21st Annual Summer Research Symposium

Sponsored by
The Bayer School of Natural and Environmental Sciences

Keynote Address:
David Dausey, Ph.D.
Provost and Vice President for Academic Affairs
Duquesne University

“The Road from Undergraduate Research to a Career as a Researcher.”

Friday, July 27, 2018
9:00 a.m. – 4:00 p.m.
Power Center,
Bayer Learning Center & Mellon Hall of Science
Duquesne University
Welcome to the 2018 Summer Undergraduate Research Symposium!

It is a pleasure and privilege to welcome you to today’s 21st Annual Summer Undergraduate Research Symposium at Duquesne University. Each year the number of student participants and the quality and breadth of the research presented at this symposium continue to grow. The abstracts in this year’s program highlight the remarkable quality of the student research that we will see and discuss at today’s symposium. In an era in which we hear persistent concerns regarding our nation’s ability to sustain global competitiveness and global pre-eminence in the STEM disciplines, events such as today’s conference should reassure all of us of the superb caliber of the scientific research and training that occurs on a daily basis in our colleges, universities and research centers. Today’s presentations reinforce our conviction and confidence that we are preparing an emerging cadre of future scientific leaders who will possess the creativity, motivation, and intellect to meet and solve the challenges that our society faces. On behalf of the faculty, students, and staff of the Bayer School and Duquesne University, I am pleased to offer my sincerest congratulations to each of the student researchers participating in today’s symposium and to convey our best wishes for continued success in your academic and professional careers!

Sincerely,

Philip Reeder,
Dean, Bayer School of Natural and Environmental Sciences

Schedule:

9:00 AM  Registration and Poster Set-Up  Dougherty Ballroom, Power Center
Continental Breakfast  Rotunda, Bayer Learning Center

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

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

1:00 PM  Picnic Lunch  Mellon Hall Patio and Lawn

2 – 4:00 PM  Poster Session  Dougherty Ballroom, Power Center

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Instructions to Authors:

Authors presenting posters should locate their abstract number in the index of this program and then find the poster board space marked with that number. Authors with even numbered poster assignments must be present from 2 p.m. to 3 p.m. to answer any questions. Authors with odd numbered posters must be present from 3 p.m. to 4 p.m. Authors presenting talks during the Plenary Session should report to Pappert Hall no later than 9:15 a.m. A tech assistant will be available to download your PowerPoint presentation.
10 a.m.  Opening Remarks, President Ken Gormley, Duquesne University

Keynote Address, Dr. David Dausey
Provost and Vice President of Academic Affairs, Duquesne University
“The Road from Undergraduate Research to a Career as a Researcher.”

11:00 AM Student Presentations

Daniel Gray  Modeling Water with 2D Mercedes-Benz Particles
Franciscan University of Steubenville

Mary Joens  A Dynamical Mathematical Model of Cystic Fibrosis Airway Epithelium
Liquid and Ion Transport
University of Massachusetts at Lowell

Wencesalo Martinez  Does Resveratrol Prevent Sarcopenia and Preserve Oxidative Capacity with Aging?
Western Michigan University

11:45 AM  Short Break

Sophia Bakar  Fluoride Removal from Water Using a Calcium Carbonate-Based 3D Printed Filter
Duquesne University

Jahnavee Mittal  Generating Forbidden 10-Fold Symmetry Quasicrystals Using an Optical System
Duquesne University

Caleb Reagor  Modeling Information Transmission in G Protein-Coupled Receptor Signaling
University of North Texas

Adam Gargano  Mapping the Rat Serotonin Transporter through Single Cysteine Point Mutations with Cross-Linking Mass Spectrometry
Duquesne University

Session Moderator  Joshua Imperatore, Ph.D. Candidate;
Department of Chemistry and Biochemistry, Duquesne University
David J. Dausey (Ph.D., Yale University) began serving as Provost and Vice President for Academic Affairs on July 1, 2018. Prior to joining Duquesne, Dausey served as Provost and Executive Vice President of Mercyhurst University in Erie, PA. He was also a Distinguished Professor of Health Policy and Management at Carnegie Mellon University where he served as Senior Director of Health Programs and Initiatives.

Dausey is an internationally recognized epidemiologist. He was appointed a fellow of the American College of Epidemiology in 2012. He has worked closely with senior health officials in more than twenty countries and experts at international organizations and foundations such as the World Health Organization, the United Nations, the Global Health and Security Initiative and the Rockefeller Foundation. Domestically, he has collaborated with more than 100 state and local public health agencies and health care organizations in every region of the country and with large federal agencies such as the U.S. Department of Veterans Affairs and the U.S. Department of Health and Human Services. He has led and directed more than $10 million in externally funded research grants and has written a large number of books, research papers and reports including articles in top-tier journals such as the *American Journal of Public Health*, *Health Affairs*, and the *American Journal of Psychiatry*.

Dausey is regularly consulted as a health expert by regional, national and international news media providers on a wide variety of health issues including: health care reform, diet and exercise, and toxic chemicals. He is most frequently contacted by the news media for his expertise in infectious disease epidemiology that includes diseases such as: West Nile Virus, HIV/AIDS, Ebola and novel viruses. For example, Dausey was contacted by the media during the 2016 U.S. Presidential election when it was announced that Hillary Clinton had pneumonia. Dausey has served as a guest commentator on health topics for national and international television news providers including CNN, BBC, and Canadian Television. He has also served as a guest commentator on health topics for national and international radio news providers such as NPR, BBC and Beijing Today. Dausey is a guest writer on health topics for regional and national newspapers including USA Today, the Washington Post, the Pittsburgh Post-Gazette and the Buffalo News.

Dausey is an award-winning professor and teacher. He began his teaching career at Yale University where he was a teaching fellow. His first role as a professor was at the University of Pittsburgh School of Medicine where he was a Clinical Assistant Professor of Psychiatry. At the University of Pittsburgh, Dausey was actively engaged in the Center for Research on Health Care. During this time, Dausey made significant contributions to the literature in the fields of Psychiatry and health services research. For example, Dausey conducted research on the predictors of suicide among individuals with severe mental illness. Dausey and colleagues Robert Rosenheck and Anthony Lehman developed a new mental health performance measure known as “preadmission care” in 2002.

Dausey’s teaching focuses on health systems, health policy, program evaluation and epidemiology. He was recognized for teaching excellence at Carnegie Mellon when he was awarded the Martcia Wade Teaching Award in 2010. He was later recognized for teaching excellence at Carnegie Mellon’s “Celebration of Education” in 2011. Dausey was awarded both the Alpha Theta Mentorship Award and the Panhellenic Intramural Council Role Model Award for his active role in mentoring and advising students. He also has extensive experience teaching study abroad and experiential learning courses. He has advised or led study abroad initiatives in a number of countries including Mexico, Vietnam, Ireland, Ghana, Uruguay, Bangladesh and Tanzania.

As Provost at Mercyhurst, Dausey oversaw a major restructuring of the academics, including the establishment of four new colleges, restructuring the faculty body, and the development and implementation of a new core curriculum. He worked with donors to fund and establish new academic programs at Mercyhurst. For example, he was instrumental in securing a $1.25 million gift to establish the F.W. Hirt Erie Insurance Risk Management program for the Walker College of Business. He helped Mercyhurst to secure a $1 million gift to develop a Cyber Center for the Ridge College of Intelligence Studies and Applied Science. Dausey has also been active in securing funding for academic departments and initiatives. In 2017, he assisted in securing a gift of $1.5 million to support the Mercyhurst History Department and the initiatives of the Public History Program.

A Pittsburgh native, Dausey grew up in Jefferson Hills, PA. He earned both his master and doctoral degrees in Epidemiology from Yale University. He completed post-graduate training in higher education administration at Harvard University.
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City Colleges of Chicago
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Franciscan University of Steubenville
Franklin Regional High School
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Harvard University
Harvey Mudd College
Lebanon Valley College
Lincoln University
Lipscomb University
Marlboro University
Mt. Lebanon High School
Ohio University
Otterbein University
Pittsburgh Sci-Tech Academy
Rice University
Rutgers University
San Francisco State University
Seton Hill University
Skidmore College
Slippery Rock University
Taylor Allderdice High School
The George Washington University
The Ohio State University
University of Central Oklahoma
University of Dayton
University of Massachusetts - Lowell
University of Minnesota - Morris
University of North Carolina
University of Notre Dame
University of Pittsburgh
University of Puerto Rico - Mayaguez
University of Puerto Rico - Rio Piedras
University of Rochester
University of Rochester
University of South Carolina
Vassar College
Washington & Jefferson College
Waynesburg University
Western Michigan University
Westminster College
Water resource management requires accurate collection of water data over time, including river flow, but these data have been deficient in rural regions. Rural areas generally depend on smaller river systems, often where no remote-gaging capabilities exist. This is especially true in low- and middle-income countries. A relationship between flow and river width has been previously demonstrated in attempts to record and monitor this data remotely using satellite measurements; however, current methods have focused on rivers with a width of > 30m and have shown extreme errors when compared to historical gaging records. A new technique for monitoring river flow remotely is presented here, allowing for the creation of an improved river flow record (given historical satellite data), which uses minimum ground-based measurements for calibration. Buffalo Creek, located in Freeport Pennsylvania, and the Mutale River, located in the Limpopo Province of South Africa, were used as preliminary testing sites for this method.

Coronary Heart Disease (CHD) affects many worldwide and arises from plaque formation and build-up in the arteries. In response to CHD, stents are typically placed to give additional mechanical support to the lumen and oral antiplatelet drugs are given to the patient to inhibit blood clotting. Coating the stent material through immobilization of a biomolecule used as an anti-platelet drug may increase blood clot inhibition at the site of stent placement. Self-assembled monolayers (SAMs) are comprised of molecules that contain both a head and tail group and can be used to coat metal. Alkyl-chain ordered self-assembled mixed monolayers of 16-phosphonoheptadecanoic acid (16-PHDA) and methyl terminated molecules were formed on the surface of SS316L, a commonly used stent material. Diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy was used to evaluate the attachment of the self-assembled monolayers. The carboxylic acid tail group of 16-PHDA was free at the interface for additional reactions.

TiO₂ is important in the aerospace, medical, and aircraft industries. The surface of amorphous TiO₂ is not well characterized computationally or experimentally. The computational models of the crystalline polymorph rutile give a lower theoretical surface energy than that derived experimentally of TiO₂. It is hypothesized that modeling a TiO₂ surface using a quasi-amorphous computational model will give a surface energy that is in better agreement with the experimentally determined surface energy of rutile (110). The quasi-amorphous model was constructed using LAMMPS code with the ReaxFF force field. Our models are compared to the experimental radial distribution functions, and the quality of our models will be discussed in the presentation. Density functional theory was used for analysis with the PBE basis set and D3 dispersion correction. The reported work provides the structural framework to further investigate surface properties and binding with common substrates.
Intrinsic Reactivity of Ions Derived from Anionic Uranyl Complexes That Contain a Mix of Carboxylate and Halide Ligands
Iacovino, Anna; Tatosian, Irena; and Van Stipdonk, Michael
Department of Chemistry and Biochemistry
Duquesne University

In this study, tandem mass spectrometry was used to generate species with composition \( [\text{UO}_2((\text{CH}_3)_2(\text{Ac})(\text{Cl}))^n\text{X}^{m-}] \) for examination of collision-induced dissociation and ion molecule reactions (IMR). For the uranyl-acetate-halide complexes, decarboxylation is favored over loss of carboxyl radicals. Reaction of \( [\text{UO}_2((\text{CH}_3)_2(\text{Ac})(\text{F}))^n\text{X}^{m-}] \) caused loss of HF to make \( [\text{UO}_2((\text{CH}_3)_2(\text{Ac})(\text{OH}))^n\text{X}^{m-}] \); while reaction of \( [\text{UO}_2((\text{CH}_3)_2(\text{Ac})(\text{Cl}))^n\text{X}^{m-}] \) with \( \text{H}_2\text{O} \) caused the loss of acetic acid to leave \( [\text{UO}_2((\text{CH}_3)_2(\text{OH})(\text{Cl}))^n\text{X}^{m-}] \). Decarboxylation was the dominant pathway for the uranyl-formate-halide ions. Complexes with two formate and one halogen ligand eliminated \( \text{CO}_2 \) and formaldehyde in consecutive dissociation steps. For complexes containing one formate and two halide ligands, initial decarboxylation was followed by reductive elimination of a hydrogen radical. The reaction pathways for the entire group of precursor and products ions will be presented, along with preliminary density functional theory calculations to predict possible ion structures and vibrational spectra.

The second reaction involved the hydrolysis of the analogous proton transfer step of hydrolysis to produce \( [\text{MOH}^n\text{X}^{m-}] \). Density functional theory (DFT) and second-order Møller-Plesset (MP2) calculations were used to investigate three reactions. The first was the reaction of \( [\text{M}-\text{F}^+] \) with \( \text{H}_2\text{O} \), and the proton transfer step of hydrolysis to produce \( [\text{MOH}^+\text{HF}]^- \). The second reaction involved the hydrolysis of the analogous \( [\text{M}-\text{Cl}^+] \) ion pair. The final reaction involved hydrolysis of \( [\text{M}-\text{CH}_3]^- \). The structures and energies of relevant minima and transition structures were determined. Our results predict that the halogenated species should be endothermic, while hydrolysis of the methides are exothermic. The calculations also predict that the TS energy relative to the starting complex decreases with increasing cation size. The structures and energetics for all species will be presented, along with a comparison of results obtained using DFT and MP2 calculations.

Theoretical investigation of proton transfer energetics in the gas-phase: monohydrates of group II metal complexes
Rissler, Scott; Metzler, Luke; and Van Stipdonk, Michael
Department of Chemistry and Biochemistry
Duquesne University

This study focused on the hydrolysis of ion-pairs with general composition \( [\text{M}-\text{X}]^+ \) \( [\text{M} = \text{Mg, Ca, Sr and Ba}; \text{X} = \text{F, Cl and CH}_3] \). Density functional theory (DFT) and second-order Møller-Plesset (MP2) calculations were used to investigate three reactions. The first was the reaction of \( [\text{M}-\text{F}]^+ \) with \( \text{H}_2\text{O} \), and the proton transfer step of hydrolysis to produce \( [\text{MOH}^+\text{HF}]^- \). The second reaction involved the hydrolysis of the analogous \( [\text{M}-\text{Cl}]^+ \) ion pair. The final reaction involved hydrolysis of \( [\text{M}-\text{CH}_3]^+ \). The structures and energies of relevant minima and transition structures were determined. Our results predict that the halogenated species should be endothermic, while hydrolysis of the methides are exothermic. The calculations also predict that the TS energy relative to the starting complex decreases with increasing cation size. The structures and energetics for all species will be presented, along with a comparison of results obtained using DFT and MP2 calculations.

Exploring the Fragmentation of Copper (II) Cationized, N-terminally Modified Peptides using Tandem Mass Spectrometry and Density Functional Theory Calculations
Kline, Susan; Bubas, Amanda; Metzler, Luke J.; Van Stipdonk, Michael J.
Department of Chemistry and Biochemistry
Duquesne University

Tandem mass spectrometry is one of the most useful tools for identifying peptides and proteins. Our group has found that derivatization to create N-terminal imines may significantly improve de novo peptide sequencing/identification by enhancing ion yields and sequence coverage. In this study, N-terminally modified peptides cationized using \( \text{Cu}^{2+} \) were examined by multiple-stage mass spectrometry to determine if metal cationization also enhances de novo sequencing of peptides. A group of small model peptides were used to establish general fragmentation patterns using the N-terminal modification and \( \text{Cu}^{2+} \) cationization. For each peptide, losses of 44 mass units (loss of \( \text{CO}_2 \)) and 46 mass units (loss of \( \text{H}_2\text{O} \) and \( \text{CO} \)) were observed, and sequence of fragmentation pathways for the two dissociation channels were investigated. A range of sequence ions and non-sequence ions were observed and density functional theory (DFT) calculations were performed to identify probable structures of precursors and products.

Probing for high momentum protons in \( ^4\text{He} \) via the \( ^4\text{He}(e,e'p)X \) reaction
Boyd, Courtney; Benmokhtar, Fatiha
Physics Department
Duquesne University

The continuous electron beam at Thomas Jefferson National Accelerator Facility was aimed at a cryogenic Helium-4 target in Hall A. The aim of the experiment is to collect information on the \( 4\text{He}(e,e'p)X \) reaction. Data was collected on missing momentum ranging from 153 MeV/c to 632 MeV/c and missing energy ranging from 0.353 GeV/c to 0.632 GeV/c. The data from the two high resolution spectrometers in Hall A must be analyzed and the background noise must be removed in order to successfully find the Physics data. Using ROOT, an object-oriented analysis software, five variables were cut to deduct the background noise. Missing energy is used to determine if the nucleons were in two-body or multibody breakups. Missing Energy spectra for two body breakup are used to determine proton cross sections and compared to theoretical models.
Creating a Zero Waste 3D Printing Recycling System
Sutton, Karli; Goldschmidt, Benjamin S. PhD
Department of Biomedical Engineering
Duquesne University

Where do 3D printed objects go when they are no longer in use? Previously, they would have been thrown out and sent through the waste collection system here at Duquesne. The goal of this project was to create a 3D printing filament recycling system that could not only recycle 3D printed objects, but could also recycle plastic generated throughout the campus. The challenging part of this is finding a combination of melting temperatures, gear speeds, and spooling techniques that can provide usable filament from recycled plastics such as plastic cups. Another aspect of this project is determining how many times a sample can be recycled before deteriorating to the point where its structural integrity is compromised. The end goal for this project is to be able to turn plastic bottles and cups into functional prosthetics and other biomedical devices, thus lowering the waste production throughout Duquesne University's campus.

Investigation of Stability Trends in Bimetallic CuAg/CuAu/AgAu Nanoparticles via a Bond-Centric Model
Ramadan, Mahmoud; Estes, Jonathan; Dean, James; Mpourmpakis, Giannis
Department of Chemical and Petroleum Engineering
University of Pittsburgh

Metal nanoparticles (NPs) have attracted tremendous scientific interest over the last several decades due to their diverse technological applications, among which is catalysis. Compared to monometallic NPs, bimetallic NPs allow for a greater variation of local chemical environments and thus, control of potential catalytic sites. However, this local site variation also results in a significantly larger search space when investigating NPs of even the same bimetallic nanoparticle composition, size, and shape. Using a previously-developed bond-centric model as a means to calculate computationally fast a NP’s cohesive energy, a code was developed to efficiently determine potential ground-state structures for any given bimetallic NP. The cohesive energy was determined for 55- and 147-atom icosahedral and cuboctahedral NPs, consisting of CuAg, CuAu, AgAu ranging from 0-100% in metal composition. At each given composition and morphology, atomic identities within the NP are shuffled several thousand times, calculating the cohesive energy for each sampled microstate. Additionally, a comparison is made between observed trends and literature results.

Efficacy of Biocides Against Microbes from Fracking Waste Water
Miller, Mackenzie; Roth, Kristen; Cantlay, Tetiana; McGough, Cecilia; Stolz, John F.
Department of Biological Science; Center for Environmental Research and Education
Duquesne University

Unconventional gas extraction with hydraulic fracturing and horizontal drilling has revolutionized the way natural gas from “tight” reserves such as the Marcellus Shale is obtained. The process requires immense amounts of water, chemicals, and sand (i.e., proppant) to be pumped into the wells. Although there are biocides added to these fluids, the wastewater from hydrofracking is rich with microbes. A previous study done by our group showed that the common biocides used are not only ineffective, but can stimulate microbial growth. Here, we have tested several different biocide formulations for their efficacy under conditions simulating produced water using two different enrichment cultures, LP1 and SWPA, both from fracking operations. Three concentrations of biocides (low, medium, high) were tested with different salt (NaCl) concentrations under aerobic and anaerobic (nitrate or sulfate reducing) conditions. The high concentration was found to be most effective for inhibiting growth, with LP1 showing the greatest resistance.
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Predicting NMR chemical shift anisotropy of cimetidine with dispersion corrected plane-wave DFT.
Engl, Olivia1, Iuliuici, Robbie J. 1, Holmes, Sean T. 2, and Harper, James K1.
1Washington and Jefferson College
2University of Windsor

Correctly assigning NMR peaks to corresponding atoms in molecules is a difficult process when similar nuclear sites exist. Predicting the chemical shifts from molecular modeling can provide this essential information. By studying pharmaceutical cimetidine form A, a polymorph with a well-known x-ray diffraction structure, a solution to assigning 13C peaks can be achieved by using DFT1. Several DFT functionals with a plane-wave basis set were considered along with coordinate and lattice optimizations using the Castep2 module of the Materials Studio software. NMR parameters were calculated with the Gauge Included Plane Augmented Wave method (GIPAW)3. Dispersion interactions were included using the Grimme4 D2 method with the d-parameter optimized by NMR quadrupole data. The Perdue-Wang 91-D25 functional outperformed the others with a root-mean-square deviation of 3.2 ppm for the 13C principal values. A single solution to the NMR peak assignment is attained and disagrees with the previous literature assignment.

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Preforming Electronic Structure Calculations for Chalcogenide Quaternary Diamond-Like Semiconductors
Deverant, Kristianne1; Bonnioni, Allyson1; MacNeil, Joseph2; Aitken, Jennifer A1.
1Department of Chemistry and Biochemistry, Duquesne University
2Department of Chemistry, Chatham University

Quaternary diamond-like semiconductors are compounds that crystallize with structures that can be derived from diamond. Depending on their specific composition and structure, this class of semiconductors exhibit bandgaps that span the near infrared, visible and UV regions, generating a wide range of potential applications in fields such as photovoltaics, non-linear optics and thermoelectrics. Traditionally in the Aitken lab, diamond-like chalcogenide semiconductors have been created with the I2−II−IV−VI4 configuration. Although this is a common stoichiometry for diamond-like semiconductors, there are other formulas, such as IV−II−IV−VI4. Density functional theory computations (using the WIEN2k platform) were performed on analogous compounds of both formula to calculate their total and partial density of states (DOS) and the band structures. Comparing the data from both calculations allowed for the impacts of the stoichiometric variations on the DOS and band gaps of the compounds to be estimated.

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Analysis and Certification of a Low-level Cr(VI) Soil Matrix Reference Material by Speciated Isotope Dilution Mass Spectrometry, EPA Method 6800
Pereira, Laury3, Weier Hao1, Logan Miller1, Matt Pamuku2, Teresa Switzer3, Bob O’Brian4, Larry Tucker5, and H. M. “Skip” Kingston1
1Department of Chemistry and Biochemistry, Duquesne University
2Applied Isotope Technologies Company, Pittsburgh, PA
3Ministry of the Environment, Canada, Ontario
4Sigma-Aldrich, Wyoming, USA
5Metrohm, Houston, TX

In Ontario, Canada a new mining site is under development for the extraction of a deposit of chromium. Chromium is used for everything from making stainless steel to dietary supplements. Two forms of chromium exist in the environment, trivalent chromium [Cr(III)] and hexavalent chromium [Cr(VI)]. Cr(III) is known to be carcinogenic to humans. Assessment of the environment requires quantifying the low levels of Cr(VI) that may be in the mining site naturally before mining begins. The indigenous groups, that own the land, and the Canadian government have agreed upon the site being mined so long as contamination that may happen is remediated to the original Cr(VI) levels. A new low-level Cr(VI) soil reference material is required to allow for the quantitation of pre-contamination Cr(VI) levels currently in the soil the mining site area.
17 Investigating the degradation pathways of nucleotide binding domain protein truncations
Burns, Grace, Hilal, Olivia, Needham, Patrick, Guerriero, Christopher, and Brodsky, Jeffrey
Department of Biological Sciences
University of Pittsburgh

Protein folding is essential for cellular function as protein aggregation can result in disease. In the cytoplasm, aberrant proteins are degraded by cytoplasmic quality control (CytoQC), which we previously delineated in the model organism, Saccharomyces cerevisiae. Using the second nucleotide-binding domain (NBD2) of a plasma membrane transporter, we discovered that a 42 amino acid truncation leads to rapid degradation. To understand how truncations impact NBD2 folding and CytoQC, a truncation series was generated. We first found that truncation length impacts the degradation of NBD2. Next, three truncations with fast, intermediate and slow degradation rates were characterized. Using a cycloheximide chase assay, we discovered that each truncation “class” is dependent on the proteasome for degradation, but differentially rely on Hsp70 and Hsp104 chaperones. Understanding the degradation mechanisms of these phenotypically diverse truncations will help cultivate a greater understanding of the roles of chaperones in CytoQC and potentially human diseases.

19 Modeling information transmission in G protein-coupled receptor signaling
Reagor, Caleb
Department of Computational and Systems Biology, School of Medicine
University of Pittsburgh

G protein-coupled receptors (GPCRs) are cell-surface receptors that can transduce diverse extracellular signals involving many small molecules involved in autocrine, paracrine and endocrine signaling. Although GPCRs comprise the largest gene family in the human genome, their information transmission capabilities are still poorly characterized. Due to experimental design limitations, previous investigations into the channel capacity of GPCRs likely underestimate the upper limit of GPCR information transmission. In this study, I used a published mathematical model of GPCR signaling and a novel sensitivity-based analysis pipeline to identify which parameters in the mathematical model must be tightly constrained in multidimensional parameter space to elicit realistic GPCR behavior. Published single-cell data was then used to implement realistic constraints on the mathematical model. The results of this analysis demonstrate that three parameters that control generation, degradation and activity of Phospholipase C primarily determine the information transmission capabilities of GPCRs.

20 Analysis and Confidence Scoring of Detection Waveforms from Photoacoustic Flow Cytometry
Minard, Austin1 ; Edgar, Robert1,2 ; Viator, John1,2
1Biomedical Engineering Program, Duquesne University
2Department of Bioengineering, Swanson School of Engineering, University of Pittsburgh

Photoacoustic flow cytometry (PAFC) is a method that generates ultrasound waves by absorbing laser light from objects to detect cells faster than standard methods. Previously, a detection was recognized strictly when the waveform’s magnitude passes a certain threshold, for any type of cell being tested. The resulting detections are marginally accurate, however the detections could be refined. The goal of this research was to develop a computational method to analyze the waveforms, and gain a better understanding of each detection structure. Completing this research will provide a better differentiation between a noisy and detection waveforms. This decreases the probability of false positives confirming or denying the resulting waveform as a detection. The types of PAFC detection waveforms analyzed were bacterial cells with a high and low concentrations of bacteriophage, and melanoma cells. The new system guarantees the certainty of detections will be greatly increased, and more accurate results.
Bacterial detection and identification is a long process that takes 3-4 days to complete. Currently, a patient’s blood sample is tested in a laboratory for identification of bacteria present. Bacteriophage are viruses with the ability to attack and destroy specific bacteria based on their antigen binding capabilities. The goal of this work is to produce bacteriophage particles with magnetic beads for quicker identification of bacteria from an unknown sample. Bacteriophage are built from repeating protein subunits and therefore prime targets for biotinylation. Biotinylation bacteriophage allows the functional amino acids of the biotin reagent to react with the surface proteins of the bacteriophage. Through highly affinitive biotin-avidin interactions, the biotin labeled bacteriophage are attached to magnetic streptavidin beads and separated with a strong magnet. Ultimately, biotinylation and extracting highly concentrated bacteriophage without affecting their infecting capabilities allows for quicker separation from leukocytes and other particles present in patient’s blood sample.

Insight into subatomic particles can be attained through understanding electric and magnetic form factors that describe charge and magnetization distributions inside the nucleon. By increasing the energy used in a particle accelerator, higher precision measurements can be attained. Towards this goal an upgrade was required to the BigBite spectrometer in Hall A at Jefferson Lab. This upgrade consisted of assembling and installing 90 hodoscope bars into BigBite. Hodoscopes consist of a plastic scintillator in between two light guidescopes attached to photo multiplier tubes (PMTs). The bars were marked, and carefully centered within the detector to ensure that they are were aligned. At the end of the project, all of the bars were inserted into BigBite and affixed. This upgrade adds accuracy to measuring higher momentum values within the Super BigBite Spectrometer (SBS). SBS consists of the BigHAND nucleon detector, BigBen proton deflector, and BigBite electron spectrometer. Moving forward, the SBS should now be able to utilize the 12 GeV laser upgrade that recently came to Jefferson Lab.

Cytosolic DNA is an indicator of a multitude problems at the cellular level. The detection of cytosolic DNA in cells is achieved by a protein known as cyclic GMP-AMP synthase, or cGAS. This protein is critical in activating a type I interferon response in the innate immune system, which, in turn, induces the transcription of hundreds of genes, responsible for inflammation, immune cell activation and apoptosis. Unfortunately, the mechanism that regulates this pathway is still poorly understood. This focus of this study was to better understand the production and diffusion of type I interferon and its involvement in cellular resistance to viral infection. To accomplish this goal, an agent-based modeling software called NetLogo was used. Using NetLogo, we modeled the effects of the cGAS pathway and gained better insight into the time-scale in which interferon is produced and diffuses out of epithelial lung cells under various parameters.
Fragile X syndrome is a genetically inherited disorder which causes intellectual defects in humans during development. This disorder is caused by a trinucleotide overexpansion within the Fragile X mental retardation (FMR1) gene, resulting in transcriptional silencing and subsequent downregulation of the Fragile X mental retardation protein (FMRP). The FMR1 mRNA contains 15 exons which can undergo alternative splicing, resulting in up to 20 different isoforms of FMRP. This research focuses on alternative splicing at exon 12 and how secondary structures within the FMR1 mRNA sequence may affect this splicing. In this study, we hypothesized that the formation of a G-quadruplex structure within the FMR1 exon 12 mRNA sequence would block the binding of the spliceosome U1 RNA, and hence affect the FMR1 alternative splicing. The FMR1 exon 12 mRNA sequence was biophysically characterized and its binding to a truncated portion of the spliceosome U1 RNA was monitored using gel electrophoresis.

In general, when small particles such as proteins are studied, a large group of them are examined as a whole. However, we can gain a deeper understanding of nature by studying and observing a single particle. Recent advancements in science and engineering have allowed for trapping a single nanoparticle using fluid flow. When two opposing fluid streams meet at the intersection of two perpendicular channels, a "stagnation point" is created along the interface of the streams. At this point, the fluid flow virtually stops, forming a tiny pocket in which a single particle can be trapped. By precisely controlling the fluid flow at the channel intersection, a single particle can be trapped. By coupling many of these channel intersections in series, it is possible to trap multiple particles and predict each particle’s position by merely using fluid flow. This new technology opens the doors for capturing and observing single particles as well as particles interlinked with polymers in a way yet to be explored.

The serotonin transporter (SERT) is an integral membrane protein and member of the neurotransmitter sodium symporter (NSS) family. It is responsible for the reuptake of serotonin from the synaptic cleft. Dysfunction of SERT is implicated in mood disorders. Current structures of SERT contain bound ligand and have truncated loops. To better understand SERT the full length transporter must be studied in a native, apo state. Single cysteine point mutations were inserted into a plasmid containing rSERT cDNA with eight active cysteines removed (X8C) to produce V310C, L406C, and V489C SERT mutants. A MTS benzophenone based cross-linker can probe the local environment of the cysteine in purified, reconstituted SERT by specifically bonding with the mutant cysteine and nonspecifically bonding with peptides within ~20Å upon photoactivation. Subsequent protein digest, MS, and MS/MS studies can elucidate residues with bound cross-linker. Comparison of cross-linked peptides between mutants can refine SERT apo state models.

Stainless steel 316L, used in marine and aerospace applications is a low carbon steel that is susceptible to corrosion. In industrial utilization, deterioration of the metal can lead to mechanical failures. To decrease corrosion on SS316L, a polymer coating was employed. By providing a barrier to reduce electrochemical activity on the surface the coating will increase oxidation resistance. A self-assembled monolayer (SAM) on the surface of the metal and surface-initiated atom transfer radical polymerization (SI-ATRP) was used to synthesize the coating. Diffuse reflectance infrared Fourier transform spectroscopy and contact angle analysis data was obtained for the surface characterize of bare, SAM-modified, and the polymer formation on SS316L. Cyclic voltammetry will be used to measure the ability of the polymer coating to inhibit corrosion.
**29**

**LCMS Method Development for the Identification and Quantification of Illicit Drugs Introduced into Correctional Facilities**

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As illicit drug use continues to rise in America, there is an increased need to detect drugs being smuggled into correctional facilities. More and more individuals attempt to conceal illicit materials in articles of mail, believing that facilities will be unable to detect the presence of these substances. This project’s focus is to develop LCMS methodologies to identify and quantify commonly trafficked drugs: methamphetamine, ketamine, heroin, cocaine, PCP, fentanyl, and methadone. This project is in collaboration with ChemImage Corporation, in Pittsburgh, PA, to improve their hyperspectral imaging system, the VeroVision™ Mail Screener. Excisions from positively screened mail materials were extracted using sonication in 500 μL in 80:20 water:acetonitrile. Upon extraction, the solutions were syringe filtered, then identified and quantified with the developed LCMS method. Analytical figures of merit for the methodology will be discussed.

**30**

**Modeling Serum Creatinine Dynamics During Acute Kidney Injury**

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Acute kidney injury (AKI), or a sudden decrease in renal function, is common among critically ill patients. A decline in kidney function is often linked to a decrease in glomerular filtration rate (GFR), which is tedious to measure directly. Reduced urine output along with increased serum creatinine (SCr) can estimate changes in GFR, and hence the magnitude of AKI. SCr, a concentration measurement, is dependent on the retained fluid volume. Therefore, an accurate prognosis of AKI relies on the relationship between patient hydration status, SCr, and GFR. A low-order compartmental model of SCr dynamics informed with patient-specific fluid administration and collection has been developed. A normalized, time-variant GFR (1= health; 0= no kidney function) is fit to patient-specific SCr and volume electronic health record patient data via nonlinear least squares using MATLAB (©2018, the Mathworks). This proof-of-concept model could shorten the delay to AKI diagnosis in critical care.

**31**

**Epibatidine 7-Azabicyclo[2.2.1]heptane Core Synthesis by 3+2 Cycloaddition**

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Epibatidine is a toxin secreted from the skin of poison dart frogs which has the potential to procure a family of non-opioid, non-addictive pain killers. However, this toxin’s synthesis is limited due to complicated synthetic routes. Through a computational analyses, a new strategy to synthesize the epibatidine 7-azabicyclo[2.2.1]heptane core has been hypothesized. When doing a 3+2 cycloaddition between N-methylpyrrolidine N-oxide and a symmetrical trans-alkene, two reactions become possible: an addition across the pyrrolidine ring carbons adjacent to the nitrogen or an addition with the N-methyl carbon. Addition across the adjacent pyrrolidine ring carbons forms the 7-azabicyclo[2.2.1]heptane epibatidine core. Through computational analyses, the activation energies of the non-epibatidine-like product is lower and expected to be major. With this understanding, it was confirmed computationally that if the starting pyrrolidine N-oxide has an N-t-butyl group instead of an N-methyl group, then the only product formed will be the epibatidine-like 7-azabicyclo[2.2.1]heptane core.

**32**

**Modeling of Macroautophagy to Study Alpha 1-Antitrypsin**

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Antitrypsin deficiency, which is often abbreviated to ATD, is a genetic disorder that can culminate in liver disease. Antitrypsin deficiency is an autosomal co-dominant disease. Having two defective alleles causes a worse case of disease compared with only having one defective allele. Antitrypsin deficiency is caused by a point mutation in the SERPINA1 gene for alpha 1-antitrypsin, a plasma protease inhibitor. The mutated alpha 1-antitrypsin, commonly referred to as ATZ, builds up in the endoplasmic reticulum. This buildup is caused because mutant alpha 1-antitrypsin is misfolded, resulting in autophagic dysfunction. The process of macroautophagy leads to the production of alpha 1-antitrypsin. The software Copasi has been used to create a model of macroautophagy. This model of macroautophagy is being used to learn more about the dynamics behind alpha 1-antitrypsin production.
Transcription is the process by which RNA polymerase is recruited to a promoter DNA sequence, synthesizes mRNA, and then dissociates upon reaching a terminator sequence. To adequately predict transcriptional behavior in synthetic circuits, having multiple strong terminating sequences is imperative. In prior research, correlation between terminator strength and structure has been identified, and this trend can be used to produce machine learning models to predict terminator strength. Furthermore, machine learning models such as Recurrent Neural Networks have been successfully used to predict RNA secondary structure. Thus, we developed a novel dual-encoder model that combines structure and strength data by learning latent spaces to represent both facets of terminator sequences. Currently, only 582 terminator sequences have known terminator strength values. Motivated by the scarcity of data, we aim to facilitate synthetic circuit development by using our model to produce a larger and more robust library of strong terminator sequences.

**Detection of Cherenkov Radiation Produced by Aerogel Tiles**

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The Ring-imaging Cherenkov Detector (RICH) located in Hall-b at Jefferson Lab is used to detect charged subatomic particles such as electrons, pions, kaons and protons. Aerogel is a dielectric material made up of silica and residues of metal oxides. Placing a beam of charged pions at 6 GeV behind the aerogel will produce Cherenkov radiation in the UV to visible range. When a charged particle travels through the aerogel at a very high speed, the particles inside become dipoles. This polarization stretches the shape of the particles and if the incoming particle is moving faster than the speed of light in the medium, Cherenkov radiation is produced. My work consisted on the partition of the aerogel tiles, and the study of emitted Cherenkov radiation. This process is important for event reconstructions that will help with particle identification.
37
Analysis of the Effects of E-Fluids on Cultured Lung Cells
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Viewed as a healthier alternative to smoking, vaping and e-cigarettes are gaining popularity amongst teenagers and adults. In 2016, the CDC reported that 8% of high school students regularly use cigarettes, a drop from the 15.8% reported in 2011, while 12% use e-cigarettes, an increase from 1.5% in 2011. Companies advertise the e-juices, comprised of vegetable glycerin, propylene glycol, and some concentration of nicotine, as having little to no effect on the health of the users; however, few studies have been performed to back this statement. This study will examine the effect of LD22 murine lung cells treated with various concentrations of e-juices to analyze the impact of each to the viability of the cells. Results of this study could be used in the future to inform the general public of the health risks associated with e-cigarette use.

38
Observations on how a Dementia Activities Room (DAR) Affects Individuals Suffering from Dementia
Martin, Stephanie T.
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Dementia is a chronic neurological disorder that affects the cognitive function of the brain, such as memory. Millions of individuals over the age of sixty-five suffer from this disorder and the numbers are increasing every year. In today's society, there tends to be a stigma toward those suffering from dementia where they are perceived as agitated or aggressive. This preconceived misconception leads to a marginalization of individuals with this disorder, which causes feelings of rejection, frustration and loneliness. Through personal experiences volunteering at UPMC Mercy in the Dementia Activities Room (DAR), the behavior and emotional effects, and willingness to participate in activities and conversation of dementia patients was observed. Through the course of the summer, many patients seemed more positive, calm and engaging as they spent more time in the DAR. It is important to correct misconceptions regarding dementia patients so that they can live a fuller, happier and healthier life.

39
A Dynamical Mathematical Model of Cystic Fibrosis Airway Epithelium Liquid and Ion Transport
Joens, Mary A.¹,²; Serrano Castillo, Florencio¹; Corcoran, Timothy E.¹,³; Bertrand, Carol A.⁴; Shapiro, Monica E.¹; Parker, Robert S.¹
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Cystic fibrosis (CF) is a genetic disease that causes the absence or malfunction of the cystic fibrosis transmembrane conductance regulator (CFTR), an anion channel in epithelial cells. This defect results in a transepithelial osmotic imbalance, which leads to airway surface liquid (ASL) dehydration, impaired mucociliary clearance, and eventual respiratory failure. Experimental data alone cannot fully characterize the mechanisms of CF pathophysiology; coupling this data to a mathematical model provides additional insight.

We describe a model of airway epithelium ion and liquid transport using physiologically-motivated conservation relationships. The model is informed with ASL and paracellular transport data obtained from human bronchial epithelial cell cultures. APT-MCMC, a Python-based Markov Chain Monte Carlo parameter fitting package, returns patient-specific parameter distributions. These parameter settings establish population-level differences between CF and non-CF cultures, ultimately isolating mechanistic causes for differences in airway surface hydration and ion transport in health and disease.
41 RICH Calibration Analysis
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Physics Department
Duquesne University

A Ring Imagining Cherenkov (RICH) detector has been installed in Hall B of Jefferson Lab. The purpose of the RICH detector is to distinguish pions from kaons within the momentum range of 3 to 8 GeV/c. The detector utilizes aerogel tiles, spherical mirrors, and 391 multi-anode photomultiplier tubes (MAPMT) along with readout electronics. Large momentum particles passing through the aerogel tiles emit Cherenkov radiation, which are redirected by the spherical mirrors to the PMTs. The PMTs are split into 64 channels, making a total of 25024 channels for the detector. To ensure the PMTs work for the experiment, calibration runs were taken from January to May. The calibration data included tests with various conditions of gains, high voltages, and thresholds. Analysis of the readout from the PMTs included the study of the pedestal and single photoelectron signals. The channels have been determined to be stable throughout the course of the calibration testing. Also, improvements of the calibration procedure for the PMTs have been made. This calibration analysis produced the configuration parameters to be used in August runs.

42 Development and Application of a Game Theoretic Model for Competition Among Bacterial Strains in a Spatial Domain
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Evolutionary game theory is an application of mathematical games to the biological theory of evolution, the study of which can lead to a better understanding of competition between individuals. Here we work with two existing models consisting of coupled, nonlinear, first order differential equations that describe the evolution over time of fitness-seeking strategies adopted by competing populations. Our contribution is the addition of a spatial component to these models (a variable that describes where individuals exist in space), analysis of both models, and application to an existing problem: the competition between two strains of salmonella and commensal bacteria present in the gut. We developed a space-independent model, but it did not fully explain the co-existence of the three bacterial strains. Therefore, our objective is to develop a spatial model that explains the roles for two separate strains of salmonella and allows for the existence of all three bacterial populations simultaneously.

43 Resolving the Properties of Type Ia Supernova Host Galaxies
Cilento, Meghan and Dr. Wood-Vasey, Michael
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My research focuses on the preparation of Integral Field Spectroscopy data and the analysis of host galaxy properties to map the locations of Type Ia Supernovae (SNe Ia) with their host galaxy ages and explore correlations with local properties. SNe Ia are standardizable for measuring cosmological distances, however, their observed properties are known to correlate with the physical properties defining their host galaxy stellar population. We study the environmental dependencies of SNe Ia, which point to remaining systematic errors in the standardization of SNe Ia, to improve our cosmological distance measurements, and thus our knowledge of the expansion history of the cosmos.

44 Photoacoustic Flow Cytometry Oil Removal by Superhydrophobic and Oleophilic Powder
Douglas, Madeline; Edgar, Robert; Viator, John
Biomedical Engineering Program
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Photoacoustic flow cytometry allows for circulating melanoma tumor cells to be captured. Oil is used to enable capture, and is therefore present alongside the aqueous cell suspension. The presence of oil, however, is detrimental to future sample processing, such as immunostaining and PCR. Precipitated calcium carbonate and palmitic acid were used to produce a powder with superhydrophobic and oleophilic properties. Pipette tips were coated with this powder. When the oil and cell suspension of the flow system is drawn up by the coated pipette tips, the powder absorbs only the oil, and the pipette subsequently releases just the water and melanoma cells. The removal of the oil ultimately decreases the difficulty of performing other aspects of molecular biology on the sample, such as cDNA extraction, which was negatively impacted by the oil’s presence.
2018 Summer Undergraduate Research Symposium

45  The impact of anti-dandruff compounds on the human scalp microbiota
Sophia Li1, Zoe Moses2, Swagatika Bhattacharya1, Jason Chen1, Barathi Subramonian1, Melissa Echard1, Tanja Cupac1, and Wook Kim1.
1 Department of Biological Sciences, Duquesne University
2 Franklin Regional High School

The human body is colonized by a vast amount of diverse microorganisms whose interactions have significant effects on our health. The bacteria Propionibacterium acnes and Staphylococcus epidermidis and the fungus Malassezia restricta make up the bulk of the scalp microbiota. In contrast to the popular notion that dandruff is a manifestation of a fungal infection, recent metagenomics studies suggest a radically different cause: dysbiosis of the microbiota that reduce P. acnes. We thus hypothesize that anti-dandruff shampoos do not exclusively target the fungus, but rather impact multiple species to ultimately promote P. acnes and mitigate dandruff. We tested the impact of commercial and natural anti-dandruff compounds on mono- and mixed-cultures of the three major microbial species. We demonstrate that these compounds indeed have the potential to restore the symbiotic balance by promoting P. acnes. We suggest alternative preventative strategies beyond a life-long commitment to commercial anti-dandruff shampoos.

47  Characterization and Regulation of Steroid Sulfatase Activity in NIH-3T3 Cells
Ojha, Sanjana and Selcer, Kyle
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Steroid hormones circulate as inactive sulfated forms, which steroid sulfatase (STS) converts into active forms at the tissue level. We have previously characterized STS in human and mouse breast and bone tissues. This study was designed to characterize STS in the mouse NIH-3T3 fibroblast cell line. We found high STS activity in cultured cells that was blocked by the STS inhibitor EMATE. We also found that microsomes of NIH-3T3 cells had high STS activity and that cytosols had low activity. Western blotting confirmed the presence of STS in microsomes, consistent with the known distribution of STS to the ER. Steroid treatments of cultured cells revealed that glucocorticoids decreased STS activity, as we have found for other cell lines. However, estradiol also decreased STS activity, which has not been shown previously. These results may have important implications with regard to local steroid conversions by STS in fibroblasts.

46  Generation and characterization of a mitochondrially-directed, dominant negative P2X1 receptor
Andrea Lebron-Figueroa; Richard Steinman, MD, PhD
Department of Biological Sciences, University of Notre Dame1
University of Department of Pharmacology, School of Medicine, University of Pittsburgh2

The P2X1 receptor (P2RX1) is an ATP-gated ion channel with a high permeability for Ca2+. This receptor is known to localize to the cell membrane. However, the Steinman lab has shown that P2RX1 does localize to mitochondria and that P2RX1 in mitochondria inhibits mitochondrial function. The goal of this study is to generate and characterize the effect of a mitochondrial targeted dominant negative (dn-) P2RX1 on mitochondrial function. I hypothesize that this dn-P2RX1 will increase mitochondrial function. A P2RX1 with dominant negative function has been isolated from blood cells of a patient with a bleeding disorder. This mutated P2X1 lacks one leucine within amino acids 351 through 354. I am using PCR mutagenesis to generate this dn-P2RX1 fused with a mitochondrial localization tag and red fluorescent reporter protein. I will also make a second putative dn-P2RX1 containing a proline at amino acid 351. These constructs will be transfected into HEK293 cells and mitochondrial localization of the dn-P2RX1 fusion proteins and mitochondrial energetics will be compared with that of cells bearing a similarly transfected construct containing the wild type P2RX1 protein. Should we find that inhibiting P2RX1 increases mitochondrial energy production, follow-up studies would be performed on how cells function with and without mitochondrial P2RX1 signaling.

48  A Model-Based Clinical User Interface for Continuous Glucose Monitoring and Control in Critically Ill Patients
Dennis, Jason A.1,2; Clermont, Gilles3,4; Parker, Robert S.3,4
1TECBio REU, Department of Computational and Systems Biology, School of Medicine, University of Pittsburgh
2Department of Chemical and Petroleum Engineering, Swanson School of Engineering, University of Pittsburgh
3Department of Bioengineering, George R. Brown School of Engineering, Rice University
4Department of Critical Care Medicine, School of Medicine, University of Pittsburgh

In the U.S., approximately 5.7 million patients are admitted annually to ICUs for life threatening medical problems, invasive monitoring, and restoration to stable health status. Stress hyperglycemia associated with insulin resistance and high glycemic metabolic variance are common in critically ill patients in the intensive care setting. Tight glycemic control schemes have been proposed, but these increase rates of hypoglycemia, which increases mortality. We propose an interface for intensive care use that may mitigate hyperglycemia while avoiding hypoglycemia by incorporating a comprehensive model of insulin-glucose dynamics. The accuracy and predictive capability of the model has been previously validated with in silico testing on a virtual patient cohort derived from clinical care data at UPMC. Our interface provides a real-time decision support tool for nurses and clinicians to visualize the impact of current and future insulin and nutrition administration and to manage stress hyperglycemia safely for critical care patients.
Phospholipids are major components of cellular membranes and their biophysical properties, such as fatty acid composition, help define membrane structure and function. Phosphatidylethanolamine (PE) is the most abundant phospholipid in cellular membranes and is synthesized primarily by two well-defined metabolic pathways. Gpc1 is a novel acyltransferase involved in PE biosynthesis and PE remodeling. Remodeling is the process of removing fatty acids from phospholipids (via phospholipases) and replacing them with new fatty acid species (via acyltransferases). These changes can impact lipid and membrane properties, such as fluidity. Gpc1 activity results in the addition of saturated fatty acids during PE remodeling. To investigate the physiological role of Gpc1, we examined growth upon deletion and overexpression of GPC1 at various temperatures. We report, among other things, that the loss of GPC1 negatively impacts growth under normal temperature conditions and positively impacts growth at elevated temperature.

The glycine receptor (GlyR) is a chloride-dependent ligand-gated ion channel found primarily in the spinal cord and the brain stem. Although there are crystal structures available for GlyR and its pentameric homologues, a more refined structure is needed, as flexible portions of GlyR are omitted from current crystal structures. Further insight into the receptor’s protein interactions and allosteric changes can provide necessary information for designing drugs that regulate its activity in order to treat pain and diseases. In this study, crosslinking mass spectrometry is used to define structural information about GlyR in three allosteric states: resting, open, and desensitized, relative to a specific inserted cysteine site (K206C) in the pre-TM1 loop of the receptor. Intramolecular and intermolecular crosslinked peptides within approximately 25 Å of K206C are identified. MS/MS is used to further refine sites to single amino acids. This information may be used to identify information about GlyR’s conformational changes and to resolve current models.
53  Measuring Dynamics of Structure and Subcellular Location of Lysosomes and Endosomes
Thompson, Timeka., Kangas, Joshua., Murphy, Bob
Computational Biology Department
Carnegie Mellon University

All life is composed of cells containing organelles. Some of these organelles such as lysosomes and endosomes are very dynamic in nature meaning they change size, shape, and location quickly. Measuring the dynamics of these organelles can help us to understand more about their function. Lysosomes are membrane-bound organelles that possess degradative enzymes to break down cellular material (proteins, nucleic acid, etc). Endosomes are specialized intracellular transporters. In their initial form “early” endosomes sort and assign cargo to various cellular destinations occurs, while in their mature form “late” endosomes possess a defined spherical shape and ultimately integrate with lysosomes. Through the use of time-series fluorescence microscopy images (movies), our team built 2D models of the dynamics of lysosomes and endosomes over time. To build models, the ever-changing dynamics of these organelles were measured within single cells. Lastly, the team has developed tracking algorithms within MATLAB to analyze the generated images.

55  Insight into Cannabinoid Receptor Type 2 (CB2) through Computational Modeling and Bioassay Validation
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Cannabinoid receptor type 2 (CB2), a class A G-protein coupled receptor (GPCR) located in the endocannabinoid system, plays a major role in the pathobiology of diseases such as osteoporosis, cancer, and Alzheimer’s disease. Rational design of agonists has been hindered by lack of a CB2 crystal structure and information related to key/selective residues. In this study, a homological model of CB2 was created and validated using the recently reported crystal structures of CB1, a closely related receptor. Then, agonist design was investigated. Based on results of docking studies, we suggest Ser19/Asn20/Met22 in the N-terminus may play important roles for CB2 selectivity. Based on MD simulation and bioassay validation results, we suggest that Trp258 at CB2 may have an important role in distinguishing agonist from antagonist. These studies provided new insight into the crystal structure of CB2 and can serve as a basis for future functional studies and drug design.

54  Recombinant expression of protein fragments from primate semenogelin genes.
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Duquesne University

The most abundant protein in human semen is semenogelin 1 (SEMG1), accounting for at least 25% of total protein. It is also among the most rapidly evolving male reproductive proteins in primates. In order to understand the evolutionary significance of differences in SEMG1 among humans, chimpanzees, and other primates, we are working to express short fragments of this protein using an E. coli expression system and longer fragments in human 293T cells. For this, we have cloned portions of the coding sequence into plasmid vectors, and are currently optimizing conditions for maximizing protein expression. After expression and purification, these protein fragments will be used in functional assays to characterize differences among species.

56  Structural Analysis of Crosslinked rSERT using Mass Spectrometry
May, Henry; Castellano, Elizabeth; Cascio, Michael
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Duquesne University

The serotonin reuptake transporter (SERT), a member of the sodium-dependent monoamine transporter superfamily, is responsible for transporting serotonin from the synaptic cleft to the presynaptic neuron. SERT is targeted by selective serotonin reuptake inhibitors (SSRIs) but its structure is not entirely known. Better understanding of SERT could lead to more specific binding of novel SSRIs, increasing the benefit of these drugs. My project works to enhance the understanding of the structure of SERT. Single cysteine mutations were introduced into X8C at site 564, in the TM11-12 loop. After purification, the crosslinker is attached at 564, then photocrosslinked to nearby loops. With the crosslinker attached, the protein is reduced and digested by trypsin and Glu-C. These extracted peptides are analyzed by mass spectrometry and tandem mass spectrometry. From this the structure of SERT can be refined, and potentially allow for development of better anti-depressants.
Oxidative DNA lesions and loss of genome integrity are key determinants of cellular survival and are profoundly affected in disease states and with natural aging processes. The nuclear enzyme APE1 plays a role in the repair of oxidative DNA lesions and maintains redox equilibrium. Here we report that normal aging does not influence the expression of APE1 in the rat olfactory bulb, piriform, hippocampal, and entorhinal allocortex, or sensorimotor neocortex. However, in a primary neuron model of Parkinson’s disease pilot data demonstrate that loss of the redox function of APE1 slightly increases the formation of Lewy pathology. Preliminary data also suggest that APE1-expressing cells are slightly more vulnerable than cells not expressing APE1. These findings support a modest role for APE1 in modulating Lewy-related inclusions and cell survival in Parkinson’s disease.

### Abstracts

#### 57
**APE1 is not modified by natural aging but may modulate Lewy-related inclusions in experimental Parkinson’s disease**
Gongaware, Rachel N.; Bhatia, Tarun N.; Vijapurapu, Sandhya; Eckhoff, Elizabeth A.; Luk, Kelvin C.; Leak, Rehana K.
1Graduate School of Pharmaceutical Sciences, Duquesne University
2Department of Pathology and Laboratory Medicine, University of Pennsylvania

#### 58
**Mass Spectrometry Structural Analysis of Crosslinked rSERT**
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Department of Chemistry and Biochemistry
Duquesne University

The serotonin reuptake transporter (SERT) is a monoamine, sodium-dependent transporter. Selective serotonin reuptake inhibitors (SSRIs) bind to SERT and inhibit the movement of serotonin back into the pre-synaptic cell, but can bind to other transporters emphasizing the importance of developing more selective drugs. My project focuses on learning more about the structure of rSERT in its apo state. Purification was performed on rSERT X8C containing a single cysteine mutation that was previously introduced in the extracellular TM3-4 loop at location 252. A crosslinker containing a benzophenone group was attached to the purified, reconstituted SERT via disulfide bonds to the cysteine and then crosslinks were introduced through photoactivation. The protein with the crosslinker was digested with trypsin and Glu-C. The mass shifted peptides were identified using mass spectrometry. Specific attachment sites were analyzed by tandem mass spectrometry, thus allowing for the identification of sites close in space to residue 252.

#### 59
**Pre-Treatment of Solid-Phase Extraction Cartridges for Quantification of Barbiturates in Forensic Toxicology**
Dryzal, Dana E.; Cook, Amy E.; Miranda, Colette C.; Wetzel, Stephanie J
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Duquesne University

Toxicology is a forensic discipline that allows for the detection and quantification of controlled substances in cases of poisoning, drug use, and death. Knowing the concentrations of drugs can infer the effect they have on an individual and aid in legal investigations; thus, it is critical that lab results are accurate and reproducible. The numerous steps involved in sample preparation often result in inconsistencies between different workers and laboratories. This research focused on verifying a method of pre-treating solid-phase extraction (SPE) cartridges to shorten preparation time and reduce error. SPE cartridges were pre-treated with a mixture of barbiturates and stored in various environmental conditions for two weeks, one week, and one day. Synthetic urine was spiked with an internal standard and applied to the cartridge to determine the percent recovery of barbiturates using liquid chromatography-mass spectrometry (LCMS).

#### 60
**The Effects of Pre-Loading and Storage Time on Percent Recovery of Amphetamines**
Cook, Amy E; Dryzal, Dana E; Miranda, Colette C; Wetzel, Stephanie J
Department of Chemistry and Biochemistry
Duquesne University

Forensic toxicology is used to identify drugs or chemicals and determine their concentrations in the human body. As a quantifiable science, toxicology assists in the investigations of poisoning and drug use, especially relating to death. High precision and high accuracy methods of sample preparation can be improved by pre-loading standards onto Solid-Phase Extraction (SPE) cartridges. In these experiments, SPE cartridges were conditioned and then pre-loaded with a standard mixture of amphetamines, which was followed by one of three different methods: air-dry (AD), water-rinse (WR), or methanol-rinse (MR). The pre-loaded cartridges were stored for different time periods. The SPE cartridges were used to extract a synthetic urine sample spiked with a deuterated standard. SPE was completed, and the eluate was dried, reconstituted, and analyzed with Liquid Chromatography-Mass Spectrometry (LC-MS) to determine percent recovery.
Visualization and determination of hSERT cholesterol interactions and potential domains for drug targeting
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Department of Chemistry and Biochemistry, Duquesne University1
Seton Hill University School of Natural and Health Sciences, Greensburg, PA2

The serotonin transporter (SERT) is a monoamine transporter responsible for the reuptake of serotonin from the synaptic cleft following an excitatory neurotransmission event. Low concentrations of serotonin in the synaptic cleft can lead to depression and anxiety among other mood and health disorders. Crosslinking mass spectrometry (CXMS) can be used to identify potential lipid accessible domains by probing with a photoactivatable cholesterol analog. In earlier studies, these data were mapped on LeuT, a bacterial homolog of neurotransmitter transporters. In 2016, a crystal structure of human SERT was solved, and CXMS data are now visualized on this model using PyMol. This new visualization reveals a striking pattern of cholesterol binding limited to the interfacial regions of the bilayer. Additionally, systematic cysteine point mutations are being generated for use in CXMS studies to determine the structure of the extracellular loops, as these flexible regions were truncated in the crystal structure.

Expression of the Glycine Receptor (GlyR) for Crosslinker Mass Spectrometry Studies
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The glycine receptor (GlyR) is a Cys-loop pentameric ligand gated ion channel and is responsible for the inhibition of the action potential in lower brain and spinal cord. The structure of GlyR has been determined by cryo-electron microscopy, but the structure needs further refinements, which can be accomplished with crosslinking mass spectrometry (CXMS) studies. A single cysteine is introduced into a Cys-null background (C41S/C290A/C345S) or an Ivermectin background (Cys-null+F207G/A288G), and is attached to a MTS benzophenone crosslinker. After irradiation, the crosslinker will bind to nearby amino acid, approximately 25 angstroms away. In this study, two mutations I412C and G23C, were introduced into the two backgrounds via PCR mutagenesis. This mutated GlyR cDNA was then transferred into bacmid DNA. The bacmid DNA can be transfected into insect SF9 cells to isolate and purify the amplified recombinant virus, which then will be used to express the protein for our CXMS studies.

Structural Analysis of SERT Extracellular Loops via Mass Spectrometry-Crosslinking Studies
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The serotonin transporter (SERT) is a membrane protein responsible for the reuptake of serotonin, a neurotransmitter associated with mood regulation. Selective serotonin reuptake inhibitors block SERT and increase the amount of serotonin available to counteract depression and anxiety. Structural analysis of SERT will be accomplished through point mutations of modified SERT devoid of reactive cysteines (X8C). A single cysteine was previously introduced in the TM3-4 extracellular loop for crosslinking studies, which was then overexpressed through baculovirus infection of insect cell. This was then purified, reconstituted, and reacted with crosslinker. SDS-PAGE bands corresponding to monomeric and oligomeric apo SERT were digested in-gel using trypsin and GluC protease. Extracted peptide fragments were analyzed by tandem mass spectrometry. The data obtained can be used for structural insights of SERT and help develop better SSRIs.

Investigation of Oxidative DNA Damage in an Animal Model of Parkinson's Disease
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Lewy body disorders such as Parkinson's disease are characterized by reactive oxygen species. However, the impact of oxidative stress on genomic integrity is not well understood in this family of conditions. The dopaminergic nigrostriatal pathway degenerates in Parkinson's disease and dementia with Lewy bodies, and can be modeled with infusions of the oxidative toxicant 6-hydroxydopamine (6-OHDA) in the mouse striatum. Here we report that a marker of DNA damage, 8-hydroxy-2'-deoxyguanosine (8-OHdG) is increased in the mouse substantia nigra following infusions of 6-OHDA in the striatum. These findings suggest that free-radical toxicity in Parkinson's disease may contribute to oxidative lesions in DNA and perhaps contribute to loss of the nigrostriatal pathway.
65 Identifying genetic interactions between α-arrestins Aly1 and Aly2 and autophagic machinery identified through screening of the Saccharomyces cerevisiae Ubiquitin Interactome (ScUbl) gene deletion library
Chera, Karandeep; Malik, Faba; Bowman, Ray W.; and O’Donnell, Allyson F.
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α-Arrestins, a family of protein trafficking adaptors, play a pivotal role in the selective redistribution of membrane proteins. Regulation of the α-arrestins and their protein trafficking function remains poorly defined. We performed a targeted screen of the Saccharomyces cerevisiae Ubiquitin Interactome (ScUbl) gene deletion library to identify specific α-arrestin regulators associated with ubiquitination, a post-translational modification which plays a pivotal role in protein trafficking decisions. The ScUbl library is a collection of 376 strains, each of which containing a gene deletion annotated as important for ubiquitination or ubiquitin interaction. We assessed the growth on rapamycin medium for each of these gene deletions when α-arrestins Aly1 or Aly2 were over-expressed and identified ATG7 as a strong candidate for modified growth. Using serial dilution growth assays and biochemical approaches, we have begun to define the genetic interactions between the autophagic machinery and α-arrestins Aly1 and Aly2.

66 Development of a Homemade Device to Measure Color Concentration in Water Samples
Graves, Spencer; Aguilar, Ross; Corcovilos, Theodore A.
Department of Physics
Duquesne University

A common method for finding impurities in water involves measuring the color of a sample after a chemical sensor has been added. We developed an all-purpose color sensing device that is small, portable and economical allowing water samples to be tested on site instead of in a lab. The device utilizes a color sensor measuring light intensity at six wavelengths: Violet (450 nm), Blue (500 nm), Green (550 nm), Yellow (570 nm), Orange (600 nm), and Red (650 nm). The device flashes a known amount of white light from an LED onto a sample and measures the transmittance of each color through the sample. Concentrations are found using a calibration curve generated from measuring known samples. The results are displayed on the device’s LCD screen. This device has the flexibility to conduct a wide range of color tests for contaminants such as fluoride, chloride, and metals.

67 In-vitro flow visualization in patient-specific left atrial geometries and medical image segmentation
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The left atrial appendage (LAA) is an anatomical extension originating from the main body of the left atrium (LA) which experiences poor contractility in atrial fibrillation (AF) which is hypothesized to be a principal location for intra-atrial thrombus formation. Despite known causes of AF, flow analysis of LAA shape on hemodynamics and flow stasis have not been quantitatively analyzed. DICOM models of the LA were generated, which were subsequently refined by surface-clipping in 3D. A combination of iterative surface clipping, smoothing and finishing techniques were employed in Geomagic Studios until a final LA geometry was created. Inlets and outlets were extended and added to the finished LA geometries for CFD studies. The final printed models were integrated with an in-vitro mock circulatory flow loop in order to visualize fluorescent nano-particles flowing through them, using particle image velocimetry hardware. The focus of flow visualization efforts is to quantitatively determine risk of thrombus formation in the LA appendages of each studied LA, by examining regional particle stasis / residence in the appendage.

68 Causal Network Analysis of Breast Cancer Pathology Data
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University of Puerto Rico

Bryan Andrews
Department of Biomedical Informatics
University of Pittsburgh

Gregory F Cooper, M.D., Ph.D.
Department of Biomedical Informatics
University of Pittsburgh

There has been significant research progress in understanding cancer, but many open questions remain about its mechanisms. Causal discovery algorithms provide a method for exploring these mechanisms. Such algorithms can find patterns in observational data that support some of the variables having a causal relationship. We applied the FGES causal discovery algorithm to 1000 pathology reports that were extracted from the UPMC cancer registry for the years 2015-2018 and converted to UMLS CUI codes using NLP processing by the TIES system. We are currently examining the causal graphs output by FGES to seek insights about the causal mechanisms and processes involved in breast cancer. We also plan to apply to this data the GFCI algorithm, which models the possible presence of latent confounder variables.
69
Conformational analysis of chiral hydrogen-bond donor organocatalysts
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Ecofriendly dual hydrogen-bond donor organocatalysts, such as chiral urea and thiourea complexes, are becoming increasingly popular catalysts for enantioselective organic reactions. As a general principle, the dual hydrogen-bond donor forms a stereodifferentiated environment to control selectivity. Specifically, we investigate the thiourea-catalyzed alkylation of α-chloroethers through anion-abstraction. Two modes of anion-abstraction with two molecules of catalyst, the “4H-” and “2H-” configurations, have been proposed, yet a systematic and thorough conformational study of the catalyst or configurational study of the binding modes has not been reported. Computations using Stewart’s PM7 semi-empirical method and Truhlar’s M06-2X functional with Dunning’s jul-CC-pVDZ basis set were performed to scan soft dihedral angles and generate various conformations of the catalyst. Our work provides a foundation for understanding how organocatalyst conformation develops a stereodifferentiated environment to control stereoselectivity of the alkylation of α-chloroethers.

71
Biophysical characterization of oligouridylated histone mRNA degradation intermediates
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Replication-dependent metazoan histone mRNA contains a highly conserved 3’ stem loop instead of a poly(A) tail. This stem-loop is bound by the stem loop binding protein (SLBP) through a highly specific interaction, and together these two elements control all aspects histone mRNA metabolism. In the cytoplasm, the stem-loop/SLBP complex is bound by the human 3’ hexonuclease, which initiates mRNA degradation when RNA replication ends by trimming the 3’ end of histone mRNA and allowing for oligouridylation by a cytoplasmic enzyme. The stem-loop stays intact after uridylation by base-pairing the 5’ end of the stem with the oligo(U) tail to create a longer stem-loop. In order to determine the nature of the interaction between SLBP and the longer, uridylated stem-loop, two stem-loops (wild type and uridylated) were synthesized via in vitro transcription and characterization of the RNA and the RNA/SLBP complexes will be carried out with a variety of biophysical methods.

70
Classifier-based approach for detecting reliable variant calls across DNA and RNA breast cancer sequencing data
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The identification of single nucleotide variants (SNVs) within cancer cells is crucial in understanding the progression and recurrence of malignant tumors. Using matched tumor-normal tissue data from breast cancer patients, the aim of this study is to quantify the differences between DNA-seq and capture-method RNA-seq based variant calls and to assess the amount of variant information that can be reliably extracted from the sequencing data. We assume that the presence of a SNV in both RNA-seq and DNA-seq sources is more reliable than variants specific to RNA-seq. From this, we take a supervised learning approach using a gradient boosted decision tree to classify variants as RNA-seq specific or common to both RNA-seq and DNA-seq using the genomic context and confidence of the variant call. We expect this approach to help researchers prioritize reliable RNA-seq SNVs in cases where no matched DNA-seq data is available.

72
Biophysical Characterization of BACE1 mRNA and its Interactions with the FMRP RGG Box
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Fragile X syndrome (FXS) is a neurodegenerative disease caused by a trinucleotide overexpansion within the FMR1 gene, resulting in downregulation of Fragile X mental retardation protein (FMRP). FMRP targets mRNAs within the brain to regulate their translation. Specifically, the RGG box domain of FMRP recognizes G-quadruplex structures within mRNAs. This research focused on the b-amylloid precursor protein cleaving enzyme 1 (BACE1) mRNA, which is proposed to form a G-quadruplex structure. A 44 nucleotide BACE1 mRNA fragment was transcribed in vitro and was characterized using CD spectroscopy and UV thermal denaturation spectroscopy. To monitor the binding between BACE1 mRNA and the RGG box peptide, native gel electrophoresis was implemented using both the wild type BACE1 mRNA, as well as a 2-aminopurine fluorescent analogue of the sequence. These interactions were further characterized using steady-state fluorescence spectroscopy.
Regulation of the high affinity glucose transporter Hxt4 by α-arrestin Rog3 and the AMP-activated kinase Snf1
Kenny Callahan, David Augustine, Daksha Chandrashekarappa, Leo Garnar-Wortzel, Martin Schmidt, and Allyson O’Donnell
Department of Biological Sciences
Duquesne University

To maintain homeostasis in response to environmental changes, cells reshuffle the complement of transmembrane proteins at their cell surface and in intracellular membranes. Conserved from yeast to man, the α-arrestins are a family of protein trafficking adaptors that drive this selective protein reshuffling by linking protein cargo to the machinery for protein trafficking. Here we focus on the role of α-arrestins in regulating glucose transporter trafficking in response to changes in glucose abundance. Our earlier studies showed that the α-arrestins Rod1 and Rog3 are regulate Hxt1 and Hxt3, the low affinity glucose transporters, in response to exposure to the toxic glucose analog, 2-deoxyglucose, which is thought to stimulate glucose starvation in cells. While Rog3 plays a role in Hxt3 internalization, Rod1 is responsible for the majority of this trafficking. Here we identify Rod1 and Rog3 as regulators of Hxt4, a high-affinity glucose transporter, and show that Rog3 is a substrate for the AMP-activated kinase, Snf1. Snf1 controls Rog3 abundance in cells and this regulation appears to be important for Rog3-mediated trafficking of Hxt4 upon acute glucose starvation.

Immobilization of Anti-Platelet Molecules via Cross-Linking with Self-Assembled Monolayers Formed on Stents
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2University of Pittsburgh Medical Center PGY-1
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Coronary heart disease, a condition caused by the buildup of plaque in the arteries, affects over 3 million Americans. Stents are put into place to open blood flow in the obstructed arteries. However, a complication of stent usage is thrombosis, or platelet aggregation, which can lead to blood clots. To prevent this potentially deadly complication, the immobilization of Ticagrelor, an anti-platelet medication, may prevent clot formation. Ticagrelor can be immobilized through the reactive tail groups of self-assembled monolayers, which uniformly coat stents. Self-assembled monolayers were composed of 11-hydroxyundecylosphosphonic acid, 16-phosphonoheptadecanoic acid and tetradecylphosphonic acid, to provide the necessary tail groups for future reactions. These monolayers are deposited on stainless steel 316L foils and stents and then sonicated to remove all physisorbed compounds. Diffuse reflectance infrared Fourier transform spectroscopy (DRIFT) and contact angle were used to characterize the formed monolayer.

Survey of Transiting Extrasolar Planets at the University of Pittsburgh (STEPUP)
Richie, Helena and Dr. Wood-Vasey, Michael
Department of Physics and Astronomy
University of Pittsburgh

STEPUP is an undergraduate research group lead by Helena Richie that makes photometric observations of stars of variable brightness. These targets can be systems such as AG Draconis, a symbiotic binary that STEPUP has been studying since April 2018 as it exhibits unusual behavior in its fourth minor outburst of its most recent active phase. They can also be targets that have variable brightness due to a transiting exoplanet. STEPUP has recently joined the KELT Follow-Up Network (KELT-FUN) and the TESS Follow-up Observing Program Sub-Group 1 (TFOP SG1) in order to contribute photometric observations that confirm or deny exoplanet candidates detected by these two surveys. Observations made by STEPUP contribute to both the understanding of Type Ia Supernovae, as symbiotics are a suspected progenitor of these events, and the discovery of new worlds through the study of KELT and TESS candidates to detect exoplanets.

Removal of Excess Fluoride from Drinking Water by Adsorption
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Drinking water that contains high concentrations of fluoride is a prominent issue in developed and developing countries around the world. Consuming fluoride in concentrations above 1.5 mg/L can lead to the development of dental and skeletal fluorosis; unfortunately, removal of fluoride from drinking water systems is a complicated and still unsolved issue. Various techniques have been used in an attempt to remove excess fluoride, such as using activated alumina and filtration systems. These techniques tend to be expensive and have varying, low success rates. Various compounds were tested as potential fluoride removal materials including powdered calcium carbonate, a local smectite clay, and dried leaves from Dieriocayum ericarpum (the devil’s thorn plant). Clay and the devil’s thorn leaves showed great promise in treating drinking water that contains high concentrations of fluoride.
Social media can play an important role in informing health care providers with the unmet patient needs on a large scale. The challenge is the large amount of free text that must be filtered through to find the relevant health information, which is labor-intensive and time consuming. The purpose of this study was to classify dialog act in online postings regarding to the needs of patients and caregivers for developing an automated classification model.

The data was from the online support forum sponsored by the American Cancer Society, which involved patients and caregivers with ovarian cancer. Two annotators annotated 339 posts based on the need displayed in the post and then each sentence was classified by one of the follow dialog act categories: request information, explain, opinion, describe experience, express emotion, suggest, and other. Inter-rater agreement between the two annotators will be measured to evaluate whether manual identification is feasible.

The poor usability of electronic health records(EHR) systems has been a common complaint by clinicians. The rise in popularity of virtual assistants in consumer devices has made speech recognition(SR) a viable and trusted input modality that can increase the efficiency and usability of multiple systems. That's why we sought to address this issue by creating an EHR system with SR at its design core. Our work includes creating a rudimentary SR interface that allows the clinician to specify flexibly what information and formatting they want to see, using a composable approach. We will then test the system's usability in comparison to popular EHRs through test cases and clinician users, measuring time, cognitive benefits or disadvantages, efficiency, usability, and overall clinician appraisal. For this we will use standard usability testing think-aloud protocols. The SR's accuracy and need for standardized phrasing while giving commands will also be tested.

Designing a SNP panel for comparative genomics the snow leopard subspecies to examine high-altitude adaptations.

Recent advances in next-generation sequencing have been important for understanding species. This approach enables the analysis of whole genomes to identify informative genetic variants. Our lab recently delineated three subspecies in the snow leopard, Panthera uncia, that each inhabit distinct high-altitude regions of Asia. Our objective was to identify single-nucleotide polymorphisms (SNP) using 5 low-coverage snow leopard genomes, focusing on the EGLN1 gene, which regulates the hypoxia response pathway. The CLC Genomics Workbench was used to map trimmed reads to the 7.5 Mb tiger scaffold containing EGLN1 and identify polymorphic variants. The number of fixed differences between snow leopards and tigers, and polymorphism was estimated. Primers were created to genotype 32 select SNPS, and amplified in scat samples. These will be used to test for a selective sweep in EGLN1. Our preliminary study provides a foundation for examining range wide genome differences in the snow leopard.
Malaria infected over 200 million people in 2016. It is caused by parasitic protists belonging to the genus *Plasmodium* and transmitted by the *Anopheles* mosquito vector. Insect and parasite resistance to current strategies highlights the need for new control strategies. One strategy is paratransgenesis, in which symbiotic bacteria within the mosquito midgut can be transgenically modified to affect the mosquito’s phenotype. With this method, engineered bacteria strains can spread through mosquito populations to inhibit infection of the mosquito. Ideally, these modified strains will not be outcompeted by the wild type within the midgut of the mosquito. Scorpine, a strong antiplasmodial effector protein, was fused to various other carrier proteins and these plasmids were transformed into our target bacterium, *Asaia bogorensis*. The maximum growth rates of these strains were assessed, which indicates how fit they are and if they will be outcompeted by the wild-type.

The development of miniaturized mechanical systems is growing, along with a need for lubricants to improve efficiency and longevity of the devices. Organic self-assembled monolayers (SAMs) have been used to lubricate the interface between moving parts of these systems. Changing molecular structure and chemical composition of the monolayer would influence its lubricity substantially. In the present study, SAMs of octadecanoic acid (C18H) and perfluorooctadecanoic acid (C18F) were formed on single crystalline sapphire substrates by solution deposition. Diffuse reflectance infrared Fourier transform (DRIFT) spectra indicated the formation of highly ordered monolayers with mixed mono- and bidentate binding. Atomic force microscopy (AFM), employed to measure the interfacial frictional properties of the two monolayers, showed the C18H monolayer was twice as frictional as C18F monolayer. Water wettability of monolayers was determined with contact angles. While both films exhibited hydrophobicity, C18F showed more hydrophobic (108.9° ± 1.9°) than that of C18H (90.6° ± 2.2°).

**83 Frictional Properties of ODCA and Perfluorinated ODCA SAMs**

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Persistent organic pollutants (POPs) are toxic organic chemicals that have adverse effects on human health. Dietary supplements (DS) made of botanical materials have been found to contain POPs. In this study, thirteen POPs were quantified in eight commercial dietary supplements. Stir-bar sorptive extraction (SBSE), GC Triple Quad MS with multiple reaction monitoring (MRM), and isotope dilution mass spectrometry (IDMS) was used to extract and quantify the POPs. SBSE is a novel and effective extraction method for the POPs. Following the extraction, the POPs were automatically thermally desorbed into the GC Triple Quad MS. Quantification was accomplished by using IDMS (MRM). By adding isotopically enriched forms of the analyte into the extract, the isotope ratio and transition fractions were measured. The results from IDMS were compared to calibration curves. The percent errors and relative standard deviations of the measurements were significantly lower when using the IDMS method especially at lower concentrations.

**84 Quantification of Persistent Organic Pollutants in Commercial Dietary Supplements Using Stir-Bar Sorptive Extraction, GC Triple Quad MS, and Isotope Dilution Mass Spectrometry**

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Detecting cancer-causal genetic structural aberrations affecting aromatase inhibitor-resistance in luminal breast cancer patients
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Genomic alterations such as structural variations have long been known to be key drivers in especially aggressive types of cancers such as luminal breast cancer. With the advent of Whole Genome Sequencing (WGS), identifying significant recurrent genomic alterations in such oncologic phenomena is a reality. In particular, the development of specific drug therapies to target the products of these genomic alterations is of great clinical interest. In the present study we use Structural variation Analysis by Assembly (SvABA), a structural variant calling tool, to identify such recurrent alterations in WGS data from various patients of aromatase inhibitor-resistant luminal breast cancer. This study will investigate highly recurrent genetic mutations that are directly involved in aromatase inhibitor therapy resistance. Our study also describes the genomic landscape of such tumors and paves the way for further studies that can lead to the development of treatments for these types of breast cancer.

86
Biophysical Characterization of Drosha mRNA G-quadruplex Binding to FMRP RGG Box
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Fragile X Syndrome (FXS) is the most common form of inherited mental retardation and the most common cause of Autism Spectrum Disorder. The underexpression of Fragile X Mental Retardation Protein (FMRP) leads to FXS. FMRP contains an arginine-glycine-glycine (RGG) box domain which is known to bind specifically to RNA secondary structures, including the G-quadruplex. The G-quadruplex is a dynamic secondary structure that forms in guanine-rich regions of RNA. A previous study has shown that FMRP binds to the messengerRNA of Drosha, an RNase III enzyme responsible for microRNA processing in the nucleus. This messengerRNA contains a guanine-rich region in its 5’ UTR. We hypothesize that this guanine-rich region can form a G-quadruplex structure and that FMRP binds selectively to this structure via its RGG Box. In this study, we used ¹H NMR, Circular Dichroism, Fluorescence, and UV-Vis spectroscopies alongside Native PAGE assays to characterize this binding mechanism in vitro.

87
Dealing with missingness in causal discovery by utilizing test-wise deletion, the FCI algorithm, and a modified causal independence test
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Incomplete samples are not uncommon in causal discovery; whether it’s due to values missing at random or values which are missing not at random, such as a dataset with hidden selection bias. Several current approaches are to eliminate all samples with missing data or to perform a type of imputation. Eliminating data is inefficient, and if the missingness is severe, it hinders the performance of the causal discovery algorithm. On the other hand, imputation isn’t always correct and may lead to artifacts which confuse or bias the results. We developed software that simulates datasets with missing values from random graphs that modeled conditional selection bias based upon observed values. Then we applied different parametric and nonparametric causal discovery algorithms in order to test their ability to work with datasets that have missing data, and we compared their performance with different metrics, such as Structural Hamming Distance and sample size efficiency.

88
Use of Classification Trees for Prognosis of End Stage Renal Disease
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According to statistics from the National Institutes of Health, over 600,000 Americans have experienced end stage renal disease (ESRD), with over 40,000 associated deaths annually. One of the major contributors to kidney disease is polycystic kidney disease (PKD), where abnormally large cysts grow on the kidney, and cause a number of health complications. To identify people who are at greatest risk for these outcomes, a number of studies have collected and analyzed biomarker data (which are objective measurements used to assess normal biological function, pathogenic processes, or responses to treatment). In particular for PKD, the Consortium for Radiological Imaging Studies of PKD, or CRISP, collected data on several hundred, initially healthy participants over nearly a 15-year period. This current study applied classification trees to a simulated data set (with 400 observations) based on CRISP (with 46 different urine, serum, and genetic biomarkers) to identify subgroups of PKD patients who are at higher ESRD risk. The tree model was built using R which was used as means for analyzing the data. It repeatedly partitions the data into different subsets with either the highest or lowest percentage of cases in each subgroup. For our simulated data, the tree created five different (either high risk or low risk) subsets based on the estimated glomerular filtration rate, uric acid excretion, age, and alkaline phosphate levels.
89 Diagnosis of Attention-deficit/hyperactivity disorder by Causal Influence Strength
Learned from Task Related- fMRI Data
Computer Science
University of Puerto Rico Rio Piedras Campus

The goal of this study is to determine if Attention-deficit/hyperactivity disorders (ADHD) can be identified with causal inference connectivities within the brain using fMRI task-related data and machine learning algorithms. Using causal inference algorithms, FASK and Two-Step, directed connectivities and coefficient values were estimated within a set of regions of interest spanning the whole brain using task fMRI data. Once identified, the coefficient values were input into a support vector classifier in order to determine if ADHD and control individuals can be classified based on their connectivity patterns.

91 Fluoride Removal from Water Using a Calcium Carbonate-Based 3D Printed Filter
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Duquesne University

Groundwater containing high amounts of fluoride is the most common source of drinking water in rural areas in parts of east Africa, India, and China. The elevated levels of fluoride cause skeletal and dental fluorosis, which is weakening and decay of bone structures due to the leeching of calcium from the body. Over 150 million people are suffering from some form of fluorosis due to the consumption of groundwater. Calcium carbonate has been demonstrated to influence fluoride removal in several forms. To make fluoride removal a cost-effective and user-friendly process, a study has been done to test the efficacy of a 3D printed water filter using E.P Smartfil Filament, composed of 30% calcium carbonate and 70% PLA. The influence of varying conditions concerning the removal of fluoride from water, such as the initial fluoride concentration of the water and time spent in contact with the filter have been investigated.

92 Bioactive Diaporthe strains found in rosy periwinkle
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Catharanthus roseus is a species of plant grown in the Hainan province. Dr. Yan and his team of the Chinese Academy of Forestry in Beijing, China isolated four endophytic fungi strains from Catharanthus roseus belonging to the Diaporthe genus, due to the genus' known bioactivity. Genomic DNA was extracted from each fungus strain. Five loci: ITS, TEF1, CAL, HIS, and TUB regions, were amplified using PCR. The sequences were analyzed and the strains were identified via maximum likelihood and maximum parsimony phylogenetic analysis. The four stains were designated Diaporthe sp. Strains (FPYF3053-3056). The VOCs produced by each endophytic strain showed antifungal activity against nine pathogenic test fungi, exhibiting growth inhibition ranging between 10% and 60% within 72 hours of initial exposure. The VOCs were examined using SPME fiber-GC/MS techniques to determine their antifungal bioactivity. Terpenoids were found to be the major component in VOCs of each fungus strain.
93 Characterization of Spore-Associated Protein A Assembly onto the Spore Surface in *Streptomyces coelicolor*
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*Streptomyces* is a soil-dwelling bacteria that is known for its production of antibiotics. *Streptomyces coelicolor* has a complex life cycle that involves sporulating aerial hyphae. *S. coelicolor* has spore associated proteins that are secreted and localized to the spore coat. Previously, recombineering was used to fuse the gene for *E. coli* *ltb* to 3’ end of *sapA* and conjugated into *S. coelicolor*, and a full length SapA fused to Ltb and a C-terminal truncation of 38 amino acids was shown to be secreted and localized to the spore surface. The goal was to learn more about SapA by characterizing different Ltb fusion mutations to better understand SapA incorporation into the spore coat. Currently, we are trying to further characterize the secretion and localization pattern of the SapA-LTB fusion by performing an in frame deletion of a conserved motif (CGSGY) in the SapA protein sequence and a complete deletion of the gene. With more understanding of SapA secretion and assembly onto the spore surface it could provide a future alternative vaccination mechanism.

95 Generating Forbidden 10-Fold Symmetry Quasicrystals using an Optical System
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Quasicrystals are non-periodic arrangements of atoms, first discovered in the 1980s, that possess no translational symmetry but still maintain long-range order. The empirical mechanical, thermal, and electronic properties of quasicrystals match neither those of true crystals nor amorphous materials, making these properties difficult to predict theoretically. We will study the quantum mechanical properties of quasicrystals by building analogs to them using atoms at nanokelvin temperatures in an optical potential equal to that of a quasicrystal. We numerically simulated a quasicrystal with 10-fold symmetry built by the interference of five nearly co-propagating laser beams using Fresnel propagation software written in Python and constructed a simple optical setup to demonstrate the potential. The quasicrystal structure of the laser interference pattern is experimentally verified using the Fourier transform of a photograph of the pattern, which clearly shows “forbidden” 10-fold rotational symmetry.

94 Use of a SapA Protein Fusion for Pertussis Toxin Vaccine Delivery
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This study aims to develop an alternative method of vaccine delivery through the use of spore-associated proteins of *Streptomyces coelicolor* as a potential vehicle to carry the major pathogenic determinant from *B. pertussis*. The major goal of this project was to create a fusion of pertussis toxin PtxA to the C-terminus of the SapA protein. A fusion was constructed using the spore-associated protein SapA because it is secreted through the standard signal sequence-dependent pathway. Once the strain expressing the fusion was isolated, it was analyzed using various methods, including: SDS-PAGE and Western blot analysis using a commercial polyclonal antibody to PtxA and testing in a mouse model. The Western blot analysis of spore proteins extracted with a non-lethal detergent wash indicated that SapA-PtxA is localized to the surface of the spore. The spores are currently being tested in a mouse model to see if recombinant spores will protect against a *B. pertussis* Challenge. In the future, the use of Sap protein fusions to passenger proteins might lead to recombinant *Streptomyces* with epitopes displayed on the spore surface creating an additional method of vaccine delivery.

96 Development of Contaminant Detecting Mobile Application UtilizingPhotographic Color Analysis
Aguilar, Ross; Graves, Spencer; Corcovilos, Theodore A.
Department of Physics
Duquesne University

Our work sought to determine a method via software development to compute the concentration of a given contaminant in water based on the optical intensity of the color of a sample of water. This methodology can simplify work in Chemistry and Environmental Science to analyze water in various ecosystems. In lab, red food dye was used to mimic a color-change test on contaminated water and varying concentrations of dye were analyzed. The samples were photographed with a mobile device through a RAW photo application to preserve all color data. Software was developed in Python to determine the color of the water based on an RGB scale and the data was fit along a variation of Beer’s Law. Blind tests of unknown samples were then used to verify the method. Further work includes the development of a mobile application to simplify this testing procedure and make it publicly accessible.
Effects of Silica Nanoparticles on the Mechanical and Transport Properties of hydrosiloxane-based Nanocultures

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Organosilanes contain hydrocarbon backbones, allowing them to react with silicone-based agents in the presence of a catalyst and polymerize into membranes with tunable transport and mechanical properties. Poly(dimethylsiloxane) membranes, like Sylgard 184, have properties suitable for delivery of hydrophobic substances, gas permeability, trace organic compounds removal, and microfluidic device fabrication. Here, we design new siloxane-based membranes to study microbial dynamics. We develop a culture system referred to as nanoculture to encapsulate microbes in semipermeable membranes or grow challenging species in environmental conditions. We explore the permeability of the membranes to signalling biomolecules, sugars, and antibiotics to understand their effects on microbial growth. We screen a wide variety of Poly(methylhydrosiloxane) membranes to a controlled selectivity. The mechanical properties of the membranes are reinforced with silica nanoparticles, which enable the nanocultures to withstand high shear stress similar to environmental conditions while maintaining transport properties essential to microbial communication and growth.

Examining the Relationship between Patient Centeredness of Care (PCC) and Symptom Management Strategies During Breast Cancer (BC) Chemotherapy Clinical Visits

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University of Pittsburgh School of Nursing

Breast cancer is the second most common cancer in women. Although there have been advancements in cancer therapies, there is an increasingly wider gap in cancer mortality rates between black and white women. Though some studies propose that the disproportionate breast cancer outcomes for black women may be due to non-biological factors, more recent research points to patient-center communication (PCC) as an underlying factor in cancer outcomes. Further research into PCC in cancer patients may provide novel insights regarding health communication.

Aims: We propose to:

Aim 1: Qualitatively explore and code for PCC using Four Habits Coding scheme during the chemotherapy clinical visit of women undergoing breast cancer chemotherapy and compare by race

Aim 2: Describe and racially compare the patient factors and symptom experience among a cohort of women receiving breast cancer chemotherapy

Aim 3: Explore relationships between patient factors, symptom experience, and PCC.

Accurate Mapping of miRNA reads

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Mature miRNAs are short RNAs that are ~ 21 nucleotides long. After being transcribed from the DNA and processed into mature miRNAs, miRNAs may undergo further modifications because of mutations. It is difficult to distinguish these modifications in RNA sequencing from errors introduced during sequencing. Mapping the complementary RNA sequencing reads back to their reference genome is difficult. The best workflow strategy, designed primarily for tRNAs, was used to overcome this barrier. We attempted to improve variant calling in miRNAs by combining sequence data from pri-miRNAs and mature miRNAs.

Results: An accurate mapping strategy was developed to handle the mapping of RNA sequencing reads to miRNA. A modified target genome was used in which studied miRNA loci were masked and precursors were appended as artificial chromosomes. This research would help identify what microRNA is likely to help post-transcription modifications and see if they are tissue-specific or correlated with a disease.

Feline Infectious Keratitis Leading to Eye Rupture – Molecular Determination of Possible Pathogens

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Duquesne University

Upper respiratory infections (URIs) are common in felines. Typical signs of URI include sneezing, nasal discharge, ocular discharge, and conjunctivitis, inflammation of the sclera and lining of the eyelids. Keratitis, inflammation of the cornea, is a less common sign of URI, and can cause scarring and rupture of the eye. Feline herpesvirus 1 (FHV-1) is currently considered to be the most common primary pathogen associated with the ocular manifestations of URI, however, *Clamydophila felis* (*C. felis*) and *Mycoplasma felis* (*M. felis*) are also prevalent in cats with conjunctivitis. Feline calicivirus (FCV) and other opportunistic bacteria may also be present. Twenty ruptured, enucleated eyes were evaluated for the presence of bacteria, FHV-1, and FCV using PCR with universal bacterial primers and FHV-1 primers, qPCR with FCV primers, and Next-generation sequencing (using universal bacterial primers). These techniques allow detection of typically culture-resistant bacteria and insight into co-infections associated with severe ocular disease.
Aminophosphines, which can be represented as $R_2N–PR_2$, participate in a wider range of chemical interactions compared to phosphines ($PR_3$). For example, the nitrogen atom can participate in binding to transition metals or serve as a Lewis base. Thus, aminophosphines are versatile compounds with potential for application as ligands in homogeneous catalysis. However, their complex behavior has also served as a barrier to research. With the aim of better understanding these compounds, a family of monoprotic aminophosphines (MAPs, $RHN–PR_2$) with systematic variation of the ligand structure were studied both computationally and experimentally. Computations employed Stewart’s PM6 semi-empirical method and Kohn-Sham’s MN15 functional with a def2TZVP basis set to determine isomerization equilibrium constants and relative enthalpies of the structures. Complexes containing nickel were synthesized using Schlenk air-free techniques, and subsequently characterized using NMR and IR spectroscopy methods. This research serves to elucidate some of the fundamental characteristics of MAPs.

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Experimental and Computational Studies of Nickel-Aminophosphine Complexes
Frederic, Wrebekah; Pros, Gabrielle; Evanseck, Jeffrey D.; and Bloomfield, Aaron
Center for Computational Sciences and Department of Chemistry and Biochemistry
Duquesne University

Bacteria form dense communities known as biofilms that cause a plethora of chronic diseases due to their recalcitrant nature. These dense communities also inherently pose significant space and resource constraints to individual bacterial cells. How do bacteria solve this intrinsic problem? Our recent work suggests that multiple secretions that are regulated by a post-transcriptional regulator, RsmE, function to capture space and optimal positioning in a dense colony. We hypothesize that various secretions play discrete roles to compete for space. We have identified a mucoid polymer and biosurfactant that are RsmE-regulated and have engineered respective mutants to explore their function. Epifluorescence microscopy reveals that the mucoid polymer pushes away neighboring cells while the biosurfactant physically prevents their encroachment into the newly created space. Our work shows that bacteria produce specific structures to compete for space and understanding the molecular underpinnings could pave way to develop therapeutic strategies to eradicate biofilm infections.

**102**
Characterization of bacterial secretions that function to create space and optimal positioning in dense bacterial colonies
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**103**
Isolating and characterizing null mutants of a putative chromosome segregation protein in *S. venezuelae*
Woodward, Braden, Orr, Erin, Sallmen, Joseph, Bennett, Jennifer, McCormick, Joseph
Biological Sciences
Duquesne University

*Xylenomyces venezuelae* is a Gram positive soil bacterium that produces a variety of secondary metabolites, such as antibiotics. The *Xylenomyces* genus is also of interest because of its complex lifestyle and close relation to medically relevant bacteria, such as *Mycobacterium tuberculosis*. In the past, our research focused on the species, *S. coelicolor*, where a random mini transposon reaction mutant of a gene, that encodes a putative membrane protein was isolated. These mutants were shown to have a severe DNA segregation phenotype. Recently, we have made complete deletion of the orthologous gene in *S. venezuelae*, a relative of *S. coelicolor*, but one that can sporulate in liquid medium. The overall goal was to see if the mutant phenotype was reproducible in *S. venezuelae*. Preliminary fluorescence microscopy was used to analyze spores of *S. venezuelae*. The new mutants have a less severe genome segregation phenotype. Currently, construction of a genetic complementation vector is underway to show that the segregation phenotype is the result of the introduced mutation.

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Preliminary characterization of a thermoresponsive gel for treatment of open globe injuries
Lauren A. Krzystostwczyk (5), Michael A. Washington (1), and Morgan V. Fedorchak (1,2,3,4)
Department of Ophthalmology (1)
Bioengineering (2)
Clinical and Translational Science (3)
McGowan Institute of Regenerative Medicine (4)
University of Pittsburgh
Vanderbilt University (5)

Open globe injuries are full-thickness injuries to the cornea or sclera resulting in loss of intraocular pressure (IOP), inflammation, and possible permanent vision loss. Studies suggest that proper treatment and protection of traumatic ocular injuries at the point-of-injury are critical to preserving the form and function of the eye and its supporting adnexa. However, the current standard of treatment used by first responders is taping a cup over the eye. The purpose of this study was to evaluate the rheological, anti-inflammatory drug release, and IOP stabilization properties of a thermoresponsive poly(N-isopropylacrylamide-co-ethyl acrylate) (pNIPAAm-co-EA) hydroxypropyl methylcellulose (HPMC) gel. Rheological properties of various gel formulations were evaluated using a dynamic temperature ramp methodology on a parallel plate rheometer. *In vitro* drug release of the corticosteroid, dexamethasone, was monitored over a 5 h time period and IOP stabilization efficacy was assessed using an *ex vivo* bovine eye model for full thickness stellate lacerations.
2018 Summer Undergraduate Research Symposium

Developing a model to study the functional impacts of putative high-altitude snow leopard adaptations in the hypoxia response pathway
Nelson, Brionna; Sree Puluguulla; Dr. Deb Galson; Dr. Phil Auron; Dr. Brian Davis; Janecka, Jan, Department of Biological Sciences Duquesne University

Hypoxia, defined as low levels of oxygen, is one of the most stressful conditions for cells as it can rapidly lead to death. Snow leopards have a unique mutation in EGLN1, a gene which acts as the oxygen sensor for the primary regulator (HIF1a) in the hypoxia pathway. Research was conducted last summer to observe gene regulation in the hypoxia pathway of the snow leopard and showed upregulation of EGLN1 and some of its target genes, including VEGF, which is a primary regulator. We wanted to examine the expression of these genes in other felines that lack the putative molecular adaptation to high altitude. Therefore, RNA was extracted from bobcat tissue, converted to cDNA, gene expression patterns in hypoxia related genes examined. In addition, we developed a model using a domestic cat macrophage cell line to examine expression of hypoxia related genes under different conditions including LPS treatment and growth in a hypoxia chamber. Expression differences under hypoxic conditions will enable us to better understand the potential beneficial effects of the putative molecular adaptation in snow leopard.

Using Evolutionary Rate Covariation as an Computational Tool to Identify α-Arrestin Cargo Pairs
David A. Macar¹, Tova Finkelstein¹, Abdullah Malik¹, Alexiy Nikiforov¹, Uthman Fadu¹, Hilary Serbin¹, Zelia Ferreria², Nathan Clark², and Allyson F. O’Donnell¹
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2) Dept. of Computational and Systems Biology, University of Pittsburgh

α-arrestins, a class of protein trafficking adaptors, have been shown to regulate endocytosis and intracellular trafficking of transmembrane proteins in response to environmental changes. To identify transmembrane candidates whose trafficking is regulated by α-arrestins, we employed a comparative genomic sequence analysis, Evolutionary Rate Covariation (ERC), across 18 yeast species to identify genes with similar evolutionary histories. From this list of candidates, 5 of the known cargo for ldb19 were identified as having a high ERC value, ERC > 0.5, validating this approach.

To assess the regulation of these new cargos by α-arrestins, we examined changes in fluorescence intensities and localization of GFP-tagged cargos in cells lacking α-arrestins compared to wild-type cells suggesting that these cargos may be α-arrestin-dependent. Using this approach, we have confirmed that 36 new cargos are regulated by the α-arrestins. In conclusion, the ERC approach is a powerful new tool that can define protein trafficking regulatory networks.

THE EFFECT OF THE LOCAL NUMBER DENSITY OF GALAXIES ON ANGULAR MOMENTUM OF QUIESCENT GALAXIES IN THE LEGA-C SURVEY
Justin Cole¹
Department of Physics and Astronomy
University of Pittsburgh

Galactic environment has recently been shown to affect galaxy properties such as mass and star formation rate. We use the LEGA-C survey in the COSMOS _eld and the projected number density catalog from ULTRAVista from Darvish et. al. (2015) to create an integrated catalog with the photometric and spectroscopic information from LEGA-C and the density parameters from Darvish (2015). Using this new, unique catalog, we analyze the e_ects of local number density (N) on the angular momentum of quiescent galaxies. We_ _d tentative relationships in angular momentum plotted as a function of _xed mass and again as a function of _xed stellar velocity dispersion. The results show it is possible that quiescent galaxies with few neighbors maintain their angular momentum better than quiescent galaxies in dense regions of the universe. This could have implications for the role environment plays in the evolution of a quiescent galaxy’s angular momentum.

Combining molecular and morphological characters to reconstruct phylogenies and understand diversification of placental mammals in the Paleocene
Frontera, Manuel; Wible, John R.; Wilson, Thomas; Brusatte, Stephen; Spaulding, Michelle; Shelley, Sarah; Janecka, Jan E. Duquesne University Department of Biological Sciences (Janecka, Frontera)
Carnegie Museum of Natural History (Wible, Shelley)
Purdue Northwest University (Spaulding)
New Mexico Museum of Natural History and Science (Wilson)
University of Edinburgh

Our research aims to resolve disparities between molecular dating approaches and fossils. Relaxed molecular clocks, used to date divergence times, have supported more ancient origins of many mammalian Orders, dating back to the Cretaceous. However, these results clash with fossil observations that suggest crown mammals arose at, or shortly after, the Cretaceous-Paleogene (K-Pg) extinction event. We have put together a preliminary molecular matrix of 14 genes and 45 mammals. The white-bellied tree pangolin is being added by sequencing the whole genome on an Illumina MiSeq. The phylogeny and divergence times of major mammals will be compared to a previous family-level analysis. Subsequently, morphological traits will be added for both living mammals and fossils discovered at the beginning of the Paleogene for a total evidence phylogeny reconstruction and molecular dating analysis. Our study will shed light on the temporal pattern of diversification of placental mammals after the extinction of the dinosaurs.
The Effect of Urban Runoff on Conductivity in The Nine Mile Run Watershed
Krebs Nicholas, Martin Mackenzie, Glancey Kathleen, Kahler David
Center for Environmental Research and Education
Duquesne University

The focus of this study was on urban hydrology and how road runoff affects the conductivity of a water system. A sensor recorded depth, temperature, and conductivity every 30 minutes while deployed at the end of the Nine Mile Run watershed. A nearby weather station also provided data that was used to model the hydrologic system. In addition to continuous conductivity measurements, a water sample was analyzed for anions by ion chromatography. The results showed that conductivity remained high after winter runoff, which suggests sources in addition to road salt and that, while chloride was high, the anions tested (F⁻, Cl⁻, NO₃⁻, Br⁻, NO₂⁻, PO₄³⁻, SO₄²⁻) do not explain the conductivity observed. Studies involving the Nine Mile Run watershed should be continued, focusing on a relationship to account for elevated conductivity in the stream caused by a source other than chloride.

Tumor infiltrating regulatory T cells maintain high suppressive function mediated by lactic acid in the tumor microenvironment
Palmieri, Michael; Watson, Mac; and Delgoffe, Greg
Tumor Immunology
University of Pittsburgh

Introduction: The tumor microenvironment (TME) is metabolically supporting Treg cells via lactic acid resulting in enhanced tumor immune evasion.

Methods/Results: An inducible transgenic mouse model was used to selectively deactivate MCT1 expression. A B16 melanoma cell line was used to induce melanomas. Transgenic and control mice were given B16 melanomas. Treg from transgenic mice and control mice were isolated from the TME, lymph nodes, and spleen and cultured in various concentrations of glucose or lactic acid. Flow cytometry and suppression assays were conducted to analyze Treg functionality between groups. When Treg were placed into high glucose environments they became less functional. However, in low glucose environments Treg displayed increased functionality, suggesting that Treg favor low glucose environments like the TME. When cultured in varying concentrations of lactic acid Treg remained functional regardless of high or low concentrations. This suggests that lactic acid does not negatively impact the function of Treg.

Conclusions: The TME supports Treg function and proliferation. Targeting lactate metabolism in Tregs is a promising method to improve current immunotherapy.

Genome editing of the mosquito symbiont Asaia bogorensis using I-SceI recombination
Jasmine, Sumer; Kelly, Tom; Lampe, David J.
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Duquesne University

Paratransgenesis is a technique in which symbiotic bacteria are engineered to secrete anti-pathogenic molecules within vector species, thereby altering the phenotype of the host to control zoonotic diseases. This technique has the capability to eradicate malaria, the most prolific insect-vectored disease in the world. Asaia bogorensis, a proteobacteria naturally found in the midgut of Anopheles mosquitoes, can be modified to secrete anti-malarial effectors. We used a two-step I-SceI-mediated recombination method to modify a site in the Asaia chromosome to introduce changes downstream of a native blood meal-induced promoter. The first step recombinates a plasmid into the chromosome at a fixed site using the recombination machinery of the bacterium. The second step uses the meganuclease I-SceI to cleave the chromosome, introducing the desired chromosomal change through the bacterium’s own repair mechanisms. This project is intended to demonstrate the feasibility of modifying the Asaia genome to eventually create antimalarial strains of bacteria.

Coupling Photoaffinity Labeling with Mass Spectrometry to Investigate the Serotonin Transporter
Caridi, Brandon; Castellano, Elizabeth; Cascio, Michael
Department of Chemistry and Biochemistry
Duquesne University

The serotonin transporter (SERT) is a sodium-dependent monoamine protein that transports serotonin from the synaptic cleft to the presynaptic neuron. Due to its regulation of serotonin in the brain, SERT plays a heavy role in mood disorders such as anxiety and depression. Selective serotonin reuptake inhibitors (SSRIs) target SERT and block reuptake, but can also bind to other receptors, leading to unwanted side effects. Crosslinking studies can be conducted on the structure of SERT, leading to a better understanding of the structure of its extracellular loops. A previously inserted single cysteine mutation (Y232C) located in the second extracellular loop of SERT was photoactivated, and analyzed using mass spectrometry (MS) and tandem mass spectrometry (MS/MS) to map local protein structure. A better understanding of the structure of SERT could lead to improved drug design of SSRIs and more efficacious drug targeting.
113 Relating Traits with Gene Family Expansion and Contraction
Coffing, Gabrielle; Meyer, Wynn; Chikina, Maria; Clark, Nathan
Department of Computational and Systems Biology
University of Pittsburgh

The role of gene family expansion and contraction in the evolution of convergent traits has yet to be determined. We have created a pipeline of methods that can be applied to genome-wide data to identify specific gene families that are correlated with certain convergent phenotypic traits. First, the sequences of each gene within a family is acquired from a reference species. By aligning the reference sequences with each genome of 62 mammal species, we count the gene number in the family repertoire each species has. To determine if there are correlations between the number of genes in a family and a particular trait, we conduct a Phylogenetic Generalized Least Squares (PGLS) analysis, which is a linear model that accounts for relatedness between species. By having this pipeline, our lab can apply it to various gene families and traits to analyze the roles gene families may play in convergent evolution.

115 Impacts of Thickness and Formulation Variables on Drug Release and Adhesion Properties of Drug-in-Adhesive Transdermal Patches
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Department of Pharmaceutics
Duquesne University

Drug-in-adhesive (DIA) transdermal patches are a flexible drug delivery system that provides adjustable adhesion forces and allows for controlled drug release. In order to understand the impacts of formulation variables on the critical quality attributes of DIA patches, in-vitro release studies and probe tack analysis were performed. Samples of DIA patches were changed by drug load, thickness and adhesive ratio. Samples were dissolved and stirred in a USP 5 dissolution apparatus. The solutions were taken up and run through a UV spectrophotometer. They were measured over a period of 24 hours to determine the efficacy of DIA patches. The adhesiveness of the DIA patches were analyzed by a probe tack test and the area under the curve (AUC) of the force-displacement plots were calculated. Diffusion coefficients were determined and regression analysis was carried out to determine the statistically significant effects. Drug load and thickness were found to have significant effects.

116 Investigating PAH Degradation through the Lens of Network Science
Yates, Alexis; Gilbertson, Leanne; Khanna, Vikas; Ng, Carla
Swanson School of Engineering
University of Pittsburgh

Our research applies networks analysis to the degradation pathways of polycyclic aromatic hydrocarbons (PAHs). PAHs contain two or more benzene rings, and express toxicity, mutagenicity, and carcinogenicity. They are primarily formed through the burning of organic materials, such as fossil fuels. Due to their chemical properties, PAHs adsorb to soil and sediment around petroleum mining sites, which impairs clean-up processes. However, they can degrade through metabolism/cometabolism by some bacteria and fungi. Our work focuses on the degradation of six PAHs; anthracene, phenanthrene, fluorene, pyrene, fluoranthene, and benzo(a)pyrene. Compiled empirical and predicted biodegradation data of these PAHs is used to establish networks of degradation products, which enables identification of the most stable pathways and intermediates. Ongoing analysis of these networks will provide insight into the accuracy of existing predictive tools for PAH degradation, particularly for products that are likely to occur but have yet to be experimentally observed.

114 Age-dependent expression of antiviral cytokine signaling proteins during a measles virus infection of the brain
Creisher, Patrick S., Chandwani, Manisha N., Ganesan, Priya, and O'Donnell, Lauren A.
School of Pharmacy and Graduate School of Pharmaceutical Sciences
Duquesne University

Viral infections of the brain often cause greater disease in newborns. Utilizing a model of neuronally-restricted measles virus (MV) infection (CD46+ mice), it has been shown that there are age-dependent differences in survival. Adult mice survive the infection, while neonatal mice succumb. Previous studies have shown that adults control viral spread in an IFNγ-dependent manner. Thus, we hypothesized that the adult brain may have inherently more robust IFNγ signaling. We evaluated the basal levels of canonical IFNγ signaling proteins, such as signal transducer and activator of transcription-1 (STAT1), and found that CD46+ adults had greater expression of the IFNγ receptor. However, we found that STAT1 expression and phosphorylation was upregulated in infected neonates only during infection. These results suggest that neonates activate STAT1 despite relatively lower expression of the receptor, but the extent of STAT1 activation is not sufficient to overcome the heavy viral load in the neonatal brain.
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**Network evolution using proto-gene theory with an application to genetic algorithms**
Cantave, Dominique; Carvunis, Anne-Ruxandra; Koes, David  
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University of Pittsburgh School of Medicine

De novo gene birth, the theory that coding sequences can emerge from non-coding sequences, is a relatively new field, where not much is known. Proto-gene theory proposes that new open reading frames (ORFs) acquire gene-like characteristics along a continuum. The genetic algorithm (GA) is a machine learning technique that uses mutation and fitness to evolve optimal solutions to problems. This work applies proto-gene theory to network evolution and asks how network structure is affected if growth parameters are a function of node age; simulations of network growth were run across a parameter space and parameters that affected network structure were identified. Additionally, this idea was extended GAs, and we have further investigated whether including mutation parameters that are a function of node age could affect performance; the correlation network for historical stock prices were compared to the networks evolved by the normal and modified GAs.

118  
**Examination of anchor residue in binding of p53 to MDM2**
Gerlach, Gabriella; Camacho, Carlos  
Computational and Systems Biology  
University of Pittsburgh

Many drug targets are highly flexible proteins which makes studying and targeting them challenging, but nature specifically binds flexible proteins. The mouse double minute 2 homolog (MDM2) is a negative regulator of the tumor suppressor p53 both of which are flexible proteins and targets for cancer treatment. There are significant conformational differences between unbound MDM2 and the MDM2-p53 complex. What drives these changes is difficult to examine experimentally because atomic level information is required. Molecular dynamics simulations allow viewing of atomic detail and creation of systems that are not possible experimentally. Through simulations of Trp23, a residue important to the interaction, binding to MDM2, the ability of Trp23 to induce conformational change in MDM2 toward a structure more similar to its bound state has been shown. These results suggest Trp23 is an anchor residue in the interaction and give insight into the binding mechanism between these flexible proteins.

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**USE OF BIOMARKER PANELS AND PROTEOMIC DATA FOR DETECTION OF PANCREATIC CANCER**
ADEBIYI BAZIT, DR. LANGMEAD CHRISTOPHER  
DEPARTMENT OF COMPUTER SCIENCE  
LINCOLN UNIVERSITY

Objective: To use machine learning techniques to (i) identify serum biomarkers relevant to the detection of pancreatic cancer, and (ii) to build diagnostic classifiers from those biomarkers.

Methods and Materials: A panel of 42 circulating proteins were measured in the serum of patients with pancreatic ductal adenocarcinoma (PDAC, n =230 ), and healthy control individuals (n = 227). Feature selection methods were used to identify diagnostic biomarkers. Cross-validation was used to assess the robustness with which these biomarkers were selected. Next, a Random Forest was learned from the selected biomarkers. Cost-sensitive learning was used to learn a model with 90% sensitivity to PDAC on the training data.

Results: The feature selection step identified 10 diagnostic biomarkers and the Random Forest Classifier achieved accuracy, sensitivity, and specificity of 87%, 85%, and 89% respectively.  

Conclusion: Machine Learning is capable of identifying diagnostic biomarkers from proteomic data and producing diagnostic models with good performance metrics.

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**In-Clinic Test Kit for the Diagnosis of Bladder Cancer**
O'Sullivan, James; Abhinav; Little, Steven  
Department of Chemical and Petroleum Engineering  
University of Pittsburgh

Bladder cancer is the ninth most common cancer worldwide, and an estimated 81,190 new cases will be diagnosed this year in the US alone. This cancer is the most expensive type of cancer to treat per patient because of the need for lifelong cystoscopic examinations. Herein, a rapid (less than 1 hour), in-clinic device called UroKit for the diagnosis of bladder cancer is described that can help decrease the unnecessary need for expensive and invasive cystoscopy. UroKit detects the bladder cancer biomarker MMP-9 in urine with high fidelity, accuracy and in a cost-effective manner. UroKit is consistently able to detect the presence of MMP-9 spiked phosphate buffered saline and patient urine samples by its activity on the UroKit substrate. Currently, this diagnostic kit is being utilized to detect bladder cancer in patients.
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Disentangling the functions of three paralogous post-transcriptional regulators through bacterial competition
Bana AlMoussa1, Anton Evans2, and Wook Kim2
1 Pittsburgh Science and Technology Academy
2 Department of Biological Sciences, Duquesne University

Aging colonies of the bacterium *Pseudomonas fluorescens* Pf0-1 repeatedly generate mutant patches that result from the activity of mutants where they expand space to decrease local density and push themselves up to the surface. Remarkably, a mutation in a single gene, *rsmE*, was responsible for each and every case of over 500 independently derived patches. *RsmE* and its two paralogs (*RsmA* and *RsmI*) are described to redundantly repress multiple secretions by sequestering associated mRNA, which contradicts our large mutational data. We hypothesize that *RsmE* governs at least a partially distinct set of secretions from its paralogs. We test this hypothesis through genetic engineering and RNA immunoprecipitation sequencing (RIP-seq) techniques. Here, we describe our experimental approach and present preliminary data. Importantly, our work illustrates how spatial interactions among bacteria could directly lead to the production of phenotypes of potentially broad consequences.

122
Adsorption of formic acid onto TiO2 nanoclusters using density functional theory
Santis, Garrett D.,a Carlson, Amy N.,b and Evanseck, Jeffrey D.b
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bCenter for Computational Chemistry and Department of Chemistry and Biochemistry, Duquesne University

Quantum treatment of periodic model titanium oxide (TiO2) surfaces are resource intensive. To gain accuracy, TiO2 nanoclusters have been used to model the surface of TiO2 and its binding to carboxylic acids, important to scientific and engineering applications. B3LYP/LanL2DZ was used to scan the energies of the possible binding modes. M06-2X/def2-TZVP was found to predict formation energies accurately for the nanoclusters and was used to study the best binding modes. Formic acid has been observed to prefer binding to the lower coordinated Ti sites, with enthalpies greater than 80 kcal/mol. This binding was found to decrease as Ti coordination approached values found in crystalline TiO2, which suggests that surface defects and amorphous regions promote stronger binding of carboxylic acids to the surface. This can serve as a basis for experimentalists to study surface binding as it relates to crystallinity, and improve the prediction of surface modification to create novel materials.

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Simulations of High Energy Particle Collisions with Aerogel in a Ring Imaging Cherenkov (RICH) detector
Smoot, Waymond; Trolta, Nicholas; Behary, Robert; McCauley, Collin; Dr. Benmokhtar
Physics Department
Duquesne University

Simulations for high energy collisions with aerogel radiators for experiments at Thomas Jefferson Laboratory are being taken remotely here at Duquesne University. These aerogel radiators will be used in the RICH detector of the CLAS12 spectrometer. Cherenkov radiation will be generated by electrically charged hadrons and electrons moving through the aerogel at superluminal speeds. I will be simulating different particles passing through the radiators using GEMC particle accelerator simulator. Data collected from these simulations will be stored into output files through the use of bash script, which will then be converted into evio files through the use of a groovy script.

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Natural products analysis: Identifying endophytic fungi which produce beta-bisabolol.
Haines, Trenton; Yan, Dong-hui; Iulliucci, Robbie
Department of Chemistry
Washington and Jefferson College

In nature, a large multitude of plants act as hosts to unique endophytic fungi. Studying these largely unknown fungi, which potentially produce important natural products, could lead to advancements in biofuels, pharmaceuticals and commercial products, namely cosmetics. In this study, the products of different types of endophytic fungi, all in the *diaporthe* genus, retrieved from catharanthus roseus were studied by gas chromatography mass spectroscopy (GC-MS). In order to identify the volatile organic compounds, solid phase microextraction (SPME) was used. Alternatively, the nonvolatile organic compounds were sampled using an organic extraction. Of these substances, a potential compound of interest, beta-bisabolol, was identified for further study. Beta-bisabolol was selected due to its volatility as well as because alpha-bisabolol is widely used as an anti-inflammatory agent in cosmetics. Through use of SPME-GC-MS and a beta-bisabolol standard, it was confirmed that beta-bisabolol was present in the samples.
Silica deposition on polymers - a comparison of plasma-enhanced chemical vapor deposition and sputtering
Fersner, Alvin
Department of Chemical and Petroleum Engineering
University of Pittsburgh

Inorganic materials, such as metal oxides like silica, can be deposited on various substrates using a variety of techniques including plasma-enhanced chemical vapor deposition (PE-CVD) and sputtering. In this study, we investigate the extent to which SiOx deposited onto a polymer substrate serves as a water barrier. SiOx is sputtered onto both polyethylene oxide (PEO) and an Si wafer partially covered by tape at room temperature. After deposition, the tape is removed, and the thickness of SiOx is measured by profilometry. PE-CVD is only performed on Si wafers to determine the minimum temperature at which the SiOx can be deposited. Our results show that SiOx can be deposited by PE-CVD in the temperature range of 140 °C – 220 °C, and that the thickness of the film decreases sharply below T < 120 °C. For sputtering, we find that a 200 nm thick film increases the time to dissolution in water by a factor of ~1.5, and at 400 nm it increases by a factor of ~2.6.

High-Precision Particle Tracking for the Muon Proton Scattering Experiment (MUSE) at Paul Scherrer Institute (PSI)
Adam Sneath, Fatiha Benmokhtar
Department of Physics
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The Proton Radius Puzzle is an independently verified discrepancy (7σ) between the proton charge radius measured by electron scattering and that measured by Lamb shift spectroscopy. MUSE is the first experiment to simultaneously extract radius measurements from electron-proton (ep) and muon-proton (µp) scattering. MUSE hopes to clarify if ep and µp interactions are inherently the same, in which case all experimental methods should measure the same radius. Last summer I visited PSI and assisted construction of a prototype Straw Tube Tracker (STT) particle detector and testing its resolution. This summer I will revisit PSI and assist STT data acquisition, shifts to operate the particle beam, and analysis software development. At Duquesne, I will work on a C++ software plugin to process scattered particle raw data and generate analysis via CERN ROOT software. A configuration of TRB3 field-programmable gate arrays interface with PaDiWa front end leading-edge discriminators for STT signal processing.

Screening of ScUbI Yeast Deletion Library for Modifiers of Aly1 or Aly 2 mediated Resistance to Rapamycin
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Duquesne University

We know that modification to α-arrestins by ubiquitination results in the changing of α-arrestin functions. To help identify specific α-arrestin regulators a unique yeast gene deletion library was generated called the Saccharomyces cerevisiae Ubiquitin Interactome (ScUbI) library. This library contains all the non-essential genes associated with ubiquitination and ubiquitin interaction. Over the course of the undergraduate research program ScUbI was used to screen gene deletions that altered growth phenotypes in yeast after overexpressing α-arrestins. The ScUbI library was transformed with plasmids overexpressing the α-arrestins Aly1 and Aly2, then altered these arrestins with specific gene deletions that either increased or decreased yeasts' sensitivity to rapamycin. Yeasts' sensitivity to rapamycin was measured by calculating z-scores of >1 or <1. After calculating z-scores, four candidates were chosen that expressed significant change in sensitivity to rapamycin, an inhibitor mimicking nitrogen starvation. This data proposes that α-arrestins regulate the changes of autophagy pathways in yeast.

Proposal for an Emergency EHR Alternative in Puerto Rico
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2 Heinz College of Information Systems and Public Policy, Carnegie Mellon University

Modern healthcare has come to rely on Electronic Health Record (EHR) systems to store their data, which has improved the efficiency and quality of the care provided to patients. However, these systems rely on electricity and a steady internet connection, which restricts the access that underdeveloped countries and disaster areas may have to them, as was the case with Puerto Rico after hurricane Maria struck. Months without electricity and limited communications stunted the ability to provide aid to victims. As a solution, we propose an EHR system that would be able to run on power generators, and could store basic patient data for clinicians to access while also providing statistics for government entities. Providing two separate interfaces to protect patient data, this system aims to improve the information streamline between the hospitals and federal entities during emergencies, to provide quality care and better allocate resources throughout the island.
**Symptom Experience, Management, and Outcomes of breast cancer therapy According to Race and Social determinants of health (SEMOARS)**
Margaret Rosenzweig, Amin Khan
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**Background:** Black women with breast cancer (BC) have a lower 5-year survival than all other US races due, in part to disparity in treatment toxicity and subsequent reduction in therapy dose intensity (DI).

**Aims:**
1) Compare (Black/White) symptoms and distress (incidence and distress) at baseline and over time (6 months).
2) Compare (Black/White) chemotherapy DI (full dose, on time).
3) Explore the relationship between symptoms, distress and DI and compare by race.

**Hypothesis:** Racial disparity in symptom incidence and distress is related to reduced chemotherapy DI.

**Methods:** Pilot, comparative, longitudinal descriptive study. 5 Black/5 White patients undergoing early stage BC chemotherapy for 6 months, completed baseline demographics, baseline and over time (17) symptom assessments. Chart review for DI.

**Significance:** Racial disparity in chemotherapy DI could be mitigated through tailored symptom management.

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**Computational Predictions of the Influence of Electrostatic Charged MOFs in the Diffusivity Coefficient**
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The use of fossil fuels as a primary energy source increase greenhouse gases’ concentration in the atmosphere. This buildup of CO2 has inspired the development of Carbon Capture and Storage (CCS) technology. A significant step to carry out this technology and address this problem lies in the understanding of the gas-adsorbent interactions. In this study, Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) were performed to investigate the sensitivity of the diffusivity predictions of CO2 to the strength of the electrostatic charges in high-surface area materials, Metal-Organic Frameworks (MOFs). We examined multiple methods for assigning charges —EQeq, REPEAT, and DDec — in different MOFs —IRMOF-1, HKUST-1, ZIF-8—. A computational algorithm calculate the Mean Square Displacement (MSD), from position data, to obtain the diffusion coefficient. As expected, the diffusion coefficient through IRMOF-1 decreases as the intensity of the electrostatic charges in the MOF increases.
Concentration at 340 nm. The addition of BSA at varying concentrations was measured by recording changes in NADPH oxidase activity.

The purified enzyme was used in kinetic assays containing two peak solutions. Aldose reductase (AR) is an NADPH dependent enzyme that reduces glucose to sorbitol in the polyol pathway. Since this process involves the FAD and FMN containing enzyme undergoing large conformational changes, it was hypothesized that the enzyme's electron transfer kinetics would be sensitive to macromolecular crowding. The enzyme was solubilized and purified from porcine liver microsomes. The enzyme was solubilized using the detergents Emulgen 913 and deoxycholate, and subsequently purified by DEAE cellulose column chromatography followed by a 2',5'-ADP Sepharose affinity column. The kinetics of the enzyme were measured by monitoring the rate of reduction of cytochrome c as a surrogate electron acceptor. The results of the purification and macromolecular crowding effects will be presented.

MicroRNAs (miRNAs) are small, noncoding RNAs which regulate translation and have been implicated in various neurodegenerative diseases and cancers. miRNA development begins with transcription of long primary-miRNA (pri-miRNA) sequences, several hundred nucleotides in length. Nuclear processing proteins cleave the transcript into ~80 nucleotide precursor-miRNA (pre-miRNA), which is shuttled to the cytoplasm. Final processing by the endonuclease Dicer produces ~22 nucleotide mature miRNAs. Recent studies suggest RNA-binding proteins, such as FMRP, may interact with pre-miRNAs and regulate processing. Pre-miRNA-125b-2 is one such potential target transcript which has implicated in various pathologies. In this study, we hypothesized that FMRP associates with pre-miRNA-125b-2 and subsequently regulates its processing by Dicer. We investigated pre-miRNA-125b-2 secondary structure using biophysical methods such as 1H NMR spectroscopy and CD spectroscopy. Furthermore, we analyzed the binding interaction of pre-miRNA-125b-2 with various isoforms of FMRP and its potential effects on the rate of Dicer processing using native PAGE EMSA.

135. The Effects of Macromolecular Crowding on Rabbit Muscle Aldose Reductase
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Enzymes are typically studied in dilute solutions which do not accurately simulate the interior of a cell. The intracellular matrix is crowded with macromolecules, so to better understand how enzymes function in vivo it is essential to study them in crowded solutions. Aldose reductase (AR) is an NADPH-dependent enzyme that reduces glucose to sorbitol in the polyol pathway and it is thought to cause complications in diabetes under hyperglycemic conditions. AR was purified from rabbit muscle using ammonium sulfate fractionation, gel filtration and ion exchange chromatography. The gel filtration column resulted in two peaks of activity, a high and low molecular weight peak. The purified enzyme was used in kinetic assays containing bovine serum albumin (BSA) as a crowding agent and reaction rates were measured by recording changes in NADPH concentration at 340 nm. The addition of BSA at varying concentrations resulted in changes in kinetic properties of AR.

136. Refining the Structure of the Human α1 Glycine Receptor Through the Use of a Single Cysteine Mutation (K116C) and Cross-Linking-Mass Spectrometry
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The glycine receptor (GlyR) belongs to the pentameric ligand-gated ion channel superfamily and mediates fast inhibitory neurotransmission in the spinal cord and brain stem by forming an anion-selective transmembrane channel. Neurological conditions, such as hyperekplexia, are a result of mutations in GlyR. It is hypothesized that the insertion of a single cysteine mutation (K116C) and comparative crosslinking-mass spectrometry (CXMS) analyses will further elucidate the structure of GlyR and can allow for more targeted therapeutics to treat neurological conditions. Purified, reconstituted human α1 K116C GlyR was crosslinked with MTS-benzophenone and isolated in a primarily resting, open, or desensitized state. After UV irradiation, crosslinked GlyR was digested and analyzed with electrospray ionization quadrupole time-of-flight mass spectrometry to identify unique sites of crosslinking. Differences are seen intra- and intermolecularly between the three different states of GlyR. This provides information on local topography relative to position 116, which aids in structure refinement.
2018 Summer Undergraduate Research Symposium

137 Lipidoid Nanoparticle-siRNA Delivery for Chronic Pain Therapy: Development and Validation of a qPCR Method to confirm mRNA Knockdown in Transfected Cells.
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2Graduate School of Pharmaceutical Sciences, Duquesne University
3Department of Chemical Engineering, Carnegie Mellon University

Brain-derived neurotrophic factor (BDNF) functions as a neurotransmitter in pain signaling pathways and plays a key role in the maintenance and propagation of chronic pain. Our goal is to develop a safe and effective non-opioid therapy for treating chronic pain. We hypothesize that BDNF siRNA delivered using lipidoid nanoparticles (LNPs) can decrease BDNF expression and limit its downstream effects in pain signaling pathways. To assess the effectiveness of LNP’s ability to deliver siRNA into cytoplasm, LNPs loaded with GAPDH siRNA were delivered, as a proof of concept, in a U-87MG cell line. We successfully demonstrated mRNA knockdown in LNP-transfected cells using quantitative real-time PCR. The reduction in mRNA levels was accompanied by a corresponding decrease in GAPDH protein expression, determined using standard Western blotting techniques. These results provide the basis for subsequent studies to deliver BDNF siRNA and use the developed qPCR method to validate mRNA knockdown in transfected cells.

138 Investigation of G-quadruplex Structure Formation within Truncated Sc1 mRNA
Then, McKenna1,2 & Mihaela Rita Mihailescu1
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2Neurodegeneration Undergraduate Research Program

Fragile X syndrome (FXS) is a trinucleotide repeat expansion disease characterized by loss of the fragile X mental retardation protein (FMRP), an RNA-binding protein essential for cognitive development. Previous research on FXS pathogenesis focused on a model system guanine-rich full-length Sc1 mRNA, revealing that it primarily folds into a G-quadruplex secondary structure and binds to full-length FMRP, as well as to its RGG binding domain which specifically targets G-quadruplex structures. Whereas these studies investigated the full-length Sc1 sequence, this research focuses on a truncated sequence lacking the stem portion to investigate its importance for FMRP recognition. The truncated mRNA was characterized using various biophysical techniques including 1H-NMR spectroscopy, CD spectroscopy, UV thermal denaturation, and gel electrophoresis. Our results indicate that in the absence of the stem, the Sc1 G quadruplex structure is no longer forming, and hence the truncated Sc1 sequence is no longer recognized by the FMRP RGG box.

139 Interferon gamma-induced activation of STAT1 in neural stem/progenitor cells is age-dependent
Cadiz, Mikaela1,2; Chandwani, Manisha1; Kamte, Yashika1; Creisher, Patrick1; O’Donnell, Lauren1
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2Division of Science and Mathematics, University of Minnesota

Viral infections in the brain can profoundly alter neurodevelopment in newborns, with long-lasting neurological consequences for the host. Interferon gamma (IFNγ), a critical anti-viral cytokine in the brain, influences neural stem/progenitor cell (NSPC) fate, potentially in an age-dependent manner. Our prior studies demonstrate that IFNγ reduces proliferation and increases gliogenesis in embryonic NSPCs, but protects neonatal NSPCs without enhancing differentiation during infection. We predict that neonatal NSPCs will respond to IFNγ with a STAT1-dependent (signal transducer and activator of transcription) reduction in neuronal markers. To test this hypothesis, we treated wildtype and STAT1-knockout NSPCs with IFNγ and quantified STAT1 via western blot. Unlike the sustained STAT1 expression/activation observed in embryonic NSPCs, STAT1 activation in neonatal NSPCs was transient despite sustained expression, suggesting IFNγ-induced STAT1 activation may be insufficient to activate neonatal NSPC differentiation pathways. Current studies examine whether IFNγ/STAT signaling controls expression of neurogenic transcription factors and early differentiation markers.

140 Select α-arrestins promote growth of yeast expressing the mammalian ROMK potassium channel on low potassium media
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3Department of Biological Sciences, University of Pittsburgh

Protein trafficking regulates the composition of membrane proteins at the cell surface, including potassium ion channels whose abundance changes in response to potassium availability. Our research focuses on the protein trafficking of mammalian renal outer medullary (ROMK) channel in a yeast model. ROMK regulates potassium homeostasis and thus needs to be tightly regulated – via protein trafficking. To identify new factors that control its trafficking, we expressed ROMK in yeast lacking endogenous potassium channels, Trk1 and Trk2, and assessed its ability to rescue growth on low potassium media. We find that ROMK is functional in our yeast system and that AP-1 and AP-2, two clathrin adaptor complexes, are required for optimal ROMK-mediated growth on low potassium. We further show that select α-arrestins, protein trafficking adaptors, increase this growth. Interestingly, α-arrestin Aly2 requires AP-2 complex to stimulate ROMK-trafficking to the cell surface, suggesting that Aly2 operates via an AP-2 dependent trafficking interval.
Cyanobacteria are a rich source of secondary metabolites that provide leads for the treatment of pain, neurological disorders, and other diseases. Here, we extracted a sample of Curacaon *Moorea sp.* and separated the extract into increasingly polar fractions by column chromatography. High-performance liquid chromatography of a mid-polar fraction revealed the presence of a compound with characteristic absorbances for carbonyls and aromatics. These functional groups are commonly found in bioactive molecules, suggesting the compound could possess activity at CNS and other drug targets. The compound was isolated by flash purification and analyzed with mass spectrometry and NMR. These data revealed that the compound was barbamide, a secondary metabolite originally discovered at Barbara Beach, Curacao. Barbamide is known to be molluscicidal (snail-killing), but otherwise little research has been done on its bioactivity. It is currently being tested on different neurological receptors and cancer cells to explore its biomedical applications.

**Exploring a Marine Cyanobacterium from Curacao: Extraction, Isolation, and Elucidation of a Secondary Metabolite**

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Kappa Opioid Receptors (KORs) are an alternative opioid targeting site with the potential of targeting pain without the abuse associated with Mu Opioid Receptors (MORs). KORs have been linked to nociception, motor control and mood, and modulate responses to chemical, mechanical and potentially thermal nociceptive stimuli. The KOR-Cre knock-in model is a novel method used to drive expression of the exogenous protein Cre recombinase using the endogenous KOR locus. While this model allows for study and visualization of KOR-expressing cells, the full consequences of losing either one or both KOR alleles in these mice is not well characterized. We evaluated the sensory and affective phenotype of KOR-Cre knock-in homozygous and heterozygous mice before and after chronic variable stress and the induction of pain with Complete Freund’s Adjuvant. We report sex-specific differences in the sensory, but not affective phenotype in this model, with primary genotypic variances being observed in male mice.

**Characterizing the Sensory and Affective Phenotype of Kappa Opioid Receptor Knock-in Mice in Response to Chronic Variable Stress**

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With chronic pain affecting over 100 million Americans and the opioid epidemic on the rise, characterization of non-pharmacological pain treatments is critical. Many clinical studies have suggested that aerobic exercise may contribute to the management of chronic pain. However, it is not fully understood if exercise has preventative effects on the development of chronic pain. Published results are contradictory in the few animal studies that exist involving exercise pre-training before injury. This study tested the hypothesis that voluntary wheel running would prevent inflammatory pain in adult male C57BL/6J mice. A model of inflammation using Complete Freund’s Adjuvant (CFA) was first piloted until a robust pain-like effect was achieved. This model was then applied to sedentary and active mice after 8 weeks of exercise pre-training. von Frey mechanical sensitivity testing was then employed to determine differences in pain-like behavior. Results will indicate the impact of long-term exercise pre-training on pain-like behavior.

**The Effects of Long-Term Exercise Training on Inflammatory Pain in Mice**

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Low levels of chlorpyrifos, an organophosphorus pesticide, are found in many different habitats. These low levels of pesticide, although considered safe by the government, shape neurodevelopment of Northern Leopard Frogs (*Lithobates pipiens*) tadpoles, a common vertebrate model. We hypothesized that increased corticosterone contributed to the pesticide-induced changes in neurodevelopment. To test this, we exposed tadpoles to corticosterone or vehicle for one week and measured tadpole corticosterone, brain morphology, brain mass, and behavior. As expected, corticosterone levels were higher in the corticosterone-treated tadpoles. Also, relative diencephalon width was larger in corticosterone-treated animals, although there were no behavioral or other differences. Ongoing studies are examining the role of apoptosis in the effect on diencephalon width. In summary, our results support our hypothesis that corticosterone contributes to the effects of chlorpyrifos on the developing vertebrate brain.

**Neurodevelopmental Effects of Corticosterone in Northern Leopard Frog (*Lithobates pipiens*) Tadpoles, a Common Vertebrate Model**

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145 α-Synucleinopathy and Aging Exert Distinct Effects on Microglial Activation
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Lewy body disorders such as Parkinson’s disease are characterized by inclusions containing aggregated, fibrillar α-synuclein. The resulting α-synucleinopathy may spread throughout cells in the brain. Microglia are brain phagocytes that respond to injury and engulf α-synuclein. We report that the introduction of α-synuclein fibrils into CA2/CA3 fields of the mouse hippocampus in vivo increases global brain expression of Iba1, a protein involved in phagocytosis in activated microglia. Fibrils increased Iba1 specifically in CA2/CA3, dentate gyrus, striatum, and substantia nigra, and all these brain regions are known to display α-synucleinopathy in human Lewy body disorders. Although age is the major risk factor for Lewy body disorders, we did not observe any changes in Iba1 expression with normal aging. These findings suggest that Lewy pathology—but not aging—activates microglia and may reflect a natural attempt at slowing α-synucleinopathy transmission between cells.

146 Combination drug treatment of kinase inhibitors J19 (MG-3-81) and Ipatasertib with BRD4 inhibitor CPI203 in glioblastoma cells
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Glioblastoma multiform (GBM) is an aggressive brain cancer with a poor prognosis of less than 15 months. Genetic aberrations of PTEN, a tumor suppressor for the AKT pathway, and inhibition of epigenetic regulator Bromodomain 4 (BRD4), which regulates proliferation, show promise as treatment options for GBM. This study examined the effects of a novel AKT inhibitor, J19, and a known AKT inhibitor, Ipatasertib, with a known BRD4 inhibitor, CPI203, on cell viability and cellular signaling using MTT assay and western blot analysis in a U87 GBM cell line. Our results indicate that Ipatasertib significantly inhibits AKT in a concentration dependent manner and in combination with CPI203, significantly decreases viability. J19 decreases viability but, in combination with CPI203, produces similar effects to CPI203 alone, indicating a sensitivity to BRD4 inhibition. Inhibitors were added simultaneously, possibly affecting their efficacy. So, future studies will examine the utility of adding inhibitors at different times.

147 Analysis of Infiltrating immune cells and Neuroinflammatory Mediators in Sciatic Nerve of Rats After Chronic Constriction Injury
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In response to the opioid crisis, many groups are working to prevent the use of opioids as a method to treat chronic pain. One target for chronic pain treatment is reducing neuroinflammation to prevent a pain response. To stimulate chronic pain, chronic constriction injury (CCI) on the right sciatic nerve of rats is performed and inflammatory agents are recruited to the site of injury. These infiltrating cells, along with resident cells, express cyclooxygenase (COX-2) producing prostaglandin E2 (PGE2), generating an inflammatory response leading to peripheral neuropathy and hypersensitivity. A non-steroidal anti-inflammatory drug celecoxib, incorporated in a nanoemulsion by Janjic (CXBNE) was injected intravenously after CCI. This therapy reduces inflammation by reducing the number of infiltrating macrophages and through inhibition of COX-2 and a corresponding reduction in PGE2. To investigate further the effectiveness of CXBNE, we assess COX-2 and PGE2 as well as other cytokines and infiltrating immune and immune-like cells.

148 Aqueous Extract of Baillonella Toxisperma with Analgesic Effect Elicits Strong Calcium Responses in Mice Primary Sensory Neurons
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Natural compounds have been historically used to treat and characterize the biological mechanisms responsible for pain. Extracts from Baillonella toxisperma, a west African species of tree, have been used by the people of Cameroon to treat a number of ailments including pain. Here, a B. toxisperma aqueous extract shown to have some in vitro affinity to the 5-HT1 serotonin receptor, was evaluated in primary sensory neurons. We used in vitro calcium imaging to monitor neuronal activity while administering various concentrations of B. toxisperma bark extract. We found that B. toxisperma increases intracellular calcium levels upon administration in a concentration-dependent manner. Activation of sensory neurons by this analgesic extract suggests that some of the efficacy of B. toxisperma may be due to desensitization of nociceptors during treatment. Future studies will focus on identifying the cell-types activated by the extract and the ultimate molecular mechanism(s) of these observations.
Chronic bladder pain evokes asymmetric behavior in neurons across the left and right hemispheres of the amygdala. An agent-based computational model was created to simulate neural behavior over time in response to bladder distention. Each agent represents one neuron and is characterized by its location and response type (excited or inhibited). At each time step, firing rates (Hz) of neurons are stochastically updated from probability distributions estimated from data collected in laboratory experiments. A damage accumulation model tracks the damage accrued by individual neurons during distended states. Model output is used to visualize asymmetric neural activity as well as temporal changes in pain attributed to repetitive bladder distention. Results quantify the sensitivity of pain to the initial distribution of neurons and demonstrate the model’s ability to predict changes in pain. Computational modelling of this type is critical to understanding pain as a complex, emergent quality of neural behavior.

151 Geometric consequences of chiral catalyst conformations on Diels-Alder asymmetric induction
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The origin of Diels-Alder optical purity differences catalyzed by chiral alkoxyluminum dichloride catalysts remain relatively unexplored, yet the conformational underpinnings are vital to understanding the stereochemical control of important organic reactions. We have recently discovered that the alpha hydrogen bond is essential to complement the formyl hydrogen bond interaction to explain the stereochemical results from reactions of cyclopentadiene with acrolein (98% ee) and methacrolein (72%) catalyzed by (S)-menthoxyaluminum dichloride (1). However in the closely related (1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)aluminum dichloride catalyst (2), both dienesphiles result in ca. 25% ee from Koga’s experiments. The striking difference in stereochemical control between 1 and 2 has been investigated using J.J. Stewart’s semiempirical molecular orbital Parameterized Method 7 (PM7) method and Truhlar’s M06-2X functional with Dunning’s cc-pVTZ basis set. Geometry optimization and conformational searches of each Lewis acid complex with dienophile resulted in low energy structures that demonstrate unhindered reaction path trajectories that uniquely explain the experimentally observed optical purities. The need to enact alpha hydrogen bonding to explain stereochemical control in organic reactions is reinforced.