1

Design and Synthesis of p25/CDK5 Inhibitors Based on Roscovitine

Gwenyth Bleasdell and Patrick Flaherty
Department of Medicinal Chemistry
Duquesne University

In Alzheimer's disease (AD) two aberrant proteins amyloid plaques (Aβ) and Neurofibrillary tangles (NFTs) have been identified. Aβ peptide is produced from soluble amyloid precursor protein (SAPP) as a result of two sequential proteolysis steps by β-secretase [beta-site Amyloid Precursor Protein Cleaving Enzyme (BACE)] then γ-secretase. NFTs, are made up of several proteins but primarily hypophosphorylated Tau.
P25/Cyclin dependant kinase 5 (p25/CDK-5), hypophosphorylates Tau at Ser 205 by using ATP as a phosphate source. This project seeks to design and synthesize inhibitors of p25/Cdk-5 based on the ATP binding site.

2

Synthesis, Physicochemical Characterization and Electronic Band Structure Calculations for $CuInS_2$:Mn

Kathryn B. Knorr, Jonathan W. Lekse, Heather A. Figore, Jeffry D. Madura and Jennifer A. Aitken
Department of Chemistry and Biochemistry, Duquesne University

$CuInS_2$ is a diamond-like semiconductor with possible applications in solar cells, nonlinear optics and spintronics. The objective of our research was to make a phase-pure sample of $CuInS_2$ and dope the compound with increasing amounts of Mn. $CuInS_2$ was synthesized by microwave irradiation, using time as a variable, to examine how the phase-purity was affected. However, it was determined that phase-pure samples were more easily prepared in a furnace. Doped samples of $CuInS_2$ were synthesized where either In or both Cu and In were replaced with small amounts of Mn. All resulting materials were analyzed using powder X-ray diffraction, differential thermal analysis and UV-Vis/NIR spectroscopy. The computer program CAESAR was used to perform electronic band structure calculations.

3

Molecular Flexibility to Explain Binding Strength between MHC and HER-2/neu Epitope (GP2)

Micker K. Samios, Edward G. Franklin, Wilson S. Meng, Jeffrey D. Evanseck
Center for Computational Studies
Department of Chemistry and Biochemistry, Duquesne University

GP2 (IISAVVGIL), a HLA_A*0201-restricted T-cell epitope and tumor vaccine candidate, binds MHC. It has been postulated that GP2 exhibits poor binding affinity MHC due to flexibility within the P5-P7 region and the P2 and P9 anchors. To gain a microscopic understanding for this poor binding, molecular dynamic simulations were used to compare the effects of the mutations and variations. V6Q and G7F, the influenza matrix protein epitope, FLU and a poly-substituted mutant, GEFF, were analyzed with respect to stable cell surface interactions, lowest energy conformations and hydrophobic/hydrophilic interactions with HLA-A*0201. Each mutation exhibited lower RMSD values, inferring greater stabilization, than GP2. The molecular reasons for reduced RMSD and tighter binding will be discussed.

4

Investigation of Septum Placement Genes in the Filamentous Bacterium *Streptomyces coelicolor*

Kathryn Pevey and Joseph McCormick
Department of Biological Sciences, Duquesne University

Streptomyces coelicolor is a filamentous, sporulating soil bacterium. During cell division, multi-nucleoid aerial hyphae divide synchronously into a chain of spores. The mechanism of cell division in *S. coelicolor* is not well understood, however many normally essential division proteins are dispensable in *S. coelicolor*. I am investigating homologues of the protein MinD, which might control position placement of the division complex during sporulation. There are several *minD*-like genes in the relatively large genome of *S. coelicolor*. I have constructed single mutants which knockout a *minD*-like gene in two wild-type strains of *S. coelicolor,* and a double mutant which knockouts two *minD*-like genes, to investigate the effects on cell division and sporulation. I am currently analyzing these division mutants with Southern blot hybridization analysis and complementation experiments.

5

Evaluation of the Structural Role of Proline In the Folding of α-Conotoxins

Heather L. Rust, KaLynn M. Kline, Alyssa M. Esposito, Jason R. Burkett and Balazs Hargittai
Saint Francis University, Loretto, Pa.

Conotoxins, disulfide-rich small peptides, may provide a crucial insight into pharmaceutical development without side-effects. The objective of this research was to investigate the effects of different amino acids in some key position in the sequence of α-conotoxins and compare oxidation results obtained under folding and denaturing conditions. Our studies focused on the folding of a α-conotoxins SI, SIA, GI, and MI. These thirteen-fourteen amino acid containing peptide amides have two disulfide bridges leading to three possible regioisomers. Most reduced forms of native conotoxins are able to fold to form the natural isomer. However, under certain conditions the oxidation of these peptides yields this native isomer in a mixture of the other two isomers. Our results indicate that peptides containing the cyclic amino acid proline had very high selectivity for the natural isomer, suggesting that this amino acid enforces a structural rigidity on the peptides.

6

Designer Drug Workbook

Christopher Sidun and Jeffry D. Madura
Center for Computational Sciences
Department of Chemistry and Biochemistry, Duquesne University

Molecular recognition is a concept used to explain how proteins selectively bind specific substrates (drugs). The workbook, aimed primarily at high school students, is an introduction to intermolecular forces, the structure and function of proteins, and to the concept of molecular recognition. Using the Molecular Operating Environment (MOE) software, and several carbonic anhydrase protein-ligand complexes, an easy to understand set of exercises were created that demonstrate the binding of ligands to the protein. Tutorials on how to use MOE and accessing the Protein Data Bank (PDB) were also developed. In conclusion, this workshop will give high school students the opportunity, knowledge, and drive to pursue a science related field, in which the use of this technology, specifically to find new drugs is used.

7

Polymer Fiber Analysis by High Performance Liquid Chromatography and Liquid Chromatography-Mass Spectrometry

Genna Andrews and Stephanie J. Wetzel
Department of Chemistry and Biochemistry, Duquesne University

It was determined that polymer fibers can be identified based on polymer additives and modifiers through High Performance Liquid Chromatography with Ultra Violet Detection (HPLC) and Liquid Chromatography-Mass Spectrometry (LC-MS). A variety of parameters were used to optimize the instrument settings. An isocratic solvent system of 100% acetonitrile with parameters set at 1.25mL/minute flow rate and 254nm and 280nm detection wavelengths for 10 minutes were optimal for liquid chromatography. Polymer fibers were extracted in a variety of solvents such as acetonitrile and methylene chloride by sonication. As a result of the identification of different additives and modifiers, such as dyes, UV additives and antioxidants, the source of the fiber may be identified.

8

Incorporation Of Novel Cyclic Amino Acids Into Peptide Sequences

Lauren N. Kulak, Joel D. Himes and Balazs Hargittai
Saint Francis University, Loretto, Pa.

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

9

Isolation and Analysis of Amides from Mammalian Tissues

Antonio J. Scatena, Korey Coulter, Mitchell E. Johnson
Department of Chemistry and Biochemistry, Duquesne University

Primary fatty acid amides (PFAM's) are an important class of bio-regulatory messenger lipids in mammals. The primary focus of this research is to study oleamide, an eighteen-carbon amide containing one double bond; denoted C18:1^9, and other PFAM's. Oleamide is one of many important bioactive lipids in mammalian systems. It was discovered in the cerebrospinal fluid of sleep-deprived cats. In this project, PFAM's were isolated through Folch-Pi extraction from various tissue samples, namely mouse stomach and liver, and most recently, bovine omentum. This extraction utilizes a chloroform-methanol solution to extract lipids from cells and tissues through homogenization. Solid-phase extraction (SPE) was employed to purify and selectively isolate PFAM's from the rest of the lipid extract. The isolated products were then diluted and analyzed using gas chromatography/mass spectroscopy (GC/MS). This method determines the identity and relative abundance of the amides isolated from the tissues samples by comparison to an internal standard. In addition, pure standard components of PFAM's are needed for method development and quantitative analysis. A PFAM library was synthesized from corresponding fatty acids and purified according to known procedures.

10

Deterministic Dense Coding Using General Quantum Operations

Michael Beran and Scott M. Cohen
Department of Physics, Duquesne University

This research considers the communication of messages (e.g., 0, 1, …, N) by sending a quantum system (Q_A) from one party to another. Dense coding utilizes entanglement of Q_A with another quantum system to increase the number of messages that can be perfectly transmitted. The dependence of the maximum number of transmittable messages on the shared entangled state was analyzed. In this protocol, the sender is allowed to use the most general quantum operations to encode their messages. It was found through numerical methods that the maximal alphabet size is an integer in the range [d,d^2], with the possible exception of d^2-1, as is the case with unitary encoding. Results show that encoding using more general operations does not increase the maximal alphabet size compared to isometric encoding. Also, for protocols where the transmitted system must be smaller than Q_A, it was found that a known upper bound on the number of messages is achievable.

11

A Mössbauer Analysis of Anatase Doped-Hematite

Ashley N. Sanns and Monica Sorescu
Department of Physics, Duquesne University

The Mössbauer Effect, which is the recoilless emission and absorption of gamma rays by atoms in a crystal lattice, has a variety of applications in nuclear, solid-state, and general physics as well as in areas of chemistry. In this experiment Hematite (Fe_2O_3) was doped with an anatase form of Titanium Dioxide (TiO_2) and studied by Mössbauer Spectroscopy. The samples were obtained by ball milling. The spectra were then fit with either two or three sextets. However, for several spectra a quadrupole split doublet was also introduced. This analysis showed that as higher levels of TiO_2 were introduced in the sample the strength of the hyperfine magnetic field decreased. At low Ti content there are various nearest neighbors in the hematite structure. At high Ti concentrations there are Fe substitutions in the TiO_2.

12

Identifying the Components of Scent Mark Production in Terrestrial Salamanders

William Largen and Sarah Woodley
Department of Biological Sciences, Duquesne University

Pheromones are chemosensory cues detected by members of the same species that affect physiology and/or behavior of the recipient. Salamanders like *Plethodon shermani* are good models for understanding chemical communication because they have simple stereotyped behaviors and rely on easily available pheromones for intraspecific communication. *P.shermani* scent mark by pressing the ventral surface of the tail base on a substrate. This area of the tail has specialized postcloacal glands not found elsewhere. Given that other pheromones in this species are proteinaceous, I attempted to characterize proteins found in secretions from postcloacal glands, dorsal tail skin glands, and muscle using SDS-PAGE gels. I found a ~31kD band unique to the in the postcloacal gland extract, suggesting that postcloacal glands secrete a pheromone that may signal gender, reproductive condition or individuality.

13

A New Method To Enhance Visualization Of Cyanoacrylate Fumed Fingerprints By Staining With Near-Infrared Dyes

M. J. Cunzolo and Mitchell E. Johnson
Department of Chemistry and Biochemistry, Duquesne University

In order to increase the level of contrast between a fingerprint and its background, scientists often utilize fluorescent dye staining coupled with laser induced fluorescence (LIF). However, conventional dyes only absorb in the UV-vis region of the electromagnetic spectrum. This poses a problem as many background surfaces also absorb in these regions. Accordingly, such surfaces may fluoresce and produce background interference. One viable alternative is near-infrared (NIR) fluorescence, which entails the staining of fingerprints with NIR dye. This method is appealing because few surfaces fluoresce when exposed to NIR radiation. Latent fingerprints were consequently fumed with cyanoacrylate, stained with various NIR dye solutions, rinsed with methanol, and excited with a diode laser at 788nm. Fluorescing prints were photographed with a CCD camera. This procedure easily visualized prints on surfaces known to be problematic for conventional development methods. Therefore, NIR-LIF represents a solution for conventional methods plagued by background interference.

14

Building a Capillary Electrophoresis/Fluorescence System

Joseph J. Rosmus and Rose A. Clark, Saint Francis University, Loretto, Pa.

Capillary Electrophoresis is a useful tool for separation of charged molecules as well as neutral molecules. Its ease of use and its speed make it a powerful tool in the separation of molecules, especially amino acids. Fluorescence detection is well known for high sensitivity and resolution. Fluorescence further adds to the power behind the capillary electrophoresis system. Details of capillary electrophoresis, fluorescence detection, and computer interfacing will be presented for the capillary electrophoresis system constructed. The newly constructed system was tested with the amino acid, valine, tagged with OPA to create an aromatic compound which fluoresces.

15

Expression and Purification of the Fragile X Mental Retardation Protein ISO1

Patrick Lackey and Mihaela Rita Mihailescu
Department of Chemistry and Biochemistry

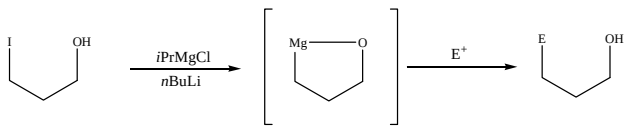
Fragile X Syndrome is one of the leading causes of inherited mental retardation, affecting 1 in 4000 males and 1 in 8000 females. The syndrome is caused by the silencing of the gene *FMR 1* coding for a protein named the fragile X mental retardation protein (FMRP). FMRP is an RNA binding protein that has been proposed to be involved in the transport and translation regulation of specific messenger RNA targets. The *FMR 1* gene has 17 exons and it has been shown that it can undergo alternative splicing that results in up to 20 FMRP isoforms. In this study we are attempting to express and purify the His-tagged FMRP isoform 1 (ISO1). Future work will involve the construction of the plasmids encoding for FMRP ISO8 and ISO9 and the study of the interactions of these different FMRP isoforms with different RNA targets.

16

Low Temperature Iodine-Magnesium Exchange at sp^3 Centers

Jenna Daggett and Fraser Fleming
Department of Chemistry and Biochemistry, Duquesne University

The chemistry of low temperature Iodine-Magnesium exchange has been examined. Halogen-Magnesium exchange at primary sp^3 centers remains a challenge in synthetic organic chemistry. Treatment of γ-hydroxy alkyl iodides with *i*-PrMgCl with subsequent *n*-BuLi generates magnesium alkoxides which readily react with various electrophiles to yield 1,3-difunctionalized asymmetric products.



17

The Investigation of Molybdenum Compounds using Cyclic Voltammetry

Alex Nunley, Dr. Barbara Serli Mitasev, Brian W. Kail, and Partha Basu
Department of Chemistry and Biochemistry; Duquesne University (Project SEED)

Cyclic Voltammetry is an electrochemical technique often used for investigating metal complexes. CV is a powerful tool for the determination of formal redox potentials, detection of chemical reactions that proceed or follow the electrochemical reaction and evaluation of electron transfer. In CV the current is measured as a function of the potential. The potential is linearly cycled from a starting potential to a final potential and back to the initial potential. The use of CV for investigating molybdenum compounds and their reactivity towards tertiary phosphines will be described. In particular the reaction between the Mo(VI) complex $TpMoO_2SPh$ (Tp = hydrotris(3,5 dimethylpyrazol-1)borate) and PMe_3 using cyclic voltammetry has been followed at different temperatures.

18

Drug-Induced Proteomic Changes in Breast Cancer Cells

Sheilah Curran, Miranda Sarachine, Billy W. Day
Department of Chemistry, University of Pittsburgh

The most common treatment for estrogen receptor (ER) positive breast cancer is tamoxifen, an antagonistic ERαligand. Although tamoxifen has been shown to be an effective treatment, about 40% of patients develop resistance to the drug. The purpose of this project is to identify the pathways employed by breast cancer cells after resistance to tamoxifen has been acquired. To identify these pathways, MCF-7, from human breast carcinoma, and MCF-7/LY2, an anti-estrogen resistant clone, cells were treated with tamoxifen. Their lysates were analyzed by difference two dimensional gel electrophoresis (DIGE), a technique wherein proteins in control and treated cultures are labeled with electrophilic dyes of differing fluorescence emission wavelengths. Gels were analyzed using DeCyder software and proteins showing altered levels of expression were analyzed using MALDI-TOF/TOF-MS. Additionally, selective ERβ agonists, genistein and DPN, are also being used in DIGE-based experiments to understand how targeting ERβ may be useful in developing a more beneficial breast cancer treatment.

19

Molecular Analysis Of The Lazy Gene In Maize

Jaime Wetzel and Mary Alleman
Department of Biology, Duquesne University

Plants that are homozygous for the "lazy" mutation in maize are disrupted in gravity sensing - mutant plants grow prostrate on the ground. Lazy mutants are negatively geotropic upon germination, become gravity-neutral as seedlings, and finally exhibit positive geotropism as adults. Other than this prostrate growth habit, lazy corn appears normal. Previous research using transposon tagging has supplied a plant-specific candidate gene for this mutation (the *la1* gene), and is supported by our data. Lazy mutations have been identified in other plant species including Arabidopsis and rice, but the mechanisms of these mutations are different from the maize gene, which is currently uncharacterized in any other plant. Thus, the significance of sequencing the maize lazy gene is that it will provide an alternate model for gravitropism in plants. Our research is to compare mutant (EMS and spontaneous) and wild type sequences of exons from the candidate *la1* gene by PCR and DNA sequencing.

20

Measuring Students' Understanding of DC Resistive Electrical Circuits

Kara Evanoff and Darryl Ozimek
Department of Physics, Duquesne University

In this study, the effects of level of instruction on student performance on the Determining and Interpreting Resistive Electric Circuit Concepts Test (DIRECT) version 1.0 were investigated. DIRECT is an instrument that assesses basic theoretical and applied understandings of DC electric circuits, energy, current, and potential difference. Duquesne University students enrolled in a conceptually-based introductory physics course for non-science majors and an algebra-trigonometry based course for life science majors participated in the study. Through individual test item and overall performance analysis, it was found that the level of instruction is not a factor whereas gender is a factor upon overall performance. Each class independently did not show any gender bias. Overall, Duquesne students scored lower when compared to a previous study; however, their scores followed a normal distribution.

21

Effects of Steroid Hormones on Growth of MG-63 Human Bone Cells

Jessica Geisler, Kyle Selcer
Department of Biological Sciences, Duquesne University

Osteoporosis currently affects 10 million people in the United States, the majority of which are women. It is a skeletal disease characterized by low bone density and a deterioration of bone, leading to fractures. Risk factors for osteoporosis include: reduced levels of estrogens in women and androgens in men, or exposure to certain medications. Steroid hormones are involved in normal bone physiology and in osteoporosis. Estrogens directly stimulate osteoblasts, the bone forming cells, and directly inhibit osteoclasts, the bone resorbing cells. In postmenopausal women, levels of estrogens decrease, leading to an increase in susceptibility to osteoporosis. In contrast, glucocorticoids result in reduced bone density and can cause osteoporosis. This is especially evident in persons requiring extensive glucocorticoid treatment for inflammation. Despite the well-known associations between bone physiology and steroid hormones, little information is available on direct effects of steroids on bone growth and metabolism. The objective of this study was to examine the effect of steroid hormones on growth of the MG-63 human bone cells line. Bone cells were grown in the presence or absence of steroid hormones (estrogens or glucocorticoids) in a steroid-free medium, after which cell number was determined using an MTT assay. The results of these experiments will be discussed.

22

Synthesis and Study of the Mn-doped, Ternary Chalcopyrite $CuInSe_2$

Carly N. Kline, Jonathan W. Lekse, Anna M. Pischera, Molly L. Gahan, Jeffry D. Madura, and Jennifer A. Aitken
Department of Chemistry and Biochemistry, Duquesne University

$CuInSe_2$ was synthesized using innovative microwave irradiation and traditional solid-state high temperature reactions. This compound is a diamond-like semiconductor, making it potentially useful in nonlinear optics, spintronics, and photovoltaics. The goal of the project is to synthesize and study a diluted magnetic semiconductor by doping $CuInSe_2$ with Mn in varying amounts to produce $CuIn_{1-x}Mn_xSe_2$ and $Cu_{1-y}In_{1-y}Mn_{2y}Se_2$ ($0.0125 \leq x = 2y \leq 0.2$). The resulting microwave and furnace products were characterized using powder X-ray diffraction, differential thermal analysis, and UV/Vis/NIR spectroscopy. Lattice parameter variations as a function of Mn concentration were also analyzed. In addition, CAESAR, a program for electronic band structure calculations, was used to determine the density of states and dispersion plots for $CuInSe_2$.

23

Identification of Carpet Fibers using GC-MS and Microwave Assisted Extraction

Nicole Navolio, Christopher Powell, Stephanie Wetzel
Department of Chemistry and Biochemistry, Duquesne University (Project SEED)

The purpose of this project was to develop the most effective fiber extraction method that would remove the polymer additives within the fibers, such as plasticizers, coatings, stabilizers and dyes. After comparing Microwave Assisted Extraction (MAE) to ultrasonication, it was determined that MAE was the most successful extraction technique. Fibers from household carpets were microwaved using a variety of different solvents and different solvent mixtures until the most efficient solution was found. Also, the time and temperature were altered and compared until the best method was verified. A GC-MS was then used to identify the components within the extracted fibers. The conclusions of this project will ultimately assist the field of Forensic Science, making it easier to connect fibers from crime scenes to criminals.

24

Biodegradable Dendritic Polymers for Biomedical Applications

Katie Murt, Toby Chapman, and Peter Bell
Department of Chemistry, University of Pittsburgh,

A new dendritic polymer is being developed from a hybrid of glycolic acid and lysine. This polymer will contain ester linkages, making it more suitable for applications like drug delivery. Dendritic polymers have gained considerable interest due to properties which make them ideal for biomedical uses. For instance, in addition to drug delivery, dendritic polylysine-poly(ethylene glycol) copolymers have been used in tissue engineering and gene therapy. However, the biodegradability of these copolymers is less than ideal. It is hoped that the ester linkages contained in the new polymer will allow for easier degradation in the body and will, therefore, be more effective for biomedical uses. In addition, the polymer will contain terminal amine groups which will allow for chemical modification of the periphery.

25

LOZENGE and its Effect on the Expression of the Downstream Genes *Brakeless* and *PTP69D* in the Developing *Drosophila* Eye

George Lincoln and John Pollock
Department of Biological Sciences, Duquesne University

The Lozenge protein influences the expression of the genes *brakeless* and *ptp69D*. Axon growth and targeting in the developing *Drosophila* eye disc are dependent upon these genes. The Lozenge protein can be categorized as a transcription factor. Transcription factors function to turn on and off a variety of subsequent genes involved in eye development. LOZENGE itself is regulated in response to the Ras/Map kinase pathways. Utilizing quantitative PCR and immunohistochemistry, it was shown that *lozenge* mutants display irregular eye development. Due to the inferred link from computer analysis between LOZENGE, *brakeless*, and *ptp69D* it is likely that the Lozenge protein influences expression of these genes.

26

X-Ray Crystallography identification of Bis-Amino Acid Oligamers

Christopher Preece, Chris Schafmeister and Graduate Student Zack Brown
Department of Chemistry, University of Pittsburgh

X-Ray Crystallography is an analytical technique used to identify the structure of molecules by the pattern in which it diffracts x-ray beams. Crystallography gives the best evidence to indicate what a substance is and its structure. This technique requires a pure crystal of your molecule. To get a crystal we used the sitting drop method, we screened over 200 different solutions to see what gave the best reproducable conditions to grow our molecule, a bis-amino acid oligamer (NapthylAlanine-Pro4-S,S- Pro4-R,R,- Pro4-R,R- Pro4-S,S-Lysine). This molecule is a rigid building block used in the Schafmeister lab to avoid the protein folding problem; this allows them to build macromolecules with many amino acids in a desirable arrangement.

27

The Isolation and Quantification of Primary Fatty Acid Amides (PFAM's) in Mammalian tissue

Geralda Joseph, Korey Coulter**,** Mitchell E. Johnson,
Department of Chemistry and Biochemistry, Duquesne University

Fatty acid amides comprise one of the important classes of bioactive lipids found in mammals. N-acylethanolamines (NAE) and PFAM's are two important families of this class. Members of both of these families consist of long chain saturated and unsaturated fatty acids which are considered as bio-regulators due to their hormone like activities.
In this experiment, PFAM's were isolated and quantified from the lipid extracts of frozen rabbit tissues and bovine samples. Isolation and separation of the amides occurs by preparation of the tissue in which the tissue sample is weighed to be greater than 0.8 g but less than 1 g. Homogenizing reduced fatty acid to particles, dispersing the tissues throughout fluids to make uniform in consistency. HPTLC (High performance thin layer chromatography) or SPE (solid-phase extraction) provided the complete separation of amides from total lipid extract and allowed their concentration for interference free and quantitative detection by GC/MS.

28

Identification of a Novel Protein Involved in the Degradation of CFTR, the Protein that when Mutated Causes Cystic Fibrosis

Lindsay R. Pereira[1], David H. Walls[1], Jennifer L. Goeckeler, Annette Ahner, and Jeffrey L. Brodsky
Department of Biological Sciences, University of Pittsburgh
[1]Co-presenters

Secretory and membrane proteins are folded and modified in the Endoplasmic Reticulum (ER). A quality control mechanism, ER-associated degradation (ERAD), recognizes and removes aberrant or unfolded proteins from the ER to the proteasome for degradation. If ERAD is insufficient to remove accumulated unfolded protein, the Unfolded Protein Response (UPR) is initiated. This signal transduction pathway leads to increased synthesis of folding and degradative enzymes, allowing the ER to manage the unfolded protein load. The cystic fibrosis transmembrane conductance regulator (CFTR) protein is prone to misfolding, and the majority is degraded by ERAD. Identification of genes transcriptionally upregulated in response to CFTR expression in yeast yielded expected results: ERAD pathway components, and also several previously uncharacterized ORFs with possible connections to ER quality control. Deletion of one of these genes inhibits CFTR degradation, indicating a role for the ORF in ERAD, however it does not induce the UPR, suggesting that overall ER quality control is not affected. We are currently examining CFTR degradation and UPR induction in the remaining ORFs.

29

Molecular Dynamic (MD) Simulations of $O_{10}H_6$ Peptide in Solution and Spectrophotometric Analysis of its Lysing Properties

Shaun-Pierre Hall, Anne Loccisano, Jeffrey Kovacs, Jeffrey D. Evanseck, Wilson S. Meng,
Department of Chemistry and Pharmaceutical Sciences Duquesne University, Pittsburgh, Pa.

A short cationic peptide, $O_{10}H_6$ (ornithine*10, histidine*6), with known DNA condensation capability has been studied for its lysing properties. The inclusion of histidines was hypothesized to provide escape from harsh pH conditions of the endosomal pathway. A hemolysis assay was used to evaluate the membrane-destabilizing activity of $O_{10}H_6$ as a function of pH, concentration, and/or states of protonation. Multiple (MD) simulations of $O_{10}H_6$ were done at three different protonation states using the micro-canonical ensemble to explore conformations over 1 ns. For each protonation state, six 1 ns MD simulations were carried out. Superimpositions, RMSDs, and quantitation were used to observe and analyze different structures to interpret the relationship between lysing properties and conformational change.

30

The Potential Transformation of Roxarsone, 3-amino-4-hydroxybenzenearsonic acid, and 4-hydroxybenzenearsonic acid Under Anaerobic Conditions by Bacteria in Chicken Litter Enrichments

Michael Gresock [1], John F. Stolz [1], Partha Basu [2], and Bryan Crable [1]
Department of Biological Sciences [1] and Department of Chemistry and Biochemistry [2] Duquesne University, Pittsburgh, Pa.

The organo-arsenical 3-nitro-4-hydroxybenzenearsonic acid (roxarsone) is often employed as a feed additive in broiler chickens. Roxarsone has been shown to transform to 3-amino-4-hydroxybenzenearsonic acid (3A4HBAA) under anaerobic conditions by bacteria in fresh chicken litter. This project attempted to determine whether bacteria in chicken litter could also degrade 3A4HBAA and 4-hydroxybenzenearsonic acid (4HBAA). Growth studies were conducted providing roxarsone, 3A4HBAA and 4HBAA as the electron acceptors and fructose as the electron donor. Growth curves, UV-VIS scans and HPLC samples were taken from the chicken litter enrichments at 0, 6, 12, 20, 28, 36, 48, 60, and 72 hours. Although the bacteria grew in the presence of each organo-arsenical, only degradation of roxarsone and 4HBAA was observed. Attempts to isolate 4HBAA transforming bacteria were made using serial dilutions and streak plating. Examination of the enrichment cultures by light microscopy revealed the bacteria responsible for transformation were motile rods.

31

The Role of *EcCad1* in Anterior-Posterior Axial Development and Gut Formation

Stephen Sandelich and Richard Elinson
Department of Biological Sciences, Duquesne University

The direct developing frog, *Eleutherodactylus coqui,* is unusual in that it bypasses the tadpole stage. We are investigating how the expression of various genes caused such a radical change in development. The caudal gene family encodes transcription factors which are involved in setting up the anterior-posterior axis in the frog *Xenopus* and are also expressed in the developing gut. I am investigating the orthologue of *XCad1* in *E. coqui, EcCad1.* Using a 680 nucleotide *EcCad1* probe, *in situ* hybridization shows posterior expression in neural tube stages, suggesting a role in the anterior-posterior axial development. *EcCad1* is also expressed in the dorsal side of the developing gut while being absent in the ventral portion. The dorsal cells form an epithelium while the ventral cells are very large and yolky. This result suggests that these ventral cells are used for nutrition and do not contribute to the developed gut tube.

32

The Continuing Controversy of Stepwise and Concerted Mechanisms of the Diels-Alder Reaction Involving Lewis Acids

Anthony Ross, Joshua Plumley, and Jeffrey Evanseck
Center for Computational Sciences and Department of Chemistry, Duquesne University

Density functional and QCISD(T) theories with the 6-31G(d) basis set were implemented to study the stepwise and concerted mechanisms of the butadiene and acrolein Diels-Alder reaction catalyzed by BF_3. Solvation was included using Tomasi's polarizable continuum model. The activation barrier for the concerted mechanism was 36.9 kcal/mol lower, in the *exo-trans* configuration, than for the corresponding stepwise pathway for the parent reaction without the Lewis acid. The Lewis acid catalyst, BF_3, lowered the activation energy difference between the concerted and stepwise reactions however; the concerted mechanism is predicted to be the dominant pathway. The computed results show that even with a polarizing Lewis acid, the concerted mechanism is followed without competition from the stepwise pathway.

33

Development of Flexible Antennae Using Single-Walled Carbon Nanotubes

Aaron Crandall and Alexander Star
Department of Chemistry,
University of Pittsburgh

In recent years, nanotechnology has become a prominent field of study, with materials showing the promise of many remarkable applications. Among these materials is the single-walled carbon nanotube, a single molecule of carbon which is built like a sheet of graphite rolled into a tube, and acts, depending on specifics of its structure, like either a metal or a semiconductor. Using commercially available spraying technologies, solutions of single-walled carbon nanotubes in different solvents were sprayed onto flexible substrates through a template of the desired structure, and the effectiveness of each method in depositing useful films of nanotubes was compared by resistivity, visual inspection, and by SEM to determine the ideal method.

34

Nucleophilic Addition Reactions Of Nitrile-Stabilized Carbanions

Sarah Gibbons, Douglas J. Fox, Jeffry D. Madura
Center for Computational Sciences, Department of Chemistry and Biochemistry
Duquesne University

Nitrile-stabilized carbanions are important synthetic intermediates, used to form carbon-carbon bonds, an essential step in preparing many organic compounds. The alkylation reaction of nitrile carbanions in solvent and in the presence of different cations is not well understood. Using the nucleophilic addition reaction of 1-methyl-cyclopentane nitrile anion with methylchloride as a model, we applied electronic structure methods to explore this reaction with and without THF and lithium. Gaussian 03 was used to calculate the geometries and energies of the reactants, transition states, and products to determine the relationship between the solvent / N-lithiated nitrile and the stereochemistry of the nucleophilic addition reaction. We were able to locate bare and solvated transition states for the reaction at the MP2/6-31+G(d) level of theory.

35

Social Organization and Migration in Feral Cat Populations in S.W. Pennsylvania.

Diana Walton, Maria Demetriou, and Lisa Ludvico
Department of Biological Sciences, Duquesne University

Feral cat numbers are estimated at over 100 million in the United States. The "feral" state describes a condition under which the animals have reverted back to their wild state. This study attempts to examine the underlying social framework of these cat colonies. Information on cat colonies in S.W. Pennsylvania was obtained from the bi-monthly spay and neuter clinics sponsored by the Homeless Cat Management Team (HCMT). Data on colony size, general location, and membership was recorded at these clinics. In addition, biological material (ear-tips; the left ear is slightly trimmed in order to identify cats that have been sterilized) was collected for genetic analysis. A microsatellite marker system was used to establish relatedness among and between cat colony members, if any existed. Also drop-off cats (recently discarded house pets) can be differentiated from migratory feral cats.

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Kinship Coefficients in Feral Cat Colonies

Maria Demetriou, Diana Walton and Lisa Ludvico
Department of Biological Sciences, Duquesne University

Degrees of relatedness among and between feral cat colonies in S.W. Pennsylvania have been analyzed in this study. Feral animals are defined as once domesticated species that have reverted back to their wild state. This study uses genetic material obtained from cats brought into the Homeless Cat Management Team's bi-monthly spay and neuter clinics. These cats are part of a Trap, Neuter and Return initiative to reduce or stabilize feral cat numbers, which are currently estimated at over 100 million in the United States. These cats are ear-tipped as a means to permanently mark them as non-reproductives. The ear tips are the source material for DNA extraction. Cat colony composition was genetically analyzed to determine if these colonies are kinship-based, or are comprised of unrelated individuals. A microsatellite marker system was employed to determine relatedness within individual cat colonies.

37

Small Molecules as a Possible Solution for Radiation Sickness and Abnormal Iron Homeostasis

Robert Joseph, Dr. Kazunori Koide (P.I.)
Department of Chemistry, University of Pittsburgh

Millions of people are sick due to excessive iron in their blood. If excessive levels of iron are maintained, death or permanent internal organ damage could result. In another study, due to the increase of proliferation of nuclear weapons, countless people could suffer from radiation poisoning and its other ill effects. These two separate problems will be addressed by using the plant extracts resveratrol and yohimbine and chemically transforming the molecules to improve efficacy. We discovered that resveratrol acts as an effective anti-radiation medicine and yohimbine has shown promise to treat excessive iron via translational activation. The poster display will describe more detailed background information, justification, recent progress, and future plans.

38

Polymer Fiber Additive Analysis by Gas Chromatography/Mass Spectrometry

Christopher Powell and Stephanie J. Wetzel
Department of Chemistry and Biochemistry, Duquesne University

Polymer additives used to manufacture fibers vary amongst manufacturers. Analysis of the polymer additives was done using Gas Chromatography/Mass Spectrometry (GC/MS). Various extraction methods and parameters were explored. Extraction techniques were found to influence the quality of data obtained. A variety of solvents were used for both Ultra-Sonification and Microwave Assisted Extraction (MAE) techniques. Extraction parameters were manipulated to optimize the efficiency of analysis for possible use in the Forensics field. The use of GC/MS for analysis would quantify fiber analysis based on additive components. This method surpasses the specificity of current quantitative fiber analysis techniques such as microscopic analysis and Fourier transform infrared radiation spectroscopy (FTIR).

39

A Population Firing Rate Model of Reverberatory Activity in Neuronal Networks

Zofia Koscielniak[1, 2] and G. Bard Ermentrout[3]
[1] Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh
[2] Carnegie Mellon University
[3] Department of Mathematics, University of Pittsburgh,

Synaptic activity based on neurotransmitters has been thoroughly described by mathematical models. Most of the existing models, however, disregard asynchronous synaptic transmission, another type of synaptic signal. Asynchronous synaptic transmission has been shown to elevate the potential of the cell slightly, causing active potentials that would not occur otherwise, and take a much longer time to return to resting state then the regular neurotransmitter signal. In this presentation, we will discuss our results in 1) creating firing rate models of neuronal networks incorporating asynchronous synaptic transmission as well as spike frequency adaptation or synaptic depression 2) creating network models with all neurons affecting each other based on the firing rate models 3) analyzing all models. These results emphasize the impact of asynchronous synaptic transmission on neural activity.

40

Effects Of Changing Self-Assembled Monolayer Composition On Cytochrome *C* Electron Transfer Kinetics

David J. Kirby, Kimberly A. Schrock, and Rose A. Clark, Saint Francis University, Loretto, Pa.

Cytochrome *c* in the mitochondria transfers electrons between inner-membrane proteins, cytochrome *c* reductase and cytochrome *c* oxidase. To study cyt *c* in vitro a mimic of the natural system is created by electrostatically adsorbing cyt *c* to carboxylic acid-terminated alkanethiols self-assembled onto a thin gold film electrode. The self-assembled monolayers that facilitate electron transfer were varied in order to compare changes in cyt *c* rate constants within each group. The rate constants were found by using cyclic voltammetry and Marcus Theory. Changes in the cyt *c* electron transfer rate for the varying mixed SAM's is related to the length of the carbon chains of the alcohol diluent thiols. Differences in cyt *c* kinetics were observed for the mixed methyl and mixed alcohol terminated diluent thiols. Comparisons of the various SAM systems will be presented.

41

A Concise Synthesis of 1,3-Disubstituted Beta-Carbolines

R. Troy Hull and Michael S. Leonard
Department of Chemistry, Washington & Jefferson College, Washington, Pa.

A robust, three-step sequence for the synthesis of 1,3-disubstituted beta-carbolines has been developed. Tryptophan derivatives are condensed with ninhydrin via Pictet-Spengler reaction. Lewis-acid induced rearrangement of the resultant spirocyclic heterocycles provides the yohimbanone framework, which is subject to oxidative ring cleavage to yield beta-carbolines. Novel analogues have been prepared by expanding this synthetic method.

42

Biophysical Study of Mixed Guanine and Adenine RNA Quadruplexes

Joshua Lipay and Mihaela Rita Mihailescu
Department of Chemistry and Biochemistry, Duquesne University

G quadruplexes, which are formed by both DNA and RNA with specific sequences, are proposed to be important in a variety of biological processes. Such structures, formed by stacking rings of four guanine residues, are stabilized by Hoogsteen H-bonds, and the presence of K^+ ions. It has been proposed that not only stretches of Gs can form quadruplexes, but also mixed purine sequences, in which adenines are flanked by guanine residues. In this study, a series of spectroscopic techniques such as circular dichroism (CD), NMR, and UV-Vis spectroscopy, along with native gel electrophoresis, were employed to monitor the impact the introduction of adenine residues has upon the structure and stability of an intermolecular RNA G-quadruplex. Three RNA oligonucleotides were used: a control, r(UGGGGGU), that easily formed a five-layer quadruplex and two others, r(UGGAGGU) and r(UGGAAGU), that contained mixed purines.

43

Development of a Powder X-ray Diffraction Laboratory Module for use in Honors General Chemistry: A Powder Identification of Unknown Household Solids

Molly L. Gahan, Jasmine Blair, Peter Wildfong and Jennifer A. Aitken
Department of Chemistry and Biochemistry, Duquesne University

Many of the items that we encounter in our homes on a daily basis are crystalline in nature. X-ray diffraction is a common method used to identify crystalline materials and mixtures, since each crystalline solid produces a unique powder pattern, like a fingerprint. In this research project, a powder X-ray diffraction (PXRD) module is being developed for use in Honors General Chemistry at Duquesne University. Students will be supplied with a white, unknown, powdered crystalline solid that they will identify using PXRD. This module will reinforce the concepts of basic crystalline solids covered in lecture. A number of household items have been studied as potential unknowns. Once a pattern has been obtained from the ground solid, it is analyzed using a software package and compared with patterns in the Powder Diffraction File. Several household items have already been identified as appropriate unknowns. Cosmetics and toothpaste have been excluded as potential unknowns due to their pattern complexity.

44

Microwave Synthesis Of Intermetallic Compounds

Tristan Stagger, Jonathan W. Lekse, Jennifer A. Aitken, Department of Chemistry and Biochemistry, Duquesne University (Project SEED)

Microwave irradiation is a unique process that can be applied to many different areas of chemistry. Microwave synthesis has a number of advantages over other synthetic techniques, due primarily to the short reaction times. Microwave reactions typically take only a few minutes. Solid-state microwave synthesis has been used to prepare carbides, complex oxides, metal vanadates, and chalcogenides, among many others. Even though solid-state microwave synthesis has been used to synthesize many compounds, it rarely has been used to prepare intermetallic materials. The goal of this research is to determine which intermetallic compounds can be prepared using solid state microwave synthesis. The microwave syntheses of intermetallics in the Cu-In, Ag-In, and Co-Sb systems were attempted. The reaction products were characterized using powder X-ray diffraction, diffuse reflectance spectroscopy, scanning electron microscopy, and energy dispersive spectroscopy. The results of these experiments will be presented.

45

Method Development for Gas Chromatography/Mass Spectrometry

Valerie Schrott, Jonathan Sirianni, and Rose A. Clark, Saint Francis University, Loretto, Pa.

Gas chromatography-Mass spectrometry is used to examine different compounds and their fragmentation. The goal of the research being done this summer was to develop experiments to be used at SFU in the chemistry department and to assist with ongoing research projects. An arson lab was designed to examine samples burnt with various accelerants. In addition, a THC lab was also developed to test suspect vegetation for the presence of the active ingredient in marijuana. A cocaine lab developed last summer was further explored to introduce quantitation features available in the XCalibur program. The GC/MS was also used to investigate self-assembled monolayer formation on gold electrodes. The SAM solution is 1:1 mixture of two different thiols, and the GC/MS can run the solution of the thiols stripped from the electrode to discover the concentration ratio.

46

Biophysical Study Of The HSV-1 ICP27 RGG Box Interactions With RNA

Medhavi Bole and Mihaela Rita Mihailescu
Department of Chemistry and Biochemistry, Duquesne University

Herpes simplex virus type1 (HSV-1) is a common human herpes virus that can cause asymptomatic infections, or can even be life threatening in individuals with repressed immune systems. HSV-1 ICP27 is an RNA binding protein required for regulating viral post-transcriptional gene expression, host cell shutoff, and HSV-1 lytic replication. The protein has been shown to use its RGG box to interact in vivo with specific HSV-1 mRNAs. It has been hypothesized that ICP27 RGG box-RNA interactions involve the recognition of RNA G-quartet structures. UL15i RNA and UL16 RNA are two such HSV-1 mRNAs, and in this study we are analyzing their interactions with the ICP27 RGG box. These RNAs are expressed and purified and the presence of G quartet elements in their structure will be tested by using circular dichroism (CD) and UV-Vis spectroscopy.

47

Inferring Modes of Selection on Copulatory Plug Genes in Chimpanzees

Michelle Marks and Michael Jensen-Seaman, Department of Biological Sciences, Duquesne University

Humans and chimpanzees differ physiologically in the consistency of their semen. This physiological difference is related to the sexual behavior of each. Humans have a gelatinous ejaculate, and typically have a one male-one female sexual relationship. Chimpanzees produce a firm rubbery copulatory plug which presumably functions to block the sperm of future males. This reflects the chimpanzee sexual behavior in which a female will mate with multiple males, fostering a high level of sperm competition. In this study, I examined the genes *KLK3*, *TGM4* and *ACPP* which are important in the formation of the copulatory plug. I sequenced 1 kilobase intronic segments of these genes in twelve chimps from three subspecies: the West African chimp (*Pan troglodytes verus*), Central African chimp (*Pan troglodytes troglodytes*), and the East African chimp (*Pan troglodytes schweinfurthii*) in order to determine levels of nucleotide diversity. The nucleotide diversity at these three genes is compared to a previously published larger set of fifty noncoding regions in order to distinguish between positive selection, purifying selection, and diversifying selection.

48

A Combinatorial Approach To The Van Leusen Multi-Component Reaction Employing Fluorous Solid-Phase Extraction For Purification

Wesley D. Carroll, Stefan Werner, Peter Wipf*
Center for Chemical Methodologies and Library Development, University of Pittsburgh

Fluorous solid-phase extraction (FSPE) provides a means to purify compounds on the basis of being fluorous and non-fluorous. Perfluorinated carbon chain tags were implemented in the van Leusen multicomponent reaction (MCR), which provides 1,4,5 substituted imidazoles *via* an amine, aldehyde, and a toluenesulphonylmethyl isocyanide (TosMIC) reagent. Following the three-component reaction, ring-closing metathesis was conducted, which cleaves the fluorous tag to provide an organic scaffold with significant molecular complexity. FSPE was employed throughout the synthesis to provide a rapid and efficient means to purify intermediates. The diversification of the van Leusen MCR will be reported.

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SAMs of Phosphonic Acids on Stainless Steel 316L

Danielle Ries, Aparna Raman, Ellen Gawalt
Department of Chemistry and Biochemistry, Duquesne University

Stainless steel is widely used in biomaterials but the only problem with it is that protein and cells attach to the surface causing a build up in cells. To prevent protein and cell attachment to the biomaterial, which may cause health problems, self assembled monolayers have been developed. SAMs of 11-hydroxyundecanephosphonic acid (OH-PA), octadecylphosphonic acid (ODPA), and 12-carboxydodecanephosphonic acid (COOH-PA) were made on stainless stee! l 316L substrates. Diffuse reflectance infra red spectroscopy was used after deposition to characterize the monolayer. Rinse and tape tests were used to determine if the self-assembled monolayers were strongly attached to the surface. VCA optima was used to determine the contact angle and hence the hydrophilicity of the substrate. Control, OH-PA, COOH-PA and ODPA modified samples were subjected to UV light to see if the formation or composition changed after irradiation. The reactivity of the OH and COOH tail before and after UV radiation were tested by reaction with dyes.

50

First Pass Monte Carlo Simulation of Oscillating Cell Cycle Regulators

Marie Wilkening and Joel Stiles
Pittsburgh Supercomputing Center

The regulation of the cell cycle inspires much interest in the scientific community due to its critical role in areas of concern such as cellular differentiation, the healing process, and cancer. This essential mechanism exceeds in complexity, and thus "quantitative tools are necessary to probe reliably into the details of cell cycle control (Tyson and Novak, 2001)". With the surmounting experimental data and detailed mathematical models available, we have started building a spatially realistic, stochastic model that takes advantage of recent functional improvements to the MCell/DReAMM simulation and visualization environment to provide the sought after quantitative, detailed view of cell cycle control. Our model expands mathematical models by incorporating local chemical dynamics, cellular compartmentalization, and important physical interactions that intimately impact the quantitative and qualitative properties of the cell cycle, yet are not explicitly addressed in a biologically meaningful way by current mathematical models based on ODE's.

51

The Synthesis of 4,4'-Amino Acid Functionalized 2,2'-Bipyridine Ligands

Joe Biedrzycki and Tomislav Pintauer
Department of Chemistry and Biochemistry, Duquesne University

The addition of enantiomerically pure alanine to a bypiridine backbone was investigated because amino acid-functionalized bipyridine ligands may have interesting applications in:

(a) Solid support catalysis
(b) Enantioselective copper(I) mediated cyclopropanation and aziridation
(c) Supramolecular organometallic chemistry

4,4'-dimethyl-2,2'-bipyridine was converted into the 4,4'carboxy-2,2'-bipyridine via a permanganate oxidation, isolated, and then characterized by IR since NMR was ineffective due to the product's limited solubility in most solvents. It was then converted to the corresponding acyl chloride, which reacted with carboxy-protected amino acids. The reaction of the amino acid and the acyl chloride has yet to yield the desired product, due to its sensitivity to air. Further investigation into the addition of the amino acid is necessary to determine the best conditions to form the desired ligand.

52

Melatonergic Ligand Binding Study

Justin M. Julius, Sarah Fetterson, Paula A.Witt-Enderby, Mylan School of Pharmacy, Duquesne University

Currently, the field of melatonin research lacks the tools necessary to explore the specific functions of the two melatonin receptor subtypes, MT_1 and MT_2, within the body. This study examined the receptor specific and high affinity binding of three melatonergic ligands, M1, NM1, and NM2, to each of the melatonin receptors. Competitive binding assays were performed which assess the ability of these drugs to compete with 2-[^{125}I]-iodomelatonin for receptor binding. Chinese hamster ovary cells, stably transfected with the human MT1 and MT2 melatonin receptors, were combined, together with 2-[^{125}I]-iodomelatonin, with various concentrations ($1x10^{-4}$M-$1x10^{-12}$M) of the test compounds. All the compounds tested showed a 100-1000 times lower affinity than melatonin (the natural ligand) for both receptor subtypes. Compounds M1 and NM1 showed little binding specificity however, NM2 displayed a ten fold higher affinity for MT_2 receptors than MT_1. These data provide the necessary information for future drug development of melatonergic ligands.

53

Applying the Wang Landau Algorithm to Clusters

Andrew Petit and Kenneth Jordan
Department of Chemistry, University of Pittsburgh

We have applied the Wang Landau algorithm to the Ar(13) Lennard Jones cluster. We partitioned the continuous energy range of this system into bins and used the algorithm to efficiently and iteratively estimate the density of states within each bin. In order to use this information to calculate thermodynamic properties, we must identify a representative energy for each bin which, because of the density of states' functional dependence on energy, is not necessarily the mid-point.

We are also developing a modified routine which divides the energy range into overlapping segments, each of which is independently subjected to the Wang Landau algorithm. The data obtained from these segments will then be pieced back together, using the information from the overlapping bins as a guide. This approach is not only readily parallelizable but also provides a natural solution to the increased complexity of larger systems like the Ar(38) cluster.

54

Coupling Hair Follicle Cycles to Produce Traveling Waves

Megan Jeans[1,2] and Bard Ermentrout[3]
[1] Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh
[2] Department of Bioengineering, Rice University, Houston, TX 77005
[3] Department of Mathematics, University of Pittsburgh, PA 15261

The hair follicle is a regenerative organ which oscillates among periods of growth, apoptosis, and dormancy. Although these cycles usually occur independently, they are clearly regulated by external factors and have been observed to synchronize in certain mutant rodents. Two common biochemical oscillator models were used to approximate the hair follicle cycle, the activator/ inhibitor model and the substrate /depletion model. The coupling function was calculated for several different modes of coupling to produce simulations of the one and two dimensional networking of hair follicles. Within these networks, the variation of relevant parameters produced traveling waves for both models and revealed interesting patterns based on the type and intensity of follicle communication. Ideally, this data will provide insight into the type of networking that really occurs in the mutant rodents.

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Computational Study Of Peptide Secondary Structure Unfolding

Pui Yee Chan and Jeffry D. Madura, Center for Computational Sciences Department of Biochemistry and Chemistry, Duquesne University

The amide vibrations of the peptide bond can be used to probe the conformation of the peptide. Mikhonin et al. have studied how the AmIII band defines the peptide secondary structure using UV resonance Raman (UVRR) spectroscopy. The results from their work uncovered a quantitative correlation between the amide III_3 band and the Ramachandran angle Ψ. They conducted another study using this correlation, for the first time, to determine the conformations of secondary structures involved during the melting of a 21-residue alanine based peptide. In this work, classical mechanics is utilized to carry out a molecular dynamics simulation of this peptide in explicit water using the CHARMM potential function. The results from these simulations will be discussed.

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Synthesis of Novel Resorcinol Derivatives via Fragmentation of Meldrum's Acid Adducts

Laura L. Tomasevich and Michael S. Leonard
Department of Chemistry, Washington & Jefferson College, Washington, Pa.

The synthetic utility of Meldrum's acid has been demonstrated throughout the literature. A particularly notable example is the formation of beta-ketoamides and esters through fragmentation of Meldrum's acid adducts. Progress toward the application of this methodology to the preparation of novel resorcinol derivatives will be described.

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Docking Studies of the Binding Mode of Dictyostatin and Its Analogues to the Taxoid Binding Site on Beta-Tubulin

Christopher B. Hackmeyer, Billy W. Day
Dept. of Computational Biology
Dept. of Pharmaceutical Sciences, School of Pharmacy
Dept. of Chemistry, University of Pittsburgh

The division of a cell's contents during mitosis is highly dependent on the dynamic growth and breakdown of microtubules. Because quickly dividing cancerous cells are especially susceptible to disruption of this process, many treatments for cancer have targeted this behavior of microtubules, hyperstabilizing the tubulin polymers they are composed of to arrest the cell cycle and trigger apoptosis. These agents have been successful in some respects, but they do face certain problems, particularly the emergence of resistant tumors.

Computer docking simulations were used to examine binding modes of the promising new antimitotic agent dictyostatin and several of its analogues with wild-type tubulin and a mutated form that is resistant to dictyostatin and some similar drugs. Our goal was to discover protein-ligand interactions that could help explain the resistance of cells expressing this mutant form of tubulin and thereby facilitate the formulation of hypotheses regarding new agents to synthesize.

58

Sequence Analysis of the Human Immunodeficiency Virus Type 1 Genome

Stephanie Lucas [1,2], David L. Corcoran [3] and Panayiotis V. Benos [1,3]
[1]Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh
[2]Department of Biology, University of San Francisco, San Francisco, CA 94117
[3]Departments of Computational Biology and Human Genetics, University of Pittsburgh

Human Immunodeficiency Virus Type 1 (HIV-1) is an RNA virus, which evolves quickly. Using its publicly available genomic sequences, an analysis of the synonymous sites was performed in order to determine whether is the various HIV-1 genes are undergoing differential selection (Kreitman and Hudson, 1991). The HIV-1 genome was also compared to genomes of similar species (HIV-2, SIV-1, and SIV-2) in order to test if the differences between species are neutral (McDonald and Kreitman (1991). HIV-1's regulatory region (U3/R) was also analyzed to test the levels of polymorphisms and the degree of selection. This data was then used to investigate the evolution of the transcription factor binding sites within the promoter region. These tests provide us with information about evolutionary constraints of the various regions of the HIV-1 virus, potentially helping us understand the evolution of its regulatory mechanisms.

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Development of a targeted DNA delivery system

Megan Mitchell, Ying Zheng, Jeffrey Kovacs, Ellen Gawalt, Wilson Meng
Division of Pharmaceutical Sciences, Duquesne University

The primary objective of my project was to develop a targeted system for delivering oligodeoxynucleotides into dendritic cells (DCs) via the major histocompatibility complex (MHC) class II molecules. We have devised and tested targeting nanoparticles by anchoring the surface with the MHC class II ligand VHA (sequence: VHASHAVHAAHAVHA-G_5-K_{16}) via ionic interactions. This approach has led to a moderate level of selectivity (2:1 comparing the targeted DCs to other cells) in vitro. We suspect that the complex in vivo environment demands a more stringent method of grafting the ligand on the particle. An EDC (1-Ethyl-3-[3-dimethylaminopropyl] carbodiimide hydrochloride) coupling method was used to form a covalent amide link between the carboxylic acid residues on the surface of the PLGA particle to the lysine ε-amines of VHA. Spectroscopic and biochemical methods were used to verify the bond formation. We will present evidence of the peptide on the particles.

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Comparative modeling plasma membrane permease Git1p from *Saccharomyces cerevisiae*

Sophie Okolo[a], Jeffry D. Madura[a], Jana Patton-Vogt[b]
[a]Center for Computational Sciences, Department of Chemistry and Biochemistry,
[b] Department of Biological Sciences, Duquesne University, Pittsburgh

The 3D structure of the plasma membrane permease Git1p has not yet been determined. However, it is predicted to have 12 membrane spanning domains and is a member of the major facilitator superfamily. GlpT and LacY were used as templates in the structural modeling of Git1p using MODELLER. In MODELLER 3D models are obtained by optimally satisfying spatial restraints derived from the 3D-Jury sequence alignment and using the coordinates from a known structure. Both templates have very similar structures even though the sequence homology is not high (21%). The computational program, MOE was used to identify the 12 transmembrane domains, three potential substrate binding sites and other properties based on the comparative models from MODELLER.

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Cloning of EcALDH1 in *Eleutherodactylus coqui*

Zachary Walton, Richard P. Elinson
Department of Biological Sciences, Duquesne University

Many tissues in development undergo retinoid-dependent differentiation. One important ligand is retinoic acid, which is formed from retinal by the enzyme ALDH1. My work involves the cloning of this gene in the direct developing frog, *Eleutherodactylus coqui*. This frog is unique, because it skips the tadpole stage and develops into a small froglet. RNA was extracted from stage TS3 (neurula) embryos. RT-PCR was then performed on this RNA using degenerate primers based on ALDH1 sequences from *Xenopus laevis*, *Xenopus tropicalis*, and *Rattus rattus*. Part of the EcALDH1 sequence was found, which consists of 491 base pairs with 78% nucleotide identity to the *X. laevis* sequence, along with 83% amino acid identity. Once more of the sequence is obtained, this gene can be used to compare forelimb development among different species.

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Git1p: Structure and Interacting Proteins

Arit Bassey, [a] Jana Patton-Vogt[b], Jeffry D. Madura[a]
[a]Center for Computational Science, Department of Chemistry and Biochemistry, [b]Department of Biological Science, Duquesne University

Git1p a plasma membrane permease for glycerophosphoinositol found in *Saccharomyces cerevisiae*, is a member of the major facilitator superfamily (MSF). Other members of the MSF have been crystallized and their structures determined. Using GlpT, (an *E.Coli* permease for glycerol-3-phosphate transporter) as a template structure and the MOE software, a homology model for Git1p was derived. The active site and binding site for the structure was found in relation to its template structures active site.

The second part of this project was to develop a method for the identification of proteins that interact with Git1p. Using a variety of methods for cell breakage and membrane protein solubilization, we are optimizing the conditions for isolating Git1p binding proteins through coimmunoprecipitation.

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Assessment of Protein Structural Similarity Statistics Against the Structural Classification of Proteins Database

Brook Chernet and Michael Sierk, Bioinformatics Program, St. Vincent College, Latrobe, PA

As biological databases grow larger automatic methods for searching them become increasingly important, since manual interpretation of the results becomes impracticable with the increasing volume of data. Pairwise sequence alignment reliably identifies relationships between evolutionarily related proteins, or homologs, allowing inferences of similar functions to be made, but is limited in its ability to detect remote homologs. Typically the three-dimensional structure of proteins is preserved much longer than the one-dimensional sequence; thus, comparison of protein structures is capable of detecting the most evolutionarily divergent homologs. However, the statistical estimates of these methods are less accurate, making it difficult to interpret the results of a structural database search. The purpose of this research is to assess the statistical estimates of homology produced by structural alignments of protein domains from the SCOP (Structural Classification of Proteins) database, with the goal of improving our understanding of structural similarity statistics and protein structure evolution.

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Synthesis and Characterization of Chloro Iron (III) Tetra (2', 6'-dimethoxyphenyl) Porphyrin

Jesse Williamson, Kellie Skoner, and Edward P. Zovinka, St. Francis University, Loretto Pa.

We are synthesizing simple model compounds of the active site of the enzyme hydroxylamine oxidoreductase, HAO, found in the denitrifying soil bacterium *Nitrosomonas europaea* (*Ne*). HAO, and the mechanism by which it oxidizes NH_2OH to NO_2^- during cellular respiration, is of particular interest because it contains a special metalloporphyrin, heme P460. Heme P460 is believed to be at the enzyme active site and transports two net electrons when every other previously studied metalloporphyrin is known to transfer only one electron at a time.[1] The current model being studied is chloro iron (III) tetra(2' , 6'–dimethoxyphenyl) porphyrin, ClFe(DMP)P. Two methods of ClFe(DMP)P synthesis were explored and the material has been characterized by UV-Vis. The lab team is in the process of further characterizing the compound using paramagnetic NMR and X-ray crystallography. The complex has been found to bind pyridine without further reaction and reactivity with NH_2OH will be explored.

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Evolution of Tumor Viruses

Angelo Kontgas[1], Bino John[2]
[1]Chemistry and Biochemistry Department, Utah State University, Logan, UT 84322 USA
[2]Department of Computational Biology, School of Medicine, University of Pittsburgh

Several viruses that predispose humans and animals to the development of cancer are known. We hypothesized that such viruses may have common genomic signatures that help promote tumorigenesis in their hosts. Therefore, we investigated whether sequence elements that are conserved between humans and a set of 12 cancer-associated viruses and can be identified. The Mouse Mammary Tumor virus (MMTV), in stark contrast to all other 11 viruses displayed significant sequence similarity to the human genome. We identified 28 instances of similarity between MMTV and human genome. Four unique segments of MMTV DNA are incorporated at 28 locations in the human genome. One of the four MMTV segments is also evolutionarily preserved in three other cancer-associated viruses. Evolutionary analysis of the viral segments and the human DNA indicate that humans were originally infected by a variant of this virus through the consumption of animal milk.

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A Kinetic Investigation of the Reaction Involving a Near Infrared Label and Fatty Acids

Kelly Ann Wilson, Mitchell E. Johnson
Department of Chemistry and Biochemistry, Duquesne University

A kinetic investigation of the reaction between a fluorescent label and a fatty acid is necessary in order to gain a more thorough understanding of the capillary electorphoretic separation of fatty acids. The reaction had an activating step involving the fatty acids being derivitized with dicyclohexylcarbodiimide (DCC) which helped to promote the linkage between the near infrared label and the now activated fatty acid. Reactions involving caproic, lauric, and stearic acids were run while varying the concentrations of acids and the label. Aliquots of reactions were quenched at specific time intervals. The progress of the reaction under pseudo first order conditions was determined using laser induced fluorescence with non-aqueous capillary electrophoresis enabling the determination of the rate law. The reactions were also performed at various temperatures to establish the Gibb's free energy and the activation energy.

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Assessment of Homolog Detection by Profile-based Protein Sequence Alignment Methods Against a Structure-based Gold Standard

Mallory Freeberg and Michael Sierk, Bioinformatics Program, St. Vincent College, Latrobe, Pa.

The ability to search large databases efficiently to extract usable information is a fundamental aspect of bioinformatics. Pairwise sequence alignment methods, such as SSEARCH, FASTA, and BLAST, are successful at this because they accurately estimate the likelihood that two protein domains are homologous, which allows one to infer functional similarities between the two domains. More sensitive profile-based alignment methods such as HMMER and PSI-BLAST can detect true homologous pairs that pairwise alignment methods may miss. However, the statistical estimates of homology produced by profile-based methods are generally less accurate than the pairwise estimates. In this study, we compare the sensitivity of the pairwise and profile alignment methods using the SCOP (Structural Classification of Proteins) database as a gold standard. We also evaluate the statistical estimates of HMMER and PSI-BLAST and discuss discrepancies between their results and SCOP with the goal of improving the efficiency of the methods.

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Tumor Cell Apoptosis and Tissue Destruction

Gabrielle Ramus,[*§Y] Huiwen Liu,[§Y] Vitaly Chibisov[§Y] and Qiuhong He[*§Y]
[*]Department of Bioengineering, University of Pittsburgh School of Engineering, Pittsburgh, Pennsylvania, [§]Magnetic Resonance Research Center, Department of Radiology, University of Pittsburgh School of Medicine, Pittsburgh, Pennsylvania, [Y] University of Pittsburgh Cancer Institute

Cancer therapy using bacteria is multifaceted due to the sophisticated bacterial interactions with the tumor microenvironment. To overcome the host immune response we have genetically engineered bacteria to act as a protein and therapeutic delivery mechanism. *Salmonella thyphimurium* that expressed the protein TNF-α was injected into the Black C57B/6J mice and CB-17 SCID mice that were inoculated with the murine tumor cell line Lewis Lung Carcinoma. Upon sacrifice of the animal the tumors were removed, fixed in paraffin, and cut into 4μm slices. The tissue was then stained with H&E, a modified version of the modified Brown & Hopps gram staining method, and for Terminal deoxynucleotidyl Transferase Biotin-dUTP Nick End Labeling (TUNEL). Results of the staining confirmed the presence of bacteria within the tumor. Upon staining for apoptosis, using the TUNEL method, we concluded that the massive tissue destruction within the tumor environment was caused by apoptotic cells.

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Density Functional Study Of Aza-Bis(Oxazoline) Copper(I) Catalyzed Cyclopropanation

Lauren M. Matosziuk, Ellen Gawalt, Jeffrey D. Evanseck
Center for Computational Sciences and Department of Chemistry and Biochemistry, Duquesne University

The concerted and stepwise mechanisms of the aza-bis(oxazoline) copper(I) catalyzed cyclopropanation reaction of carbene acetate and ethylene has been investigated using the B3LYP/6-31G(d) level of theory. Cyclopropanation occurs through the bonding of the electrophillic carbene carbon with the *pi* system of the olefin. However, it is debated whether this bond formation is concerted or occurs through the formation of a metallocyclobutane intermediate, which collapses to form the cyclopropane. A less computationally expensive model of aza-bis(oxazoline) has been used to model the reaction both in vacuum and in methylene chloride. The structure and energetics for both the concerted and stepwise processes will be discussed and presented.

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Stability Analyses of Proposed α-Helix in newly Discovered Dimerization Domain using CHARMM

Sonisha A. Warren, Charles T. Dameron, Jeffry D. Madura
Center for Computational Sciences, Department of Chemistry and Biochemistry, Duquesne University

Dimerization of the homodimeric repressor CopY is accomplished in part by a 22 residue sequence predicted to behave like a leucine zipper. Computational methods were used to estimate the potential of the 22 residue sequence from CopY, whose structure is unknown, to fold into an α-helix. In these analyses, MOE software was used to design an α-helix and subsequently create homodimers. Solvation of each structure was accomplished using the VMD program followed by an investigation of their stabilities using CHARMM. In this paper, we report data showing stability statistics in support of the proposed α-helical component of CopY. The hypothesis that this α-helix is responsible for dimerization is being further explored.

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Modeling Bipolar Disorder for Clinical Purposes

Nicole Kennerly[1], Eva Eggeling[2], Shlomo Ta'asan[2]
[1]Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh, Pittsburgh, PA 15216
[2]Department of Mathematical Sciences, Carnegie Mellon University

Successful treatment of bipolar disorder, an illness that affects mood, energy, and performance, has evaded psychiatrists for decades. To develop a quantitative understanding of the illness that addresses clinical questions, we constructed a mathematical model that employs a stochastic differential equation with two parameters, homing and volatility, which are patient-dependent. Collaborators at Western Psychiatric Institute supplied a decade of clinical data that monitors the moods of 175 patients over time. By analyzing patients' data using MATLAB, we determined that the noise has a Laplacian distribution, which has jumps that are characteristic of patients' severe shifts in mood. Treatment effectiveness was assessed by comparing patterns before and after treatment. With further testing, this model can be used to pre-select medicine and dose for a patient, to predict a next big episode, and to measure treatment effectiveness.

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Molecular Dynamics Simulation of HIV-1 Reverse Transcriptase

Abderrahmane Benghanem[1, 2] and Maria Kurnikova[3]
[1]Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh, Pittsburgh, PA 15261
[2]Rensselaer Polytechnic Institute, Troy, NY
[3]Carnegie Mellon University, Pittsburgh, PA

HIV-1 reverse transcriptase (RT) has been in the center of attention in the treatment of AIDS for many years. Understanding its structure will prove essentially useful in the design of new antiviral agents. The unliganded structure has been studied by Molecular dynamics techniques showing the flexibility and rigidity of HIV-1 reverse transcriptase. Solving the flexibility of HIV-1 RT is essential in determining controlling mechanisms of polymerases, binding of inhibitors, and developing more efficient drugs in the treatment of AIDS. The AMBER module was used to carry out the molecular dynamics studies. All calculations are performed using AMBER and its force fields as well as the Ptraj analysis package. Harlem, a locally developed simulator, is used for sample preparations and output simulations.

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Luminescent Lanthanide Reporters: Characterization of Polymetallic Dendrimer Complexes

Savannah Johnson, Stephane Petoud and Grzegorz Filipczyk
Department of Chemistry, University of Pittsburgh and Department of Sciences, Piedmont College

In recent years, lanthanide complexes have gained more attention in the scientific world due to their unique chemical properties including photostability, sharp emission bands, and long luminescent lifetimes. These characteristics make lanthanides excellent reporters in biological and medical applications, though many times their signals are weak. In an effort to make these beneficial qualities more efficient, lanthanide complexes using ligands such as dendrimers have been studied for a single dendrimer has the ability to encapsulate many lanthanide cations, making the complex's luminescence more brilliant through a more efficient means of energy transfer. By making such improvements, these complexes are better able to fulfill requirements for biomedical applications, such as *in vivo* oxygen sensing. Our investigation involves preparing dendrimer-lanthanide complexes and characterizing their properties using spectrophotometric titrations, quantum yields, triplet state measurements, and luminescence lifetimes, to better understand these special molecules and their potential for communicating vital information in bioassays.

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Phenotypic Characterization Of Intervertebral Disc Cells By Analysis Of Traction Forces And Relative Gene Expression

[1*] James J. Morrow, [2]Paulo Coelho[4]Jianxin Chen, and [4]James H-C Wang, [2,3]Gwendolyn Sowa, [2] James Kang,
[1*]Summer Intern, Pittsburgh Tissue Engineering Initiative
[2] Ferguson Lab, Department of Orthopaedics
[3]Department of Physical Medicine and Rehabilitation
[4]MechanoBiology Laboratory, Departments of Orthopaedic Surgery, Bioengineering and Mechanical Engineering

Back pain is a problem affecting a large portion of the world's population. Studies have shown that problems associated with intervertebral discs can cause this pain. The primary goal of this study was to further characterize the phenotypic behavior of intervertebral disc cells to help in guiding future treatment. It was hypothesized that a traction force gradient could be established between articular chondrocyte (AC), NP, AF, and ligament fibroblast (LF) cells from low to high respectively. This hypothesis was tested through the use of traction force microscopy and real time PCR. The trends in the data from these tests suggest that both AF and NP cells are more like chondrocytes in their phenotypic markers than previously expected. These characteristics will provide useful information in examining how the cells of the intervertebral disc change phenotype with age or after injury or to see how these cells will respond to therapeutic intervention.

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Synthetic Approaches to 4-(Hydroxymethyl)benzoates and Cyclophanes

Ashley D. Carbaugh and Michael S. Leonard
Department of Chemistry, Washington & Jefferson College, Washington, Pa.

Trisubstituted benzoates, bearing a hydroxymethyl group in the 4 position, were prepared in a single synthetic step from propargyl alcohol or its derivatives and a coumalate ester. The effect of catalysts on this tandem cycloaddition-fragmentation has been studied. Additionally, this process has been applied to the synthesis of cyclophanes.

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Proteomic Analysis of Co-polyester Degradation by *Thermobifida fusca*

David Deglau and Matthew A. Fisher
Department of Chemistry, St. Vincent College, Latrobe, Pa.

Thermobifida fusca is known to degrade simple plastic copolymers and may therefore serve as a tool for environmental remediation. Our work focuses on understanding global changes in protein expression, using 2D electrophoresis, when *T. Fusca* uses plastic as the sole carbon source. Initial challenges in this project included 1) limited growth of *T. fusca* on the minimal medium used in copolymer experiments published by Müller and coworkers and 2) accurate determination of protein concentration prior to electrophoresis. Work to date has focused on optimizing the lysis procedure for *T. fusca* grown in rich medium. Preliminary data obtained through Bradford assays and one-dimensional SDS gels will be presented.

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Two-Step Protocol for the Synthesis of Substituted Cyclic Imines via a Radical Atom Transfer / Reduction Sequence

Katherine M. Freeman, David B. Guthrie, and Dennis P. Curran*
Department of Chemistry, University of Pittsburgh

Atom transfer radical addition reactions are useful methods for carbon-carbon bond formation, and have been widely applied to many synthetic problems. We have developed an efficient atom transfer reaction wherein the attacking carbon radical is derived from inexpensive, widely available diazo compounds such as the popular radical initiator AIBN. Furthermore, the reaction avoids the use of toxic tributylstannane compounds, which are typically used in radical atom transfer conditions. This process affords α,α-disubstituted 2° γ-iodonitriles, which are extremely difficult to synthesize by other routes. Furthermore, reduction of the resulting adducts with DIBAL-H with a controlled workup results in substituted cyclic imines, which are useful for further synthetic transformations. The mechanism of the nitrile reduction/cyclization has been studied, and both the radical addition and cyclic imine formation reactions have been optimized and tested on various substrates.

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Monte Carlo Simulations of Protein Folding using Lattice Models

Ryan Cheng[1,2] and Kenneth Jordan[1,3]
[1]Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh
[2]Department of Chemistry, Carnegie Mellon University
[3]Department of Chemistry, University of Pittsburgh

Understanding the so-called native state conformation of protein molecules is of great importance due to the direct relationship between their structure and biological function. However, this native conformation is typically adopted at the global free energy minimum located among an enormous number of local minima on a complex energy landscape. As a result, locating the global minimum through heuristic optimization techniques and simplifying models has attracted considerable attention. This study involved the use of simulated annealing (Kirkpatrick et al, 1983) and the Metropolis method (Metropolis et al, 1953), which utilized the Verdier-Stockmayer algorithm (Verdier et al, 1969). Additionally, the problem was greatly simplified through the use of a two-dimensional lattice model and the Hydrophobic-Polar model (Dil et al, 1985). Results from this study provided insight on protein folding and more realistic models that have since been developed.

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Distance Dependence of Electron Transfer Kinetics of Cytochrome C covalently attached to a Self-assembled Monolayer.

Brianna Drews, David Waldeck, Hongjun Yue, Kathryn Davis
Department of Chemistry, University of Pittsburgh

Cytochrome c is an electron transfer protein that is involved in the respiratory and photosynthetic process. The electron transfer kinetics of Cytochrome c has been examined in order to further understand its role and the overall process of cellular oxidation in plants and animals. For this project Cytochrome c was immobilized by covalent attachment to a gold ball electrode surface chemically modified with self assembled monolayers (SAMs) comprised of carboxylic acid- and hydroxyl-terminated thiols. The electron transfer rate was studied as a function of the thickness of the SAMs. Carboxylic acid chain lengths of 16 and 11 methylene groups were examined. For each mixed SAM combination the electron transfer rate constant (k^o) was measured. The rate constants of C15COOH and C10COOH were much lower than those of 3, 5 or 7 methylene groups which helps to clarify the hypothesis of friction controlled electron transfer.

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Steered Molecular Dynamic (SMD) Simulation of Anthrax Edema Factor Translocation through a Protective Antigen Pore

Michael R. Lacina, Anne Loccisano, and Jeffrey D. Evanseck
Center for Computational Studies and Department of Chemistry and Biochemistry Duquesne University,

The toxin released by anthrax is made up of three proteins, protective antigen (PA), lethal factor (LF), and edema factor (EF). PA binds to the cell membrane and then oligomerizes into a heptamer ring. The heptamer ring can bind up to 3 LF and/or EF and is then brought into the cell by endocytosis, where the acidic conditions initiate the translocation. It is not yet known how the EF or LF enters from its binding site and through the pore; the translocation of EF through the PA pore was studied by steered molecular dynamics (SMD). As the N-terminal region of EF enters the pore, it unfolds, partially losing its secondary structure during translocation. Knowing this it will be possible to find new ways of fighting anthrax toxins.

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Synthesis and Characterization of Quaternary Adamantine-Like Chalcogenides

Beth M. Leverett, Charles H. Lake
Department of Chemistry, Indiana University of Pennsylvania
Jonathan W. Lekse, Jennifer A. Aitken
Department of Chemistry and Biochemistry, Duquesne University

I_2-II-IV-VI_4 compounds are of interest as potential precursors to novel magnetic materials; however lithium-containing I_2-II-IV-VI_4 materials are only beginning to attract attention. The compounds Li_2CdSnS_4, Li_2MnSnS_4, Li_2FeSnS_4 and Li_2FeGeS_4 adopt the adamantine-like structure in which all atoms possess a tetrahedral environment. These compounds were synthesized using standard high-temperature solid-state synthesis techniques. Initial reaction conditions were determined using differential thermal analysis. Further reactions were prepared to optimize crystal growth. The purity of the products was examined with powder X-ray diffraction and energy dispersive spectroscopy. Band gaps were determined from diffuse reflectance UV-Vis-NIR spectra. The crystal structure of a potentially isomorphous compound, Li_2ZnSnS_4, was determined from single crystal diffractometry. This structure possesses cationic substitutional disorder between the zinc and lithium ions. Finally, the diamagnetic Li_2ZnSnS_4 was doped with Fe^{2+} ions to create new materials with potentially interesting magnetic behavior.

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Balance Assessment for Everyday Life

Tomas F. Maldonado-Pagan, Mark Redfern and Chris Atkeson
Department of Bioengineering, University of Pittsburgh/Robotics Institute, Carnegie Mellon

Dual-Task protocols have been in used in laboratories for more than 10 years to explore the influence of cognitive processes (specifically attention) on postural control on older adults. Dual-Task protocols have been shown to be sensitive to aging and vestibular disorders by quantifying the interference between cognitive tasks and postural tasks. There is a recognized need for the ability to probe attentional impact on balance outside the laboratory (i.e in clinical settings). The goal of this project is to develop a system to be able to measure attentional influences on balance in a clinical research setting. The project is divided in two phases. The first phase, which is my current project, is develop a system to measure postural movements during standing concurrent with performance on reaction time (RT) tasks. Sway measurements are taken using a Gryo Enhanced Orientation Sensor via a laptop computer. Accuracy and sensitivity of the motion measurement system is being evaluated for standing postural sway. Dual-task RT tasks will be incorporated once the sway measurement system has been validated.

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Lipid Bilayer Fission via Adhesion to a Surface and Interfacial Tension

David Nelles, Kurt Smith, Anna Balazs
University of Pittsburgh Department Chemical and Petroleum Engineering

Fission of lipid bilayer membranes is a crucial step in many processes occuring in vesicles and cells. Examples include the splitting of a vesicle into smaller vesicles and the engulfing of a particle by a vesicle. We examine the final stages of fission through numerical simulation of a tubular neck connected two flat membranes. We consider two driving forces which can cause the neck to pinch off, allowing the membranes to separate. One is the presence of an attractive surface, analogous to a membrane fully engulfing a solid particle. As the membrane wraps around the object, it must meet itself and form a cylindrical neck. This can close and fully encapsulate the solid object. In contrast, a second type of fission occurs when a vesicle is composed of two lipid phases. A narrow neck forms to reduce their interface. The interfacial energy between the phases can cause the neck to pinch off.

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Needle Steering for Brain Surgery

Michele Fenske, Johnathan Engh, Cameron Riviere
University of Pittsburgh Physics REU, CMU Robotics Institute

Recent research has exploited the inherent bending of a bevel-tipped needle during insertion, accomplishing steering of the needle by rotating the needle shaft. Combining this technique with the observation that a straight trajectory can be accomplished by spinning the needle at a constant rate during insertion, a novel technique for proportional control of the curvature of the trajectory via duty-cycled spinning of the needle is achieved. In order to accommodate this technique to very soft tissues such as the brain, several custom needle prototypes have also been designed in order to increase the steering versatility of the system by maximizing the attainable curvature. I will discuss the needle-steering system and software and the needle prototypes, and present preliminary results from tests in an artificial brain tissue substitute.

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Characterization of Pancreas Extracellular Matrix for the Development of a Tissue-Engineered Endocrine Pancreas Replacement Device

Rena Tchen [1, 2*], Jillian Tengood [2], Hongbin Jiang [2], Stephen F. Badylak[2], Jennifer B. Ogilvie [2, 3]
[1] Summer Intern, Pittsburgh Tissue Engineering Initiative
[2] McGowan Institute for Regenerative Medicine
[3] University of Pittsburgh Medical Center

Islet transplantation is an alternative approach in the treatment of insulin-dependent diabetes, but maintaining islet viability and function after transplantation remains a significant challenge. Previous attempts have used small intestinal submucosa (SIS) and growth factors to provide an extracellular matrix (ECM) scaffold that promoted islet recovery *in vitro*. We hypothesize that decellularized pancreas extracellular matrix, along with its native structural proteins, bioactive molecules, and growth factors, is the ideal substrate to support functional recovery and growth of transplanted islets. In this study, enzymatic, mechanical and chemical methods were used to remove cells from porcine pancreas tissue to produce a completely decellularized pancreatic ECM scaffold. Developing native rat pancreata were also stained for specific ECM components such as fibronectin, laminin, and collagen IV with immunofluorescence to characterize the localization and ultrastructure of the proteins in the ECM. This pilot study demonstrates that decellularized pancreatic ECM can be produced and maintains native protein ultrastructure.

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A Bioinformatics Approach To The Structural And Functional Analysis Of The Glycogen Phosphorylase Protein Family

Jieming Shen[1,2] and Hugh B. Nicholas, Jr.[3]
[1]Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh
[2]Department of Chemistry and Chemical Biology, Rutgers University
[3]Biomedical Initiative Group, Pittsburgh Supercomputing Center

The enzyme glycogen phosphorylase plays a major role in carbohydrate metabolism by catalyzing the breakdown of glycogen into glucose subunits. In this study, we utilized computational methods to examine 282 sequences in the glycogen phosphorylase protein family. Specifically, we integrated multiple sequence alignments obtained from a variety of different algorithms into a single refined alignment using the GeneDoc program and identified twenty highly conserved motifs in the set of sequences using MEME. A phylogenetic tree, constructed using the PHYLIP suite software, SeqSpace, and GEnt, provided insight into the patterns of evolutionary descent for the protein family and organized sequences in the family into various subfamilies based on distinctive sequence characteristics. Preliminary analysis of the tree identified twelve major subfamilies as well as brain (B), liver (L) and muscle (M) isozymes within mammals in the Metazoan subfamily. Visualization of the conserved and variable features among subfamily members through Rasmol and VMD revealed their structural and functional significance to protein activity.

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The Use of S_N2' (γ-S_{AL}) Displacements in Allyl Phenyl Chlorides for Substrate Generation in Zinc-ene Cyclizations

Brianna Rossiter, Roman Ivanov and Theodore Cohen
Department of Chemistry, University of Pittsburgh

A new substrate for the zinc-ene cyclization, an allyl phenyl sulfide with appropriately situated unsaturation, can be readily generated by copper salt-mediated γ-S_{AL} (often referred to as S_N2') displacement of the chloride ion of a 1-phenylthio-3-chloropropene by an appropriate organozinc compound. Since the product of such a cyclization is itself an organozinc containing the requisite alkene linkage, this product can be used in an γ-S_{AL} reaction with another 1-phenylthio-3-chloropropene to generate a new allyl phenyl sulfide that can be used for a new cyclization (iterative cyclizations) resulting in fused ring systems such as triquinanes. The conversion of the allyl phenyl sulfides to the required allylzincs involves reductive lithiation using an aromatic lithium radical-anion followed by transmetallation with zinc chloride.

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The Effect of Cu^1L (L=Tp and Tp*) Complexes On Radical Cyclization of 6-Br-1-Hexene

Ryan Egesdahl, Marielle Bailili, and Tomislav Pintauer
Department of Chemistry and Biochemistry, Duquesne University

Free radical cyclization reactions of 6-bromo-1-hexene are conventionally carried out using radical initiators, such as 2,2'-azobisidobutyronitrile (AIBN) and *n*Bu_3SnH. Copper (I) complexes were used to influence the product distributions of these reactions to yield predominantly methylcyclopentane and trace amounts of cyclohexane and open-chain 1-hexene. It was observed that reactions at the same rate and of the same product distribution were carried out regardless of the inclusion of AIBN in the reaction system. A model for these reactions, Atom Transfer Radical Addition (ATRA), is suggested.

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Weighted-Ensemble Brownian Dynamics Simulation

Amanda McCoy, Harvard University, Daniel M. Zuckerman, Department of Computational Biology, University of Pittsburgh

It is difficult to determine high-energy conformations of proteins, because they are dynamic molecules that exist in high energy states for too short of a time to acquire laboratory data. The alternative for determining high-energy protein conformations outside the laboratory is through a dynamics simulation. Most algorithms for dynamics simulations are incapable of simulating a protein long enough to identify a protein's high energy conformation. However, Huber and Kim's weighted-ensemble Brownian (WEB) dynamics simulation surpasses its contemporary algorithms. The WEB method makes such an improvement on the standard Brownian algorithm that it can produce the same length of real-time simulation as the standard Brownian method, but at a fraction of the computing time. In order to fully appreciate the advantage the WEB method provides over the standard Brownian algorithm, we wrote a small-scale WEB dynamics simulation in Perl that assessed particle movement in an one-dimensional, double-welled energy coordinate and compared our results to the theoretical data and the standard Brownian algorithm.

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Photocatalysis of Iron and Organic Pollutants

Jessie Penich, Alex Krupey, Caiti Sherman, Steven Gravelle (Faculty of Chem. Dept & PI)
Department of Chemistry, St. Vincent College, Latrobe, Pa.

Photocatalysis is being investigated as a means of decomposing organic pollutants in the St. Vincent College wetlands. Experiments have demonstrated that one such organic pollutant, p-nitrophenol can be oxidized using photocatalysis with titanium dioxide. The TiO_2 photocatalyst has been shown to be effective both when placed in solution as a particle suspension and when coated onto the bottom of a reaction cell as a thin film. The addition of aqueous ferrous iron to the reaction increases the rate of p-nitrophenol decomposition which seems dependent upon the concentration of Fe^{2+}. Additionally, Fe^{2+} itself decomposes p-nitrophenol in the presence of ultraviolet light, even when no TiO_2 photocatalyst is present. Observation of the behavior of ferrous iron during this process indicates that it was not being decomposed, suggesting that it may be acting as a photocatalyst.

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The Isolation and Analysis of Primary Fatty Acid Amides in Mammalian Tissues

Korey Coulter, Mitchell E. Johnson
Department of Chemistry, Duquesne University

The purpose of this research was to isolate and analyze the group of lipids known as the primary fatty acid amides (PFAMs) and determine their distribution within various mammalian tissue samples. PFAMs are a unique class of biologically active lipids known for their hormone like activity. Some PFAMs of interest included oleamide ($C18:1^{9}$), stearamide (C18:0), linoleamide ($C18:2^{9,12}$), linolenamide ($C18:3^{9,12,15}$), and palmitamide (C16:0) . The isolation of the PFAMs from samples of mouse liver, stomach, heart, kidney, brain, and bovine omentum was initiated by performing Folch-Pi extractions which separated the lipids from the rest of the compounds contained in the samples. Solid phase extractions were then utilized to selectively elute the PFAMs from this lipid extract. The isolated amides were then derivatized and analyzed using gas chromatography/mass spectrometry (GC/MS). In order to properly identify and quantify the PFAMs, standards were used to determine retention times and fragmentation patterns. The amides were then quantified by comparing the relative abundance from GC/MS analysis to the known abundance of an internal standard. Improved method development, percent recovery and carryover during the extraction procedures were also investigated.

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Vortex Shedding Off Of A Rotating Circular Cylinder

Rory Cerbus, Xian-Lu Wu
Physics REU, University of Pittsburgh

My research this summer concerns the effects of a rotating cylinder on vortex street patterns and also on the boundary layer of the fluid. An essentially two-dimensional setup will be used to study these effects, using a soap film suspended between two nylon wires. Since this phenomenon occurs very quickly, a high-speed digital camera will enable me to study the altered patterns at very low speeds, since this phenomenon occurs very quickly. One of the applications of this experiment includes a better understanding of how these vortices are formed and sustained with relevance to vortices in nature such as those found in weather patterns and on planets in our own solar system. Also, a look into MSBC (moving surface boundary layer control) will hopefully yield some useful results concerning the drag and lift that is affected by mounting a rotating cylinder on an airplane wing or on a ship rudder. There are many exciting things to be discovered in fluid mechanics.

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A Search for CIV Systems in the Sloan Digital Sky Survey

Michael Daino, David Turnshek
Physics REU, University of Pittsburgh

We present preliminary results of a search for triply ionized carbon (CIV) absorption line doublets in quasar spectra selected from the Sloan Digital Sky Survey. The large number of quasars in SDSS will allow us to describe the number and absorption line strength of CIV systems with high statistical accuracy. Since CIV systems are thought to arise in moderately-ionized gas associated with galaxies along the line of sight toward the background quasars, the results from this database can be used to place constraints on models of galaxy evolution.

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Data Analysis with the ATLAS Experiment at the LHC

Kevin Kress, Vladimir Savinov
Physics REU, University of Pittsburgh

Though the Standard Model describes low-energy physics phenomena accurately, it contains limitations. The acquisition of mass is explained through interaction with a particle known as the Higgs boson, but this particle remains unseen. The *ATLAS* experiment, beginning in 2007 at the LHC, will determine its existence. Physicists predict ATLAS' functionality through *Monte* Carlo simulations, which reveal the sensitivity of ATLAS to observing real-time phenomena. I have written algorithms to determine its sensitivity to the *Higgs* boson, completing an algorithm for studying the decay of *Higgs* candidates to Z bosons. I have observed detection efficiency of 48% for the specific decay probability $H \rightarrow ZZ^* \rightarrow 4e$ and will continue measuring sensitivities by studying signal optimization and other decays of $H \rightarrow ZZ^*$: 4 muons, and electron pair- muon pair combinations. I will also study the decay of *Higgs* to pairs of bosons W+ and W- in their decays to an electron (or muon) and neutrino.

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Electrophoretic Nuclear Magnetic Resonance (ENMR)

Bradley Schorer, Qiuhong He
UPMC Radiology, Physics REU, University of Pittsburgh

My goal is to successfully perform electrophoretic nuclear magnetic resonance spectroscopy (ENMR spectroscopy). I have already made several circuits tuned to a specific frequency and performed nuclear magnetic resonance imaging on water samples. Instead of a traditional solenoid, my inductor is comprised of a simple metal strip. This is easier to make and easier to place samples on. In addition, the circuit with the strip coil showed a higher Q factor when compared to another circuit made of a solenoid and tuned to the same frequency. This method has been successful with four capillaries with a diameter of several micrometers, small enough to view proteins and molecules. To perform ENMR spectroscopy, a sample must be exposed to an electric field, physically separating out the molecules. This significance to NMR allows the separation of individual molecular resonances.

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Modeling the Effects of Rotation on Stellar Spectra

Charles Warren, John Hillier
Physics REU, University of Pittsburgh

We can determine a wealth of information about a star including its mass, its surface temperature, the abundances of elements and their ions, etc. by analyzing a star's spectrum. As all stars rotate, it is important to understand how the rotation of a star affects its spectrum. The principal effect of rotation is to broaden absorption lines in the stars's spectrum. This occurs because of the Doppler effect – in a rotating star some parts of the star are moving towards us while other parts are moving away. In the case of a slowly rotating star there are methods to easily calculate the influence that rotation has on the star's spectrum. Things become complicated in the rapidly rotating case because phenomena that were insignificant in the slowly rotating case become very important. Effects that come into play for rapidly rotating stars include: physical bulging at the equator, and a variation in surface temperature with latitude (the equator cools down). It is the goal of this project to design a computer program that will properly model the spectrum of a rapidly rotating star, taking into account the effects that slowly rotating models ignore. The result will a better understanding of rotating star's spectra, and therefore allow for better estimations of elemental abundances, surface temperature, and any other information that is derived from a star's spectrum.

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Implementation of K-Factor Algorithm and Its Application to the Identification of microRNA Regulatory Elements

Ji W. Lee[1,2] and Bino John[3]
1 Bioengineering and Bioinformatics Summer Institute, Center for Computational Biology and Bioinformatics, University of Pittsburgh
2 Department of Bioengineering, Pennsylvania State University
3 Department of Computational Biology, University of Pittsburgh School of Medicine

MicroRNAs (miRNAs) are endogenous non-protein-coding RNAs that are thought to negatively regulate gene expression. We have developed the K-Factor computational method to accurately identify sequence elements that regulate the expression of miRNAs. Our results indicate that the biogenesis of miRNAs is regulated by numerous regulatory elements that frequently occur in multiple copies in the upstream sequences of miRNAs. The number of transcription factors that regulate human miRNAs also appears to be significantly large. We have also developed an extensible implementation of the K-Factor algorithm within a desktop application written in Java. The framework of the application is constructed to provide extensibility of functionality in the form of plug-ins. The software will be generally useful in the identification of sequence motifs that regulate the expression of gene sets of interest.

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Functionalized Calcium Aluminate Ceramics as Biomaterials

Brian F. DiSalle, Ellen S. Gawalt
Department of Chemistry and Biochemistry, Duquesne University

In this study we are investigating the modification of the surface of calcium aluminate ceramics in order to improve their effectiveness as potential biomaterials. The ceramic surface has been functionalized with long chain organic acids. These organic acids serve as linkers for the attachment of biologically active molecules such as peptides and antibiotics. Additionally, powder X-ray diffraction was used to investigate the phase composition of the ceramic before and after chemical surface modification.

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Integration of Infrared-Based DNA Sequencing and Genomic Analysis into the Undergraduate Curricula

Jennifer Laco and Bruce Bethke, Department of Biology, St. Vincent College, Latrobe, Pa.

Sequencing technologies are becoming rapidly integrated into undergraduate curricula. For smaller, teaching institutions, however, DNA sequencing in undergraduate laboratories poses challenges. Automated, fluorescence-based sequencing is not economical for use in teaching laboratories; while manual methods typically require the use of radioactive isotopes associated with safety concerns. An appropriate alternative for undergraduate education and research is DNA sequencing using primers labeled with infrared dyes. The LI-COR Model 4300 DNA Analyzer employs infrared technologies for DNA sequencing as well as genomic analysis by Amplified Fragment Length Polymorphism (AFLP) and microsatellite profiling. In 2005 St. Vincent College received a Genomics Education Matching Fund Grant for the purchase of a 4300 Analyzer, however, its integration into the curriculum has been limited by the technical complexity of both the techniques and analysis software. To overcome these obstacles we have developed Standard Operating Procedures organized by technique and user time-frames that clearly define pre- and post-lab steps for gel preparation and subsequent analysis.

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Quantitative Image Analysis and 3-D Digital Reconstruction of the Right Coronary Aortic Valve Leaflet

Chi Zheng, John A. Stella and Michael S. Sacks
Bioengineering and Bioinformatics Summer Institute, Department of Computational Biology, University of Pittsburgh

Current efforts center on designing a viable replacement aortic valve as an alternative to the existing mechanical and biological prosthetics. Compared with existing prosthetics, this valve would offer better longevity and biocompatibility. To design and construct such a valve, a detailed understanding of the microstructure of the native porcine valve must first be acquired. Histological sections of the right coronary leaflet of the aortic valve, taken along the circumferential direction, were first digitally imaged using bright field microscopy. Then, the slides were scanned individually and digitally stacked to construct a 3-D volumetric rending of the entire leaflet. The results of these imaging techniques will allow researchers to visualize local variations within the leaflet in terms of cell count, cellular layer thickness, and structural protein composition. An inferred understanding of the function behind the structure will help researchers emulate the performance of the aortic valve in the tissue-engineered prosthetics.

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The Manufactoring of Probes for Scanning Capacitance and Apertureless Near Field Scanning Optical Microscopy

Matt Kanairis and Jeremy Levy
Physics REU, University of Pittsburgh

The quality of the probes used in scanning capacitance microscopes and near field optical microscopes is a limiting factor for their resolution. Both a good profile and a sharp tip are required for optimal resolution and the minimization of noise. In the case of near field optical microscopes, the tip of the probe must also possess the property of being a good reflector while maintaining a good aspect ratio and a fine point. Electrochemical etching is a common and relatively straight forward method for creating probes of high quality. Through experimentation, we codified a methodology based on previous research to consistently produce probes with a radius of curvature around 10 nanometers. However, direct electrochemical plating has not proven itself to be a viable option for treating the tungsten probes for use in near field optical microscopy. Two viable options to fill this role include a novel gold plating and etching method and the more complicated method of direct gold evaporation onto the probe.

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Motility of *E. coli* and *V. alginolyticus* Under Different Conditions

Julie Mancini and Xiao-Lun Wu
Department of Physics and Astonomy, University of Pittsburgh

The motility of two species of bacteria, *Escherichia coli* and *Vibrio alginolyticus*, was examined, studying the dependence of translational speed on several different factors including cell body size, environmental temperature, salt/ion concentration, and salt type in medium. Bacteria subjected to different conditions were studied using traditional microscopy at 500 times magnification. The translational swimming speed of *E. coli* showed no dependence on cell body size, while *V. alginolyticus* showed tendency toward an optimal length of approximately 2 microns for maximum swimming speed. When placed in a motility medium containing lithium salts, the cells swam at only about 10%of their speed in the presence of NaCl. The cells did not swim at all with only potassium salts. Current experiments attempt to verify relationships between swimming speed and salt concentration and temperature.

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Looking for Z and Z' in a Simulated ATLAS Detector

Jafet Morales and Vittorio Paolone
Department of Physics and Astonomy, University of Pittsburgh

It is thought that new physics (new particles and interactions) may exist at very high energies. When finished, the ATLAS detector will be able to probe these energies using the LHC. If there is a Higgs boson responsible for giving mass to particles, ATLAS might find it. Many other particles may be discovered. Using data generated by the ATLAS simulation, I have studied the response and sensitivity of the detector to standard model physics, specifically the production of the Z boson, which is a carrier of the weak force, by looking at its decay into leptons. Using a similar approach, I will study the production of the Z' boson, which exists in some extensions of the Standard Model, but has not been detected.

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Femtosecond Pulsed Laser Drilling in GaAs

John G. Murphy and David W. Snoke
Physics REU, University of Pittsburgh

Ultra-fast laser drilling provides a high level of precision. This study examines the use of a femtosecond pulsed laser in drilling micrometric craters in the semiconductor gallium arsenide (GaAs). The beam is focused using a microscope objective resulting in high fluence (energy/area) at the focus. When a sample of GaAs is placed in the focus with fluence above a certain threshold, material is ablated. Because energy is delivered in femtosecond pulses, thermal effects, which occur on the pico-second scale, are greatly reduced resulting in high precision. The focal length and focal spot size were found experimentally. The value for fluence threshold was taken from previous studies(1)(2). The dimensions of the damage was found using an optical profilometer.

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Turbulence Studies

Jo Ellen Narron and Walter Goldburg
Physics REU, University of Pittsburgh

A soap film approximates a two-dimensional fluid. Our setup is a vertically hanging soap film between two nylon wires. The friction factor is a measure of the Reynolds number, the relative roughness of the nylon wires, and the distance between the nylon wires. Using laser dopler velocimetry and photon correlation spectroscopy we are measuring the friction factor between the wires and the soap film in order to compare our results to those from three dimensional pipes.

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Neutrino Physics and MINERvA

Federico Pineda and Steven Dytman
Physics REU, University of Pittsburgh

My research this summer focused on neutrino physics. There are still several fundamental properties of neutrinos that are not measured. Various experiments are aiming to determine many of these properties. The first part of the project is to understand neutrino oscillations, this is, the process through which neutrinos change “flavor”. By deriving the formulas that govern oscillations we can understand some of the assumptions that are being made in the next generation of neutrino experiments.

The second part of the project is related to MINERvA, an experiment at Fermilab which aims to measure many neutrino-nucleus cross sections. These results will provide valuable data that will improve results of the more fundamental experiments. We are prototyping a light injection calibration system for MINERvA. Light from an LED is fanned out and injected into photomultiplier tubes using optical fibers. This work will provide a rapid calibration of the large scintillator system that is the core of the experiment.

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Development and Evaluation of Web-Based Tutorials to Develop Expertise in Introductory Students

D. W. Haileselassie-I and Chandralekha Singh
Department of Physics and Astronomy, University of Pittsburgh

We are developing and evaluating interactive problem-solving tutorials to help introductory physics students learn effective problem-solving heuristics and enhance their problem solving, reasoning, and meta-cognitive abilities. The self-paced tutorials provide scaffolding support for a variety of problem solving techniques, and opportunities for knowledge and skill acquisition. We discuss the assessment of the tutorials which involves control studies comparing performance of the learners using tutorials with those who learn similar content from other means.

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Characterization of Ferroelectric Thin Films for Quantum Computing Applications

Chuck Sleasman and Jeremy Levy
Department of Physics and Astronomy, University of Pittsburgh

Quantum computers do not yet exist but are known to be able to solve problems that are intractable for ordinary computers. There are many approaches, but the one I am working on involves the use of ferroelectric films grown on semiconductors. I have been characterizing various properties of ferroelectric Barium Titanate ($BaTiO_3$) films, which may be useful for realizing quantum gates in a solid state quantum computer. Using atomic force microscopy, I have imaged the piezoelectric response of the $BaTiO_3$ samples which exhibited hysteresis in accordance to the voltage written to them. Also, I have mapped the conductance which reveals certain “hot spots” that can lead to electrical breakdown of the films.

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Search for DLA Lines in SDSS Quasar Spectra

Melisa Steighner and David Turnshek
Department of Physics and Astronomy, University of Pittsburgh

Since quasars are the most distant and luminous objects observed in the Universe, they can be used as background light bulbs to study intervening galaxies. The spectra of quasars reveal absorption lines due to hydrogen and other elements such as Mg, Fe, Mn, Si, O, Zn, Cr, etc. that are believed to be formed in extended halos and disks of galaxies along the line of sight to the quasars. We are using the Sloan Digital Sky Survey (SDSS) database of quasar spectra to study correlations between neutral hydrogen and metal absorption lines. Specifically, since SDSS spectra include wavelengths between 3820 A and 9200 A, HI Lyman alpha is observed between redshifts 2.14 and 6.57, and MgII from 0.37 to 2.29. We are studying the redshift interval 2.14 - 2.29 where both lines can be simultaneously measured. Trends between HI column density, and MgII and FeII line strengths will be explored.

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Deformation of Vesicles in Shear

William Uspal and Anna Balasz
Department of Chemical Engineering, University of Pittsburgh

Understanding the behavior of cells and vesicles in driven flows is crucial to nano- and microfluidic technologies. We model the behavior of single and multi-component budded amphiphilic bilayer vesicles in simple shear using dissipative particle dynamics. Deformation of floppy and tense single component vesicles in shear is quantitatively characterized. We find that deformation of vesicles is piecewise linear with capillary number, with segments corresponding to availability and exhaustion of the reservoir of area in the floppy membrane.

Morphological change of multicomponent budded vesicles in shear is investigated and two major vesicle transformation processes are observed: 1.) Migration of the bud to the vesicle tip, followed by pinch-off and formation of a daughter vesicle, and 2.) flattening of the bud into a circular domain and circulation around the vesicle. The phase diagram is mapped out in the region of interest, and the pathway of evolution of the neck morphology during shear-driven pinch-off is closely examined.

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Modeling the Interaction Between Particle-filled Capsules and Substrates: Potential for Healing Damaged Surfaces

Prashant Kumar and Anna Balasz
Department of Chemical Engineering, University of Pittsburgh

We present an algorithm to simulate the release of nanoparticles from a single microcapsule rolling along an adhesive substrate, and the repair of a damaged area of that substrate. The capsule's shell was modeled by the lattice spring model, while the nanoparticles are modeled with a Brownian dynamics algorithm to simulate particle trajectories though both used the Lattice Boltzmann. We then exploit the fact that the adhesion strength between the capsule and the substrate could be different for an 'untreated' surface and a surface with a coating of nanoparticles. We discuss how this could be utilized to repair an area where the coating is 'damaged'. We examine how the quality of repair is affected by the capsule-substrate adhesion strength, pressure gradient, and diffusion coefficients for the particles in both the capsule wall and the fluid. The findings yield guidelines for efficient localized delivery of an active ingredient onto a substrate.