ) stretches are believed to be key players in protein aggregation due to a stable β-hairpin conformation. Experimental results indicated that polyQ10 peptides existed as a PPII structure in solution. Simulation models that mirrored current experimental protein conformation results for polyQ peptides were formulated. This project investigated the different shapes of the peptides D2Q10K2 and D2Q17K2 in varying solvent conditions using metadynamics simulations in the software package NAMD. The free energy landscape was determined using the RMSD collective variables for reference structures α-helix, β-hairpin, and PPII. The gas phase simulation results show a quick formation of a turn as the low energy structure. Aqueous phase simulations of polyQ systems are underway.

Pore formation in Vibrio cholera cytolsyn (VCC)
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The cholera disease is caused by the bacterium Vibrio cholera. A toxin, Vibrio cholera cytolsyn (VCC) is produced by this bacterium. There are two forms of VCC, a protoxin form and a pore-forming toxic (PFT) form. The PFT form is a component of a heptamer pore where a pre-stem loop unfolds from the protoxin monomer. Computer simulations were employed to test the hypothesis that the pre-stem loop in VCC underwent a conformational change from the protoxin to the PFT form upon pore-formation. A LowModeMD search was applied to the protoxin form as well as the PFT form to explore the various conformations of the pre-stem loop. There was no significant loop movement or loop extension in the protoxin form, but there was significant loop movement in the PFT form. LowModeMD was applied again to the PFT form under different conditions.

Importance of Protein Membrane Interactions in Parasite Virulence: an in Silico and in Vivo Analysis
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Toxoplasma gondii is an intracellular parasite with the ability to infect virtually any warm-blooded animal. During the infection process, the parasite injects a variety of proteins into the host cell. The invasion process results in the parasite being surrounded by a vacuole constructed of the host plasma membrane, known as the parasitophorous vacuole (PVM). Many of the secreted proteins then bind to this membrane. One family of these proteins, known as rhoptry proteins (ROP) are known to have a high affinity for the PVM. In this project, a computational analysis of ROP proteins was performed using coarse-grained molecular dynamics simulations to determine the affinity of three arginine-rich alpha helices for a model membrane. To study the importance of this process in vivo, a parasite strain expressing one of these ROP proteins with helix 2 deleted is being generated. This strain will be used in immunofluorescence assays to determine PVM affinity.

Molecular Dynamics Study of Ion Transport through a Carbon Nanotube in a Lipid Bilayer
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Ion channels in the form of integral membrane proteins are important structures for the function of multiple physiological processes. In particular, integral membrane proteins work to regulate the flow of ions across membranes in the nervous system. In order to develop a system with a constant chemical potential, a simple model was created. Rather than using complex proteins as ion channels, carbon nanotubes were used as a replacement. The ability of carbon nanotubes to facilitate ion flow was studied using molecular dynamics. A model was built with a lipid bilayer bisected by a carbon nanotube. Sodium and potassium ions were placed in water above the bilayer and chlorine ions were placed below the bilayer. To maintain separate salt baths, a unique boundary condition was required. Glide-plane boundary conditions, found in the program ESP, were used. Water and ion permeation through the nanotube were analyzed.
77 Investigating and Confirming Glycine Receptor Labeling with MTS- Benzophenone  
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As a member of the nicotinicoid super family, the glycine receptor (GlyR) is best known for its inhibitory role in neurotransmission involving the spinal cord and brain stem. Crosslinking can be used to study the allostrey of proteins, but verification of labeling with such reagents is an imperative first step. A methythiosulfonate (MTS)-benzophenone cross linking reagent modified with an alkyne tag was employed as a cross linking reagent by adding it in molar excess to a sample of pure GlyR that was reconstituted in mixed lipid/detergent micelles. The reaction time and temperature were varied to determine an optimum labeling condition. Confirmation of the labeling was then made by biotinylating the alkyne tag of the crosslinker and then probing for biotin using an IR-conjugated avidin probe.

78 Viability of the Purification of Cross-Linked GlyR  
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The glycine receptor (GlyR) is an important inhibitory ion channel found in the central nervous system. The viability of cysteine-labeling and subsequent purification of the protein was examined as a means to later shed light on the structure of an α1 homomeric wild type GlyR using crosslinking techniques. After solubilizing the GlyR protein from the extracellular membrane of Sf-9 insect cells, it was labeled with methanethiosulfonate-benzophenone crosslinker and then modified with an alkyne tag. The labeled protein was then purified. In order to confirm the success of GlyR labeling, click chemistry was employed to biotinylate the bound crosslinker and allow for probing with IR-conjugated avidin. If a label is introduced while the protein is solubilized and more structurally accessible, the presence of the label can be detected with IR-conjugated avidin.

79 A Mathematical Model of Glucose-Insulin Dynamics in Critical Care Patients  
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Elevated and highly variable blood glucose levels are commonly seen among critically ill patients and are associated with increased rates of morbidity and mortality [1]. Tight glycemic control (TGC) has been shown to improve these outcomes [2]. We evaluated the ability of our mathematical model [3] to capture glucose and insulin dynamics, using data from ten critically ill patients. The model was fit to patient data by varying parameters associated with insulin sensitivity and/or endogenous glucose production. Least squares error between model simulation and patient data was used to assess the achieved quality of fit. The patient model [3] effectively captured glucose dynamics of individual patients in the cohort. The performance of the model compared to that of Lin [4], which has also had success in fitting patient data. Further work will examine the merits of both models when utilized in a model predictive control algorithm to provide TGC.

80 Mixed Turing Patterns and Periodic Orbits  
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Since neurons are oscillators that may interact through inhibitory neurotransmitters, a theoretical knowledge of oscillators networked through inhibition underpins any knowledge of neural pattern generation, with applications to understanding movement and sensory perception. Prior experimental work on discrete Belousov-Zhabotinsky reactors, a chemical model of inhibition-linked oscillators, has uncovered an attractor with some reactors in steady state (a Turing pattern) and some oscillating. Unfortunately, this intriguing attractor appears rarely and only in certain models. Using bifurcation theory and automated parameter searches, we characterize conditions where this attractor is stable.
2012 Summer Undergraduate Research Symposium

81 Method Development: Use of NMR Crystallography to Determine True Crystal Structure
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The search for an efficient and accurate computational predictive method for determining the true crystal lattice structure of a particular substance is one that has been a challenge to physical chemists. A method using molecular dynamics calculations can accomplish this, but fails to predict the correct structure consistently. There is evidence to suggest that NMR crystallographic data can be used as a filter to determine a small set of possible structures. This set will likely contain a structure that is in agreement with a true structure known from neutron diffraction data. In addition, using density functional theory, plane-wave geometry optimization calculations, we can predict a structure with 98 percent confidence that will yield NMR principle and isotropic chemical shift values that are within 2 ppm of the neutron structure shift values. This experiment analyzes small sets of structures for four organic sugars for which reliable neutron diffraction data is available.

82 Solid State 29Si NMR study of Cyclosiloxane Crystals
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Silicon compounds have a variety of applications in many divisions of chemistry such as glass, cosmetics, and nanoparticles. Therefore, the molecular structure and electronic properties of these compounds are of great interest. The molecular structure of the compounds can be indirectly determined using solid state NMR spectroscopy by examining the observed chemical shift. Solid-state 29Si NMR experiments provide more information than liquid state experiments due to chemical shift anisotropy, which defines the localized bonding to a higher degree than isotropic values. The cyclosiloxane crystal compounds chosen for this study were selected for known crystal structures and the isotropic silicon shift changes with differing ring size. The crystals were also explored using different DFT electronic structure methods to predict chemical shift. Using the chemical shift anisotropy of silicon crystals with well-known structures, we can determine the relationship between the 29Si chemical shift and the electronic structure of the molecule.

83 Cytokine Capture for the Treatment of Sepsis
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Sepsis, a systemic inflammatory response resulting from infection, affects 750,000 Americans per year with a mortality rate of 30-50%. During sepsis, patients overproduce inflammatory mediators called cytokines, even after removal of the infection, often resulting in organ failure and death. Hemoadsorption devices engineered to remove cytokines from the bloodstream show promise in the treatment of sepsis by attenuating the dysfunctional inflammatory response. New bioincompatible sorbent materials designed for this application were studied in this work. These materials’ rate of cytokine capture over time was measured experimentally and, using an adsorption based model, the effectiveness of these materials was compared. Additionally, cytokine adsorption devices were created for in vivo animal studies to show the effect of cytokine adsorption on the survival rate of septic mice.

84 Computational Investigation of the Brucine-Derived Amino Alcohol Catalyzed Asymmetric Henry Reaction
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The enantioenriched Henry products were synthesized and analyzed from the use of metal-ligand complexes generated from Cu(I) and Zn(II) metals with readily available chiral amino alcohol. When using Cu(I) the enantioselectivity of the products generated 78-96% anti-Henry products (R,S) and 92-98% syn-Henry products (R,R). With Zn(II) the enantioselectivity generated yielded 28-60% anti-Henry products (S,R), (R,S) and 52-92% syn-Henry products (S,S). In order to understand the asymmetric origin of our catalysts, computational analysis was undertaken. Initially, the Henry reaction was modeled with aldehyde and nitro-ethane in the absence of metalated catalyst, to generate 12 plausible asymmetric Henry products. From these calculations four of the chiral products syn-(R,S), syn-(S,R), syn-(R,R), and syn-(S,S) were found to be most stable with the same activation energy. Of interest is on how the catalyst modifies the stereochemistry of the products. This study will highlight the electronic and steric considerations in explaining the role of Cu(I) and Zn(II) metalated brucine-derived amino alcohols in asymmetric Henry reactions.
A Facile Approach to Silicon Nanoparticles
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Silicon nanoparticles are ubiquitously used in various energy storage devices, semiconductors, biosensors, drug delivery etc. Mechanical milling is an attractive approach for generating bulk quantities of nano-silicon involving use of inexpensive precursors and processing equipment. Herein we report the synthesis of silicon nanoparticles by mechanically milling silicon monoxide and magnesium silicide. The product was acid washed to remove unwanted reaction products and further surface etched to generate high surface area, porous structures. X-Ray Diffraction (XRD) was used to study the kinetics of the milling induced chemical reaction between the oxide and silicide to form silicon. Results indicate a scalable alternative process to the hitherto complicated methods of Si nanoparticle generation by chemical and physical vapor deposition approaches.

Characterization of a Fluorogen Sensing Injectable Film
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The goal of this project was to investigate the interactions between the fluorogen-activating protein (FAP) dL5 and the amphiphilic peptide [AEAEAKAK]2, also known as “EAK”. dL5 is a dimer of two identical single chain antibody fragments (scFv) that has a specific affinity for malachite green (MG). When bound to the dL5 the fluorogen MG emits a strong fluorescence. EAK is a self-assembling peptide based platform that has the ability to form an insoluble film in the presence of saline. EAK can combine with similar peptides containing the same sequence. By introducing the self-assembling EAK platform to the dL5 it may transform the FAP into a biosensor that can be used for in vitro and in vivo applications. The hypothesis of this work was that the bi-functional protein, named dL5_EAK, would spontaneously integrate into films made of EAK.

Mössbauer Study of Europium Oxide Doped Hematite Nanoparticles
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Department of Physics, Duquesne University

Eu2O3 doped hematite nanoparticles were synthesized by mechanochemical activation using high energy ball milling for time periods ranging from 0 to 12 hours. High resolution spectroscopy analysis of the resulting nanoparticles was performed by transmission Mössbauer spectroscopy using an Fe-57 gamma ray source. Most spectra were fitted with two to three sextets indicating the substitution of Eu for Fe in the hematite lattice. For higher Eu2O3 concentrations, the addition of quadruple split doublet was necessary and represented the occurrence of a nonmagnetic phase. This phase corresponds to Fe substituting Eu in the Eu2O3 lattice. It was concluded that the mutual substitutions gave rise to a solid solution for the nanoparticles.

Vitamin D Receptor
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By studying the Vitamin D receptor (VDR), a member of the nuclear receptor family of transcription factor. Various proteins such as Phenylalanine, Leucine, Tyrosine were transformed and made in to alanine using NAMD. NAMD was used to run computation simulations that were then connected VDR to see how it was affected by alanine. The receptor was generated using 2D alanine scanning using CHARMM. Free energy perturbation examined the hydration of F2A and L2A. The substrate (1S,5S,Z)-3-((E)-2-(1-(2S,3R)-6-hydroxy-3,6-dimethylheptan-2-yl)-7a-methylhexahydro-1H-inden-4(2H)-ylidene)ethylidene)-5-methyl-4-methylene-n-cyclohexanol interacted with Vitamin D Receptor, results were analyzed and are to be reported in future data.
Vitamin D Receptor – Substrate Interactions
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Agonists and antagonists modulate the function of the vitamin D receptor (VDR) in such a way that can be used to control some diseases as well as improve the intake of vitamin D. The binding of substrates was studied using 2D alanine scanning to explore the VDR binding pocket. Substrate binding was also examined using interaction between active site residues and the natural hormone agonist 1,25D$_3$. The results from this natural hormone served as a control that would be compared to the effects of the interactions in which different agonists or antagonists were substituted. Using the CHARMM force field with NAMD, alanine scanning and free energy perturbations were performed. This computational approach was validated by performing simulations on the amino acid mutations D2A and Y2A. The results of the alanine scanning were compared to existing experimental data to quantify specific substrate-VDR interactions.

Interactions of a type II antagonist with the Vitamin D Receptor
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Allosteric effects on the function of the Vitamin D receptor (VDR) are of interest in the nuclear receptor (NR) superfamily. The receptor has been experimentally analyzed using a 2D alanine scanning technique. Substrate binding was investigated by computing the interactions between active site residues and specific type II antagonist (TEI9647) containing a methylene lactone with no bulky structure. The NAMD molecular dynamics program was used to carry out alanine scanning and free energy perturbation (FEP) with the CHARMM force field. Hybrid topology files were constructed for valine and glutamine amino acid residues. Validation of the hybrid topology files and the FEP method was carried out by examining the relative free energy of hydration for V2A and Q2A. The results of the computational alanine scanning of the VDR binding pocket are compared back to experiment.

Binding of the LAC67b Antagonist in the Vitamin D Receptor
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The allosteric network of the Vitamin D Receptor (VDR) has an important role within the nuclear receptor (NR) superfamily. The VDR allows for Vitamin D to be biologically active. The binding pocket of the VDR has been experimentally analyzed using a 2D alanine scanning method. Substrate binding was examined by computing the interactions between residues in the binding pocket and the antagonist substrate known as LAC67b. The molecular dynamics program (NAMD) was used to perform alanine scanning. Investigations in the relative free-energy of hydration for W2A and H2A mutations were used to validate the free-energy perturbation method. The computational analysis of the binding interactions between LAC67b and the VDR shows that there are energetic as well as structural consequences of allosteric effects on the Vitamin D Receptor’s function.
Finding the Diagonal Blocks of the Inverse of Large Matrices
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The Korringer-Kohn-Rostoker method (KKR) is a quantum mechanical approach to the electronic structure calculation for solid state materials. It is based on multiple scattering theory, in which each atomic ion is considered as an electron scattering center and the electronic states in a material are the solution of the multiple scattering processes by the atoms. The solution of the multiple scattering equation requires the inverse of a large matrix, also known as KKR matrix. Since we are only interested in the diagonal blocks of the inversed matrix, the diagonal blocks of the inverse can be individually computed by recursively applying an algorithm that only requires inverting matrices in a greatly reduced size. Because the time it takes to invert a matrix is proportional to n^3, the decrease in size of each matrix inversion greatly outweighs the increase in inversions needed. Parallelization of this technique can further improve its efficiency.

Characterization of Membrane Protein and Aqueous Protein Stabilities via Free Energy Calculations
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The classification of membrane proteins and aqueous proteins has traditionally been based on the observation that membrane proteins possess hydrophobic transmembrane regions that interact favorably with the membrane core while aqueous proteins have hydrophilic residues covering their surface. Nonetheless, there are numerous membrane proteins, such as voltage-gated channels, that must bury charged residues within transmembrane regions for proper function, which can be electrostatically unfavorable (Jan and Jan, 1990). The Grabe lab recently developed a computational model that showed that membrane bending can stabilize even highly charged voltage sensing helices (Callenburg et al., 2012). Here, I intend to use our model to calculate the stability of a set of membrane proteins and a set of aqueous proteins. I hypothesize that the aqueous proteins will be unfavorable in the membrane and that membrane proteins will be favorable. This work will help tune the model and explore physical aspects critical to membrane stability.

Biomineralization Approach to Titanium oxide coatings on AZ31 alloys
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Magnesium and its alloys are known to be extremely reactive and corrode quickly in biological environments. However, they are highly biocompatible, thereby making them potential candidates for degradable implant materials. Hence, studies are being performed to engineer the surface of these alloys with suitable coatings to allow for their controlled degradation. In this study, we are exploiting the bio-mineralization reactions of titanium (IV) bis(ammonium lactate) dihydroxide (TiBALDH) to coat titanium oxide on AZ31 alloys. The coated alloys are studied further for their surface morphology and corrosion characteristics using scanning electron microscopy, Raman spectroscopy and polarization tests. The developed coatings may also serve as scaffold materials for release of bone growth factors or immobilize biological molecules on the surface for further sensor development.

Viability and proliferation of Alginate encapsulated Human Embryonic Stem Cells into Islet cells type
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Through the application of specific culture conditions, human embryonic stem cells can be differentiated into insulin producing cells by chemical induction. This makes them a potential source for generation of pancreatic beta cells as a possible therapy for type1 diabetes. Cells are encapsulated in calcium alginate capsules due to the immunosolatation capabilities, making it a suitable platform for implantation. hESC are encapsulated as either undifferentiated or pre-differentiated definitive endoderm cells. Encapsulated cells were further matured towards the pancreatic islet cell types following a stage wise directed differentiation protocol. Viability and proliferation analysis are being conducted using the LIVE/DEAD assay and AlamarBlue at each stage of differentiation. While significant dead cells were observed after initial encapsulation, dead cells were less prominent towards the end of the protocol when small colonies of viable differentiated cells become dominant. Each stage of differentiation was confirmed by gene and protein analysis of the relevant markers.
97 Model Reduction as a Tool for Elucidating Key Dynamics in a Neutrophil Model of Inflammation and Cancer
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Mathematical models able to capture clinically-relevant dynamics and data can be powerful tools to aid clinicians in evaluating the effect of a medical intervention on patient response. We recently published a model of neutrophil and granulocyte-stimulating factor (G-CSF) dynamics that captures both fast (endotoxin challenge, inflammation) and slow (docetaxel chemotherapy, cancer) responses. This model, which reproduces the underlying biology of the neutrophil signaling cascade in both inflammation and cancer, is of high order (14 ordinary differential equations) and has multiple saturation nonlinearities. This complex structure is not a priori parametrically identifiable and is intimidating to the intended user: clinicians. We use model reduction techniques, both algorithmic and heuristic, that preserve input-output behavior of the model while simplifying the interpretation of the model states by focusing on key physical variables with clinical relevance. The result is a lower equation order with clearer interpretation and imitation into clinical observations and practice.

99 Benchmarking MPI-PHYLIP on Blacklight
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Phylogenetic study of protein sequences provides unique and valuable insights about the origins and development of physiological features in present day organisms as well as insights into the molecular and genetic basis of important medical and epidemiological problems. The MPI-PHYLIP code can help researchers perform phylogenetic study on data sets of hundreds of protein sequences. This study will benchmark the MPI-PHYLIP code on Blacklight, the world’s largest shared memory system. The alignments used in this benchmarking study include cytochrome B, cytochrome oxidase 1, cytochrome oxidase 3, ABCG transporters, and a set of G-alpha proteins.

98 Multi-Reservoir Host Model of the Evolutionary Dynamics of Influenza
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Reassortment of animal and human influenza strains has unexpectedly produced easily transmissible, lethal human strains giving rise to global pandemics. We use the Gillespie algorithm to stochastically implement an individual based simulation of the infectivity of the virus as a function of time. Our simulation captures the epidemiological dynamics by allowing for members to reproduce, die, recover, and gain immunity. We assign the degree of cross immunity between antigenic strains depending on similarity in phenotype rather than genotype. To determine phenotype similarity, we constructed a fitness landscape, which allowed for epistatic interactions between antigenic strains and recognized functionally conservative amino acid substitutions. We introduce multiple reservoir hosts such as pigs, birds, and humans to facilitate reassortment of genetic strains and consequently generate strains for which populations have little to no immunity. A more realistic viral evolution model is essential to gain insight into the frequency and severity of future pandemics.

100 Novel Tetradeutate Nitrogen Based Ligands for Atom Transfer Radical Processes
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Tris[2-aminoethyl]amine (TREN) based ligands were evaluated in copper catalyzed atom transfer radical addition (ATRA) in the presence of free-radical diazo initiator AIBN (2,2’-azobis(2-methylpropionitrile)). These studies were constructed by substituting various electron donating/withdrawing groups on the ligand. By substituting dimethyl groups and a chlorine atom on the benzyl rings of TREN based ligand, [Cu(TBEA-Me2)]Cl][Cl] and [Cu(TBEA-4-chloro)]Cl][Cl] complexes were synthesized. The study also was performed with a non-substituted ligand, [Cu(TBEA)]Cl][Cl]. It was hypothesized that the more electron donating the substituted ligand, the higher activity in ATRA. Cyclic voltammetry of the metal-ligand complexes have confirmed that higher active complexes also have more negative reduction potential (E1/2). Molecular structures of [Cu(TBEA)]Cl][Cl] complexes in the solid state have indicated that copper (II) center was distorted from trigonal bipyramidal in geometry due to the steric hindrance of the relatively large halogen atoms. Novel ligands were fully characterized using several spectroscopic techniques.
101 An Investigation of the Tribological Properties of Self-Assembled Monolayers  
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A self-assembled monolayer (SAM) is a two-dimensional molecular array that is spontaneously organized by adsorption of amphiphilic organic molecules on a solid inorganic surface. A typical SAM monomer consists of a head group that initiates binding to the substrate, a methylene backbone chain that influences the packing density of SAM by its length, and a tail group that determines the surface properties of the SAM. Interfacial properties of a SAM can be tailored simply by modifying the structure of the SAM monomer unit enabling the wide use of SAM in many fields including computer hard disk drives, micro-electromechanical systems (MEMS), etc. SAMs of n-alkyl carboxylic acids were formed on the surfaces of medical grade stainless steel (SS316L). Chain-length dependence on the frictional properties of SAMs was investigated with atomic force microscopy (AFM). The order and bonding nature of the SAM was observed with Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFT).

102 Design and Verification of a Device to Apply Shear Strain to Cell Sheets  
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Mechanical stimuli have significant effects on the behavior of cells and are linked to certain crucial events including cell differentiation and development of disease. The goal of this project was to design and test an apparatus that can controllably apply shear strain to cell sheets, as the effects of shear strain, the deformation caused by shear force, on such tissues are mostly unknown. Devices utilizing miniature springs were cut from polyester sheets using a KNKMaxx computerized cutter and attached to a computer-controlled stage which applied the necessary force. The springs' optimum parameters were estimated from the literature and confirmed experimentally through image capture and strain analysis programs in ImageJ. The shape of the spring, its dimensions, symmetry, and number of coils were all found to be important factors in how controlled the applied shear strain was. Testing of micro-scale tissue with the best spring design is ongoing.

103 Modeling the Process of T cell Differentiation  
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T cells play an important role in an adaptive immune response. Thus, understanding the process through which they differentiate from naïve to effecter cells is valuable. In this project, we use NetLogo to build an agent based model (ABM) in order to capture the dynamics of T cell survival, differentiation, growth, proliferation, and death. We start with a population of naïve cells which are stimulated by their specific antigens. Then, these activated cells express the growth factor known as interleukin-2 (IL-2) and α of the high-affinity IL-2 receptor, known as CD25, which allow them to bind with the IL-2 molecules present in the environment. After a sufficient number of bonds, T cells proliferate and differentiate into active effecter cells, which can act upon their target cells. An ABM allows for better understanding of the T cell dynamics and it can be used as a substitute for experimentation.

104 The Presence of Pseudo-Depletion Attraction in Micro-Particle Systems  
Blevins, Laura C.; Lash, Melissa H.; Little, Steven R.; McCarthy, Joseph J.  
Micro-particle based colloidal crystal structures serve as a potential architecture for biological applications due to their physiologically relevant particle/void sizes. A thorough understanding of the mechanisms governing their arrangement is imperative for fine-tuning the structures and improving their overall quality. This work investigates the forces that form hexagonally packed colloidal structures of these "large" particles by means of artificial thermalization. Prior studies of analogous systems on the sub-micron and nano-scale indicate that depletion attraction forces dominate the particle organization, but are negligible for larger particle systems, such as those examined here. In this study, we analyze the relative influence of capillary forces versus a "pseudo-depletion attraction" -- that is a consequence of our artificial thermalization -- on the packing structure of micro-particles for mono-dispersed, binary, and tertiary systems. The resulting structures demonstrate ordered hexagonal packing. These results suggest that both capillary action and a force similar to that of depletion attraction contribute significantly to the character of micro-scale colloidal structures.
Hyperglycemia is associated with, and may be causally related to, worse outcomes in critically ill patients [1]. To more closely simulate stress hyperglycemia and potential targets to modulate it, we propose a multiscale model simulating the impact of epinephrine, a key stress hormone, on glucose regulation. We integrate both cellular and whole-body dynamics of epinephrine-induced glucose regulation. Using an α2-adrenergic receptor model [4] and a pancreatic β-cell model [2], our model simulates α2-adrenergic inhibition of cyclic adenosine monophosphate production (cAMP). Decreased cytosolic calcium cAMP subsequently inhibits insulin exocytosis from pancreatic β cells. Macroscopically, our compartmental whole-body model [3] accounts for insulin, glucose, and free fatty acid dynamic interactions. In connecting these models, epinephrine data input into the cellular model curbs insulin secretion, which in turn varies dynamics of the whole-body model. In addition to identifying potential therapeutic targets which could mitigate stress hyperglycemia, our model can be used to evaluate catecholamine contributions to blood glucose changes during insulin therapy.

107 Characterization of Extracellular Matrix Secreted by Embryoid Bodies
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Extracellular matrix (ECM), the native microenvironment of cells which actively remodels throughout cell growth and differentiation, is key for cell survival. We hypothesize that ECM may be used as a platform to aid in the maintenance and directed differentiation of embryonic stem cells in vitro. The objective of this study was to characterize and compare ECM secreted by germ layers formed during spontaneous embryoid body (EB) formation and when induced by retinoic acid (RA) for enhanced ectoderm commitment. 0.1% Sodium Dodecyl Sulfate and 1% Triton-X 100 detergents were used to produce acellular murine EBs. Immunohistochemistry, DNA quantification, and protein quantification assays were used to confirm acellularity and characterize the ECM of EBs cultured under spontaneous conditions and EBs exposed to 1μM RA. Our results show that decellularization successfully removed nuclear material while maintaining ECM protein under both culture conditions; however, greater amounts of ECM protein were observed in spontaneous EBs.

106 Regulation of cell migration and differentiation by microparticle-based controlled delivery
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A characteristic symptom related to joint injury and disease is inflammation, leading to progressive tissue damage. Mesenchymal Stem Cells (MSCs) have been shown to possess a regulatory potential and to significantly reduce inflammation. Furthermore, MSCs can differentiate and promote tissue regeneration. The aim of this project is to recruit MSCs to the joint with the purpose to reduce inflammation and promote homeostasis to avoid tissue damage. To recruit MSCs, a chemokine gradient will be created; PDGF has been shown to be the most effective MSCs chemoattractant. It is encapsulated in alginate or PLGA microparticles to obtain different release profiles. The recruitment potential of each particle preparation is tested in vitro using an automated transwell system to monitor cell migration. Subsequently, controlled release of dorsomorphin, a synthetic molecule capable of avoiding the differentiation of MSCs towards bone, is also encapsulated in microparticles to achieve a controlled release and regulate MSCs differentiation.

108 Investigation of particle-level structures in oil and aqueous suspensions
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It has been shown previously in our group that adding moisture to granular materials allows for controlled mixing or segregation. This project focuses on expanding the aforementioned concept to colloidal systems consisting of discrete oil and aqueous phases with further focus on the creation of liquid bridges that cause this phenomenon. By manipulating the contact angle and particle size we can predict whether a given system will segregate or mix. Acrylic and glass beads in various hexadecane and water mixtures were investigated to identify the particle-level structure of suspensions. Many antibiotics and children medications are delivered as suspensions; therefore creating a robust method of controlling the particle-level structure of a given suspension could have implications for the pharmaceutical industry.
109
**Interdigital Alkylations: A Study of Stereochemical Control**
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Alkylations with secondary electrophiles containing two different substituents proceed with excellent diastereoselectivity. Stereochemical control results from the substituents of the chiral electrophile fitting like “digits” into the spaces of the attacking nucleophile. The two attacking enantiotopic faces of the nucleophile interdigital with the chiral electrophile results in two diastereomeric transition structures with significant energy differences. (1-Bromoethyl)-2-methylbenzene was synthesized and employed as a model electrophile, reacting with two anionic nucleophiles. A diastereomeric ratio of 100:1 was found by compound characterization, specifically ¹H NMR.

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**Forensic Analysis of Hairs: Identifying Styling Product Residues on Hairs by GC-MS**
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Forensic analysis of hairs is an important crime scene investigative tool. The residues present on hairs found at crime scenes have the potential to increase the information obtained from hair evidence. To help identify these unknown residues on a hair a Gas Chromatograph-Mass Spectrometer (GC-MS) is used. Hair products were mixed with different solvents such as Acetone, Hexane, Isopropanol, and Methanol. Then these samples were sonicated to extract soluble residues, and then analyzed by the GC-MS. After looking at these results from the GC-MS, a solvent was chosen and hair samples were collected. Finally, the ability to extract hair products from a single hair and identify the residue was tested.