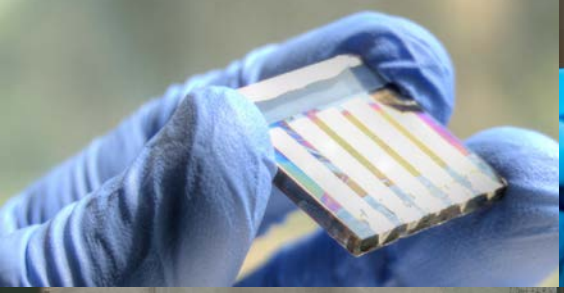
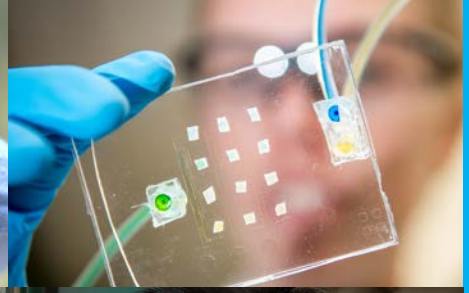
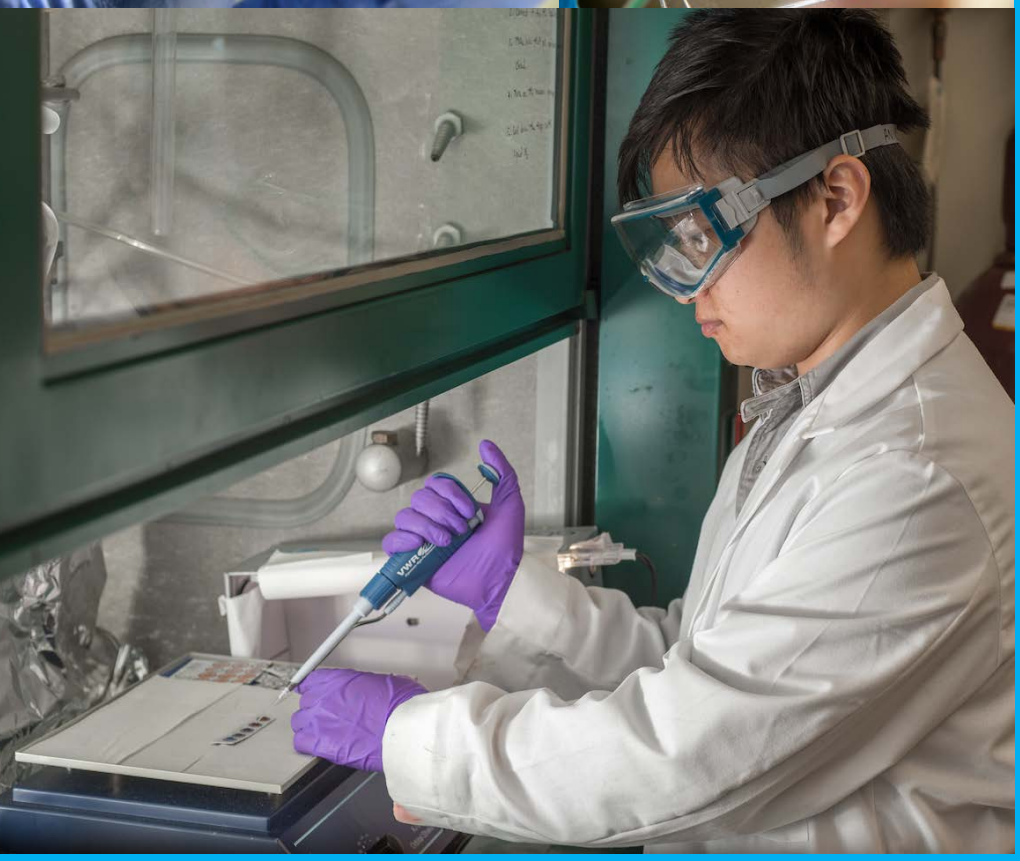
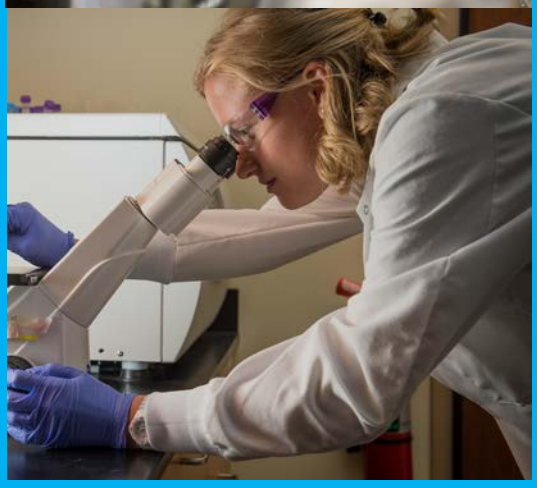




Summer 2017



Undergraduate RESEARCH Symposium



July 26
9:30 – 11:45 am
Jordan Hall of Science

ROSTER OF STUDENT RESEARCHERS

#	STUDENT RESEARCHER	PROJECT TITLE	ADVISOR
1	Emily Baert	An Analysis of Ego Network Characteristics	David Hachen
2	Catharine Brady	Development of a Microfluidic Tunable Attribute Precision Screening for Characterization of Bacterial Stress	Joshua Shrout
3	Catherine Breakfield	How to Collect 636 Samples in 28 Days	Toni Barstis
4	Caroline Brooks	Cross Sectional Time Series Analysis on the Impacts of Race on Homeownership	Richard Williams
5	Roy BrooksRivera	Perturbation of the Calcium Signaling Toolkit Impacts *Drosophila* Wing Morphogenesis	Jeremiah Zartman
6	Brendan Brown	Dispersion Curves for Plasmons in Metal Nanostructures	Gregory Hartland
7	Savannah Butler	Degradation of Chemical Warfare Agent Proxies through ZnO Nanocrystal Assisted Photocatalysis	Prashant Kamat
8	Adam Carr	Quantitative PCR analysis of LTA resistance in _Streptococcus pyogenes_ against synthetic bacteriocins	Shaun Lee
9	Carl Colglazier	Parallel Python for Global Social Simulation	Paul Brenner
10	Adam Cooper	Fighting Low Quality Pharmaceuticals through the Development and Simplification of an Affordable Paper-Medium Antibiotic Assay	Marya Lieberman
11	Jonah Cremin-Endes	Community Members are an Asset in Public Health Movements	Marya Lieberman
12	Lina Daza	Application of molecular dynamics to study the gas-liquid interfacial properties of the ionic liquid: 1-n-butyl-3-methylimidazolium acetate [BMIM] [OA]	Edward Maginn
14	Heather DiLallo	HPLC Verification of Paper Analytical Devices to Screen for Low-Quality Albendazole	Toni Barstis
13	Michael Dowd	Keep the Lead Away: Understanding the Problem of Lead in St. Joseph County, Indiana	Marya Lieberman
32	Alfredo DuarteGomez	Development of Luminescent Porous Particle for Two-Color Pressure-Sensitive Paint	Hirotaka Sakaue

16	Rebecca Dudek	Development of Novel DNA Extraction Technique for the Detection of Genetically Modified Soy Beans	Hsueh-Chia Chang
17	Kiera Dwyer	Development of a phosphate biosensor using the optical density and pressure of growing yeast.	Holly Goodson
18	Bailee Egan	Linking the Core Oral Microbiome and Gut Parasites in Long-tailed Macaques	Hope Hollocher
19	Paul Elhallal	Classifying Islamic Terrorism and its effects on US Counterterrorism	James Philpott
20	Grace Enright	Applying HTC to Economic Innovation Discovery	Kirk Doran
21	Kirstin Favazzo	Validation by LC-MS of Paper Analytical Devices of Suspect Nepali Antibiotic Pharmaceuticals	Toni Barstis
22	Caitlin Guccione	Improving the Accessibility of Bioinformatic Workflows Through Cloud Deployment	Douglas Thain
23	Amber Hannah	The role of Adenomatous Polyposis Coli (APC) tumor suppressor in intercellular junctions and cell migration	Jenifer Prosperi
24	Esther Harkness	Optical Microbe Detection Platform via Low Cost Open Source Electronics	Scott Howard
25	Bryan Harris	Analyzing Resource Metadata from High Throughput Computing in an Opportunistic Environment	Douglas Thain
26	Melissa Henry	Longitudinal Effect of Food Insecurity on Academic Outcomes	Ying Cheng
27	Connor Howington	Using computational genomics and high-throughput computing to study malaria parasite _P. falciparum_ and mosquito vector _A. funestus_	Scott Emrich
28	Elizabeth Innis	Validation by LC-MS of Paper Analytical Devices of Suspect Nepali Omeprazole	Toni Barstis
29	Mackenzie Jones	The Long Road off the Family Track: The Difficulty of Having it all	Kasey Buckles
30	Elisabeth Kerns	Effect of Low Bandgap Metal Oxides and Direct Irradiation on the Degradation of Perovskites	Prashant Kamat
31	Peter Lazorchak	ENTROPY improves admixture analyses of low-coverage sequencing data in _Rhagoletis_ flies	Meredith Doellman
15	Yutong Liu	Quantitative Analysis Using Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES) Reveal High Lead Contamination of Soil and Dust in Census Track 6, South Bend, Indiana (IN)	Marya Lieberman

33	Benjamin MacCurtain	Analysis of porosity, mineralization, and damage as contributors to fracture risk	Ryan Roeder
34	Siena Mantooth	Targeted Asparaginase for Improved Treatment of Pediatric Leukemia	Matthew Webber
35	William McCarthy	Synthesis of peptidic derivatives of 1,3,5-benzenetricarboxamide and investigation of their supramolecular-assembly	Matthew Webber
36	Brady McLaughlin	[Re]Evaluating the Cost of Electricity in Hospitals with Unreliable Energy - VSL/E Metric	Abigail Mechtenberg
37	Heather Miller	Development of a yeast biosensor for prednisone detection	Don Paetkau
38	Kate Mockler	Engineering Multifunctional Nanoparticles for Targeted Drug Delivery in Cancer	Basar Bilgicer
39	Sebastian MunizMartinez	Electrochemical Nitrite reduction using Earth abundant based catalysts	Kyle Doudrick
40	Mitchell Murphy	Using Optical Character Recognition to Assess Differential Treatment	Kasey Buckles
41	Calvin Nazareth	Self-assembly of amphiphilic tripeptides and their peptoid analogues	Matthew Webber
42	Ansley Nemeth	Synthesis of Novel Oxazoline Compounds for Use as Insecticides and the Evaluation for Mosquitocidal and Larvalcidal Activity	Mary Ann McDowell
43	Kimberly Orr	A new approach for alignment-free comparison of temporal networks	Tijana Milenkovic
44	Khayyon Parker	Sensitivity and Uncertainty analysis of Ground Water model Replacement TimML	Stuart Jones
45	Ana Quintero	Synthesis of [^13^]C-Labeled Methyl Î±- and Î²-D-Arabinofuranosides and Studies of Ring Conformational Equilibria Using Redundant NMR Spin-Couplings and Circular Statistics	Anthony Serianni
46	Rebecca Radomsky	ZnO and CdSe Dual-Emission Ratiometric Probe for the Detection of Organophosphonates	Prashant Kamat
48	Paola Rivera	Geochemical and isotopic evolution of carbonatites in Magnet Cove Complex in Arkansas	Antonio Simonetti
47	Alexander Scott	Detecting Human Eye Movements from Infrared Cameras	James Schmiedeler
49	Gregory Serapio-Garcia	Big Data & the Big Five: Computationally Predicting Personality and Psychopathology from Social Media	David Watson
50	Derek Shank	Utilizing The Cannon to Predict Stellar Parameters	Timothy Beers

51	Isabella Speedon	Comparing Tree-Based Models' Variable Predictions for School Crime	Ying Cheng
52	Natalie Spica	Field-testing of the MicroBio PAD: Detection of fecal contamination of water in Nepal	Reena Lamichhane-Khadka
53	Caroline Stanton	In Membrane Exploitation of Antigen/Antibody Interaction for Selective Purification and Quantification of Therapeutic Monoclonal Antibodies	Merlin Bruening
54	Jessica Stietzel	Deep Neural Networks for Reconstructing Particle Collisions	Kevin Lannon
55	Robert Stiller	Analysis in Energy Systems for Smart Grid Control using Multiple Storage Devices	Abigail Mechtenberg
56	Maxwell Tetrick	Algal Biodiesel Conversion and Characterization for use as Decentralized Electrical Energy in Uganda and Notre Dame	Steven Wietstock
57	Joseph Vallin	Phase Inversion Membrane System for Heavy Metal Absorption	William Phillip
58	Maura Vrabel	Determination of Crucial Immunogenic Epitopes in Major Peanut Allergy Protein, Ara h2, via Novel Nanoallergen Platform	Basar Bilgicer
59	Mitsy Wedderburn	Self-Medication in Long-Tailed Macaques (_Macaca fascicularis_)	Hope Hollocher
60	Justin Wei	CNVis: A Web-Based Visual Analytics Tool for Exploring Conference Navigator Data	Chaoli Wang
61	Taylor Wiley	Making the Grade: Change in Social Network Diversity Among First-Year Notre Dame Students	David Hachen
62	Haley Wilson-Lemmon	Syngeneia And Xenoi: The Role of Kinship in the Practice of Hospitality	John Fitzgerald
63	Elon Yates	Electrochemical performance of nickel-based electrodes: Improving urea electro-oxidation	Kyle Doudrick
64	Aristotle Zervoudakis	Phase Behavior of Complex Coacervates	Jonathan Whitmer

POSTER SESSION 1: 9:30 - 10:30 A.M.

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4	Caroline Brooks	Cross Sectional Time Series Analysis on the Impacts of Race on Homeownership	Richard Williams	Sociology
6	Brendan Brown	Dispersion Curves for Plasmons in Metal Nanostructures	Gregory Hartland	Chemistry and Biochemistry
8	Adam Carr	Quantitative PCR analysis of LTA resistance in _Streptococcus pyogenes_ against synthetic bacteriocins	Shaun Lee	Biological Sciences
10	Adam Cooper	Fighting Low Quality Pharmaceuticals through the Development and Simplification of an Affordable Paper-Medium Antibiotic Assay	Marya Lieberman	Chemistry and Biochemistry
12	Lina Daza	Application of molecular dynamics to study the gas-liquid interfacial properties of the ionic liquid: 1-n-butyl-3-methylimidazolium acetate [BMIM] [OA]	Edward Maginn	Chemical and Biomolecular Engineering
14	Heather DiLallo	HPLC Verification of Paper Analytical Devices to Screen for Low-Quality Albendazole	Toni Barstis	Electrical Engineering
32	Alfredo DuarteGomez	Development of Luminescent Porous Particle for Two-Color Pressure-Sensitive Paint	Hirotaka Sakaue	Aerospace and Mechanical Engineering
16	Rebecca Dudek	Development of Novel DNA Extraction Technique for the Detection of Genetically Modified Soy Beans	Hsueh-Chia Chang	Chemical and Biomolecular Engineering
18	Bailee Egan	Linking the Core Oral Microbiome and Gut Parasites in Long-tailed Macaques	Hope Hollocher	Biological Sciences
20	Grace Enright	Applying HTC to Economic Innovation Discovery	Kirk Doran	Economics and Econometrics
22	Caitlin Guccione	Improving the Accessibility of Bioinformatic Workflows Through Cloud Deployment	Douglas Thain	Computer Science and Engineering
24	Esther Harkness	Optical Microbe Detection Platform via Low Cost Open Source Electronics	Scott Howard	Electrical Engineering
26	Melissa Henry	Longitudinal Effect of Food Insecurity on Academic Outcomes	Ying Cheng	Psychology
28	Elizabeth Innis	Validation by LC-MS of Paper Analytical Devices of Suspect Nepali Omeprazole	Toni Barstis	Electrical Engineering

30	Elisabeth Kerns	Effect of Low Bandgap Metal Oxides and Direct Irradiation on the Degradation of Perovskites	Prashant Kamat	Chemistry and Biochemistry
34	Siena Mantooth	Targeted Asparaginase for Improved Treatment of Pediatric Leukemia	Matthew Webber	Chemical and Biomolecular Engineering
36	Brady McLaughlin	[Re]Evaluating the Cost of Electricity in Hospitals with Unreliable Energy - VSL/E Metric	Abigail Mechtenberg	Physics
38	Kate Mockler	Engineering Multifunctional Nanoparticles for Targeted Drug Delivery in Cancer	Basar Bilgicer	Chemical and Biomolecular Engineering
40	Mitchell Murphy	Using Optical Character Recognition to Assess Differential Treatment	Kasey Buckles	Economics
42	Ansley Nemeth	Synthesis of Novel Oxazoline Compounds for Use as Insecticides and the Evaluation for Mosquitocidal and Larvalcidal Activity	Mary Ann McDowell	Biological Sciences
44	Khayyon Parker	Sensitivity and Uncertainty analysis of Ground Water model Replacement TimML	Stuart Jones	Biological Sciences
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48	Paola Rivera	Geochemical and isotopic evolution of carbonatites in Magnet Cove Complex in Arkansas	Antonio Simonetti	Civil Engineering and Geological Sciences
50	Derek Shank	Utilizing The Cannon to Predict Stellar Parameters	Timothy Beers	Physics
52	Natalie Spica	Field-testing of the MicroBio PAD: Detection of fecal contamination of water in Nepal	Reena Lamichhane-Khadka	Biology
54	Jessica Stietzel	Deep Neural Networks for Reconstructing Particle Collisions	Kevin Lannon	Physics
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64	Aristotle Zervoudakis	Phase Behavior of Complex Coacervates	Jonathan Whitmer	Chemical and Biomolecular Engineering

POSTER SESSION 2: 10:45 - 11:45 A.M.

#	STUDENT RESEARCHER	PROJECT TITLE	ADVISOR	DEPARTMENT
1	Emily Baert	An Analysis of Ego Network Characteristics	David Hachen	Sociology
3	Catherine Breakfield	How to Collect 636 Samples in 28 Days	Toni Barstis	Electrical Engineering
5	Roy BrooksRivera	Perturbation of the Calcium Signaling Toolkit Impacts *Drosophila* Wing Morphogenesis	Jeremiah Zartman	Chemical and Biomolecular Engineering
7	Savannah Butler	Degradation of Chemical Warfare Agent Proxies through ZnO Nanocrystal Assisted Photocatalysis	Prashant Kamat	Chemistry and Biochemistry
9	Carl Colglazier	Parallel Python for Global Social Simulation	Paul Brenner	Center for Research Computing/Computer Science and Engineering
11	Jonah Cremin-Endes	Community Members are an Asset in Public Health Movements	Marya Lieberman	Chemistry and Biochemistry
13	Michael Dowd	Keep the Lead Away: Understanding the Problem of Lead in St. Joseph County, Indiana	Marya Lieberman	Chemistry and Biochemistry
17	Kiera Dwyer	Development of a phosphate biosensor using the optical density and pressure of growing yeast.	Holly Goodson	Chemistry and Biochemistry
19	Paul Elhallal	Classifying Islamic Terrorism and its effects on US Counterterrorism	James Philpott	Political Science
21	Kirstin Favazzo	Validation by LC-MS of Paper Analytical Devices of Suspect Nepali Antibiotic Pharmaceuticals	Toni Barstis	Electrical Engineering
23	Amber Hannah	The role of Adenomatous Polyposis Coli (APC) tumor suppressor in intercellular junctions and cell migration	Jenifer Prosperi	Biological Sciences
25	Bryan Harris	Analyzing Resource Metadata from High Throughput Computing in an Opportunistic Environment	Douglas Thain	Computer Science and Engineering
27	Connor Howington	Using computational genomics and high-throughput computing to study malaria parasite _P. falciparum_ and mosquito vector _A. funestus_	Scott Emrich	Computer Science and Engineering
29	Mackenzie Jones	The Long Road off the Family Track: The Difficulty of Having it all	Kasey Buckles	Economics
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33	Benjamin MacCurtain	Analysis of porosity, mineralization, and damage as contributors to fracture risk	Ryan Roeder	Aerospace and Mechanical Engineering
35	William McCarthy	Synthesis of peptidic derivatives of 1,3,5-benzenetricarboxamide and investigation of their supramolecular-assembly	Matthew Webber	Chemical and Biomolecular Engineering
37	Heather Miller	Development of a yeast biosensor for prednisone detection	Don Paetkau	Biology
39	Sebastian MunizMartinez	Electrochemical Nitrite reduction using Earth abundant based catalysts	Kyle Doudrick	Civil Engineering and Geological Sciences
41	Calvin Nazareth	Self-assembly of amphiphilic tripeptides and their peptoid analogues	Matthew Webber	Chemical and Biomolecular Engineering
43	Kimberly Orr	A new approach for alignment-free comparison of temporal networks	Tijana Milenkovic	Computer Science and Engineering
45	Ana Quintero	Synthesis of [^13^]C-Labeled Methyl Î±- and Î²-D-Arabinofuranosides and Studies of Ring Conformational Equilibria Using Redundant NMR Spin-Couplings and Circular Statistics	Anthony Serianni	Chemistry and Biochemistry
47	Alexander Scott	Detecting Human Eye Movements from Infrared Cameras	James Schmiedeler	Aerospace and Mechanical Engineering
49	Gregory Serapio-Garcia	Big Data & the Big Five: Computationally Predicting Personality and Psychopathology from Social Media	David Watson	Psychology
51	Isabella Speedon	Comparing Tree-Based Models' Variable Predictions for School Crime	Ying Cheng	Psychology
53	Caroline Stanton	In Membrane Exploitation of Antigen/Antibody Interaction for Selective Purification and Quantification of Therapeutic Monoclonal Antibodies	Merlin Bruening	Chemical and Biomolecular Engineering and Chemistry and Biochemistry
55	Robert Stiller	Analysis in Energy Systems for Smart Grid Control using Multiple Storage Devices	Abigail Mechtenberg	Physics
57	Joseph Vallin	Phase Inversion Membrane System for Heavy Metal Absorption	William Phillip	Chemical and Biomolecular Engineering
59	Mitsy Wedderburn	Self-Medication in Long-Tailed Macaques (_Macaca fascicularis_)	Hope Hollocher	Biological Sciences
61	Taylor Wiley	Making the Grade: Change in Social Network Diversity Among First-Year Notre Dame Students	David Hachen	Sociology
63	Elon Yates	Electrochemical performance of nickel-based electrodes: Improving urea electro-oxidation	Kyle Doudrick	Civil Engineering and Geological Sciences

An Analysis of Ego Network Characteristics

Emily Baert
College of Arts & Letters
Sociology

Advisor: David Hachen, University of Notre Dame, College of Arts & Letters, Dept. of Sociology

The social networks of college students are dynamic configurations. Over the course of the academic experience, ties form, change, and dissolve. In this study, the social networks of 673 students from the class of 2019 at the University of Notre Dame are analyzed across their first two years of college. The purpose of this study is to see how characteristics of the social networks of the students vary over time within demographic categories. Using data from texting records between students in the study and from surveys, the number of connections (network size), average activity level across the connections, and the dispersion of the activity levels are analyzed by gender, race, religion, and class across four semesters. The analysis consists of two steps: averaging the collected data then using linear regressions to test for significance in the differences between the calculated means for each demographic category in each semester. Over time and within demographic categories, the network size and activity levels decreased slightly. Students who are male, foreign, nonreligious, or have parents without college degrees had fewer connections. Additionally, foreign students, nonreligious students, and students whose parents do not have college degrees also tend to have lower activity levels. Activity levels were more disperse – with mixtures of strong and weak ties – for males, foreign students, and students with one parent with a college degree during the freshman year and for protestants and students with parents without college degrees in the sophomore year. Overall, the most significant demographic differences are seen in the amount of connections a student has rather than how active the connections are and how disperse that activity level is.

Development of a Microfluidic Tunable Attribute Precision Screening for Characterization of Bacterial Stress

Catharine Brady
College of Science
Dept. of Biological Sciences and Civil Engineering and Geological Sciences

Aleksandar Dimkovikj
College of Engineering
Civil Engineering and Geological Sciences

James Shuttleworth
University of Notre Dame

Dayi Chen
University of Notre Dame

Advisors: Joshua Shrout, University of Notre Dame, College of Science, Dept. of Biological Sciences and Civil Engineering and Geological Sciences and Aaron Timperman, University of Notre Dame, College of Science, Dept. of Chemistry and Biochemistry

There is a need for new antimicrobials to treat infectious diseases, especially with the increase in drug resistance for community-acquired infections. Research worldwide is aimed at developing and deriving new compounds for antimicrobial treatment, but current strategies that are used to probe for antibiotic activity prove to be inadequate, with existing methods being inefficient to screen for compounds that limit bacterial function under relevant pathogenic conditions. This project aims to create a microfluidic bacterial culture system that precisely characterizes bacterial stress under a broad range of environmental conditions. A two layer, hybrid polydimethylsiloxane (PDMS) and glass microfluidic device was designed and fabricated. The bottom layer contains the bacteria cultures, while the top layer is a microfluidic mixer to create chemical or biochemical gradients that reproducibly vary the environments of the bacteria cultures. Microfluidic mixing and gradient reproducibility was tested under a fluorescent microscope using fluorescein and water. The performance of the mixers was determined as a function of flow rate, channel length, and the geometry of the mixer. More uniform mixing proved to occur with lower flow rates and longer channels within the mixer. These results show reliable and reproducible gradients can be formed in the microfluidic devices to culture and observe bacteria under a broad range of environmental conditions. Future directions include analyzing the bacteria growth spectroscopically from within the device allowing measurements to be taken at multiple times due to the nondestructive nature of spectroscopy when compared to other methods.

How to Collect 636 Samples in 28 Days

Catherine Breakfield
College of Engineering
Chemical Engineering

Heather DiLallo
College of Engineering
Chemical Engineering

Advisor: Toni Barstis, University of Notre Dame, College of Engineering, Dept. of Electrical Engineering

According to the World Health Organization (WHO), SSFFC (substandard, spurious, falsely-labeled, falsified, and counterfeit) medicines are a global health issue that causes harm to patients, fails to treat illnesses, yields lowered confidence in medicines, and is particularly problematic in developing countries. The world needs a device that will screen for SSFFC medicines. For use in developing countries and to address the International Medical Products Anti-Counterfeit Taskforce (IMPACT), this device must be inexpensive, portable, easy to use, and adaptable. In response, the paper analytical device (PAD) was developed to test SSFFC medicines. Nepal lies between China and India, two countries known for production of SSFFCmedicines, making it an ideal location to collect samples. The goal of this research study is to determine if certain pharmaceutical brands or manufacturers are consistently producing SSFFC medicines. A group of Saint Mary's College researchers traveled to Nepal for 28 days to collect pharmaceutical samples to be tested via PADs and HPLCMS upon return. The chosen pharmaceuticals were metformin, metronidazole, rabeprazole, ranitidine, and paracetamol. Samples were collected per the WHO suggested protocol in three regions of Nepal from a variety of pharmacies (i.e., rural/urban, government/private, etc). Samples of the chosen pharmaceuticals were purchased by Nepali research collaborators and documented per FDAdocumentation requirements for shipment. In the 28 days, 636 samples were collected and documented. All the samples were analyzed via PADs and HPLCMS analysis is underway. While many of the samples run comparably to a standard PAD of pure API, preliminary screen shows several samples to be suspect.

Cross Sectional Time Series Analysis on the Impacts of Race on Homeownership

Caroline Brooks
College of Arts & Letters
Biological Sciences and Sociology

Advisor: Richard Williams, University of Notre Dame, College of Arts & Letters, Dept. of Sociology

Previous studies show Blacks are less likely to receive home loans than Whites, contributing to a trend of homeownership inequality in the United States. These studies have been based on data collected by various government agencies and government sponsored enterprises from entities which make or purchase the loans themselves. This data is limited; while it contains information on some demographics characteristics of the neighborhood and of the applicant, critical information regarding personal variables like wealth is usually omitted. Moreover, this work focuses only on people who have applied for home loans in a given year, which thus excludes people who have not.

To fill this gap, we examined data from the Panel Study of Income Dynamics (PSID), a longitudinal study run by the University of Michigan that interviews a nationally representative sample of U.S households, to explore if rates of homeownership reveal possible discrimination. Our work consisted of conducting a series of cross sectional analyses using data gathered every other year from 2005 to 2015 to assess the impact of the head of household being black versus not black on rates of homeownership. The majority of the analysis involved running logistic regressions using homeownership as the dependent variable and race as the independent variable. Subsequent regressions included more individual variables like age, education, income, and wealth to assess any impact these factors may have. Results across all years indicate that being black negatively impacts the probability of owning a home, even after controlling for other possible socioeconomic variables. The persistence of racial inequality even after controlling for other crucial variables reinforces fears about the role discrimination plays in homeownership.

Perturbation of the Calcium Signaling Toolkit Impacts *Drosophila* Wing Morphogenesis

Roy BrooksRivera
College of Engineering
Dept. of Chemical and Biomolecular Engineering

Francisco Huizar
College of Engineering
Dept. of Chemical and Biomolecular Engineering

Advisor: Jeremiah Zartman, University of Notre Dame, College Not Specified, Dept. of Chemical and Biomolecular Engineering

Understanding morphogenesis has been a focal point of developmental biology research. Discovering even the most basic mechanisms of developmental biology will aid us in deciphering organisms at a molecular level and will allow us to advance areas such as regeneration, tissue engineering, and others which involve degeneration through aging, and disease. Approaches to this problem have been made through the study of zebrafish eyes and embryos, the epidermis of *C. elegans*, and the imaginal discs of *Drosophila melanogaster.* For this study, we are looking at the effects of the inhibition of calcium signaling pathways in wing imaginal discs, through an array of genotypes in the *Drosophila melanogaster*, using RNA interference (RNAi) expressed in larval tissues. I characterized adult wing phenotypes, including measuring the size of each wing quantified, as well as intervein regions. Inhibition of the gap junction gene Inx2 resulted in smaller wings with an approximate 40% reduction in size, compared to control RNAi against a gene not expressed in the wing disc (Ryr). In many cases, vein abnormalities were observed, primarily in the Inx2, but also in PLCβ and IP3R knockdowns. While Inx2 did have the smallest wings, we can claim that these vein abnormalities are not due to a significant difference in wing area, as PLCβ and IP3R also presented an elevated number of vein patterning abnormalities. This data suggests a direct link between calcium signaling and morphogenesis as inhibition of calcium induced calcium release and gap junction communication leads to morphological defects.

Dispersion Curves for Plasmons in Metal Nanostructures

Brendan Brown
College of Science
Dept. of Chemistry and Biochemistry

Paul Johns
College of Science
Dept. of Chemistry and Biochemistry

Dr. Gary Beane
University of Notre Dame
College of Science
Dept. of Chemistry and Biochemistry

Advisor: Gregory Hartland, University of Notre Dame, College of Science, Dept. of Chemistry and Biochemistry

The interaction between plasmonic and molecular systems is an area of intense interest. This interest arises from the potential such hybrid plasmon-exciton systems present for manipulating the interaction of light with matter. For metal nanoparticles the interaction of electrons with light creates a Surface Plasmon Resonance, SPR, which describes the resulting oscillation of free electrons in a metal. In the case of nanowires, these electrons also propagate down the wire with specific momenta and are known as Surface Plasmon Polaritons, SPPs. When a laser is focused at the end of the nanowire, the photons are able to match their momentum with the wavevector of the SPP. Using back focal plane imaging, the SPP wavevectors can be determined for different wavelengths of light, and then plotted as a dispersion curve. Using the dispersion curves, the avoided crossing can be visualized when there is a dielectric medium for the SPP to couple to. The medium used in this experiment is the dye TDBC. The experimental results show that as the wires couple to the dye the lower energy wavevectors tend to diverge from the light line whereas the higher energy wavevectors follow the light line. The splitting energy has been found to be 150meV.

Degradation of Chemical Warfare Agent Proxies through ZnO Nanocrystal Assisted Photocatalysis

Savannah Butler
College of Science
Dept. of Chemistry and Biochemistry

Victoria Bridewell
College of Science
Dept. of Chemistry and Biochemistry

Advisor: Prashant Kamat, University of Notre Dame, College of Science, Dept. of Chemistry and Biochemistry

Oxidation/reduction reactions employing metal oxide (MOx) materials play a large role in emerging energy technologies as well as other processes such as photocatalytic remediation of wastewater and gaseous contaminants. It is well known that MOx materials such as zinc oxide (ZnO) in particular undergo proton-coupled electron transfer (PCET) mechanisms and generate hydroxyl radicals through which degradation and mineralization is possible. By employing ultra-small ZnO nanocrystals (NCs) exhibiting size quantization properties, we can broadly tune their optical properties and photocatalytic activity. The observed green emission of ZnO NCs is a direct result of exciton recombination (UV emission) and oxygen-vacancy defect recombination (visible emission). Taking advantage of photoexcitation and complete quenching of ZnO defect emission, we have established a real-time, threshold fluorescence sensor for the detection of organophosphonates and nitroaromatics. Analogously, we are developing ZnO NCs on flexible substrates such as cloth for use as photocatalysts. We have shown previously that ZnO can undergo PCET as well as hydroxyl radical generation upon above band gap excitation and photocatalytically degrade DMMP and NBT into their mineral components.

Quantitative PCR analysis of LTA resistance in *Streptococcus pyogenes* against synthetic bacteriocins

Adam Carr
College of Science
Dept. of Biological Sciences

Francisco Fields
College of Science
Dept. of Biological Sciences

Advisor: Shaun Lee, University of Notre Dame, College of Science, Dept. of Biological Sciences

Overuse and lack of novel antibiotics has led to resistant phenotypes of bacteria especially in the developing world with limited access to healthcare. Unfortunately, difficulty in innovation and minimal return on investment for development of antibiotics have caused a lack of novel antibiotics for treatment of bacterial infections. (1) Antimicrobial peptides (AMPs) synthesized by bacteria called bacteriocins hold great promise as potential scaffolds for antibiotics due to their antibacterial activity. Here we tested bacterial resistance against a novel synthetic bacteriocin with cationic properties, syn-safencin. A known resistance mechanism against cationic antibiotics in gram positive bacteria is charge modification in the cell wall through the D-alanylation of lipotechoic acids (DA – LTA) to repel cationic antibiotics. We measured the effect of this resistance mechanism against syn-safencin by monitoring the *dltABCD* operon encoding the genes responsible for this resistance. We were able to quantify the relative expression using a reverse transcription – real time PCR (qRT – PCR) approach. The expression fold changes of mRNA transcripts were calculated using the CT method where CT is the cycle threshold value obtained from qPCR analysis. The results did not show any significant expression fold changes when treated with syn-safencin compared with the vehicle control of 10% DMSO. These results suggest that the DA – LTA is not a mechanism of resistance of syn-safencin, and other mechanisms involving surface charge modification should be monitored for resistance. Finding the mechanisms of resistance against synthetic bacteriocins will allow for the design optimization of peptide candidates that account for known resistance mechanisms.

(1) Fischbach, M. A. 2010, 1089 (2009).

Parallel Python for Global Social Simulation

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We introduce a system using Python and Jupyter for performing agent-based modeling at a global scale with seven billion agents. This removes the need for artificial boundary conditions and allows for multi-scale integration of macro global effects and micro agent behaviors. To validate computational scalability, we developed the simulation platform in conjunction with a global scale human migration model based on a subset of known social and economic factors. The Jupyter simulation platform and Python programming language allows for a familiar developer and user interface via a standard internet browser and allows for the computation to be performed remotely on high performance server hardware. With complexity kept linear in proportion to agent population, we have successfully scaled the system to seven billion agents and have observed significant performance improvements by running the model in parallel using multiple Python processes.

Fighting Low Quality Pharmaceuticals through the Development and Simplification of an Affordable Paper-Medium Antibiotic Assay

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Low quality and falsified pharmaceuticals are an unfortunate reality many live with around the world, especially in Low and Middle Income Countries (LMICs). The need for comprehensive analysis in limited resource settings has turned researchers to develop inexpensive tools such as paper-based analytical devices (PADS). The antibiotic PAD (aPAD) utilizes a standard titration assay for beta-lactam antibiotics that has been downscaled to function on paper. The current aPAD methodology uses a glassware addition of sodium hydroxide, carefully prepared triiodide and hydrochloric acid followed by a reaction on the paper test card consisting of a reduction with thiosulfate and a color producing complexation with starch. Through this scheme, the aPAD has the capability to semi-quantify the quality of beta-lactam antibiotics. These drugs, such as amoxicillin and ampicillin, are crucial and widespread in any healthcare system. I performed a field reproducibility test of the aPAD in Eldoret, Kenya. This test, while successful, revealed a need to simplify the process for the end user– pharmacists in LMICs that lack capacity for postmarket surveillance. I created a shortened scheme that requires the placement of triiodide in quantitative amounts onto the aPAD, which will make the final reduction step using thiosulfate redundant. This will simplify both the creation and use of the aPAD and lower cost. Testing was performed to simulate this simplified reaction scheme which gave results similar to the current readout of the aPAD and initial degradation tests show promising results of the “shelf life” of dried triiodide, the crucial new addition to the aPAD.

Community Members are an Asset in Public Health Movements

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A 2016 Reuters study brought the lead crisis in South Bend into the spotlight by indicating the high proportion of children living with elevated blood lead level in the area. My research studied effective strategies for facing the crisis through listening to lived experiences of community members, shadowing clinics, and engaging with the literature. To understand these experiences, I conducted personal interviews with community members who received tests indicating their child had an elevated blood lead level. Out of seven interviews, six respondents had taken personal action to decrease lead exposure. All seven had received contradictory or inaccurate information regarding lead exposure. People want accurate information explaining effective methods to personally reduce lead exposure. At WIC, the Women, Infants, and Children clinic, I shadowed five nurse patient screenings of children aged 0-5. There were three cases in which a lead test was offered, with all of them being accepted. Staff at WIC, including Sue Tayler, Leciesha Briggs, and Kathleen Kraner, expressed the need for more funding for further testing. I examined current literature by analyzing the most recent handouts from the CDC1 and EPA2 on lead. I categorized the information in the handout as either an explanation of the negative impact of lead, a method for reducing lead exposure that involves another party, or a method that can be performed individually. People want to know information in the third category, individual methods, but this was less than 20% of the information given. A common narrative was that community members want to act after being informed that their child had an elevated blood lead level. During the process, they receive information that can be out of scope and contradictory. If provided with accurate and concise information, community members can become a greater asset. I have produced a concise flyer and I am producing an informational video to address this opportunity. Many other cities nationwide are facing the same lead challenges as South Bend. These communities may also benefit from more specific explanation of actions one can take to reduce lead exposure in their home.

Figure 1. House Testing Photo Credit: Barbara Johnston

Application of molecular dynamics to study the gas-liquid interfacial properties of the ionic liquid: 1-n-butyl-3-methylimidazolium acetate [BMIM] [OA]

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Ionic liquids are ionic substances whose melting temperature are below 100˚C. These substances have low vapor pressure and many favorable properties. We are interested in their liquid-gas interfacial properties, due to their application in catalysis, gas separations and other applications. Atomistic simulations are a powerful way of probing gas-liquid interfaces, as they provide a link between macroscopic experimental measurements and molecular-level phenomena. In this work, we use molecular dynamics simulations with the LAMMPS code to compute different transport, thermodynamic and structural properties of 1-n-butyl-3-methylimidazolium acetate [BMIM][OA], with an emphasis on the liquid-gas interface. Our objectives were to understand the system's structure at the liquid-gas interface, while water was added to the ionic liquid mixture. Numerical simulations were computed at 300 K and 400 K. The radial and spatial distribution functions were calculated to observe structural properties. The mean square displacement was determined to study the dynamics of the cations, anions, and water. We find that water tends to accumulate at the interface.

HPLC Verification of Paper Analytical Devices to Screen for Low-Quality Albendazole

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Parasitic worm infestations (e.g., tapeworms, roundworms, hookworms, and pinworms) are common to children of developing countries and are considered to be a roadblock to the social and economic development of these countries. These effects range from mild (e.g., discomfort, diarrhea) to life-threatening (e.g., anemia, malnutrition, or death). Albendazole is a commonly used oral medication for the treatment of parasitic worm infestations. Because albendazole is a safe and effective medication, the World Health Organization (WHO) placed albendazole, a benzimidazole carbamate anthelmintic, as an essential medicine, meaning that all people should have access to albendazole in sufficient amounts at all times. Unfortunately, in developing countries such as Nepal, the quality of this essential medicine is suspect. In an extensive sample collection study in Nepal in summer 2016, including 180 samples of albendazole, Barstis found that albendazole was often stored improperly (e.g., open to the heat and humidity) and distributed past its expiration date. Additionally, DiLallo conducted a preliminary sample collection study in China in summer 2017, collecting 55 samples of albendazole in two diverse regions. China is one of the largest manufacturers of counterfeit medicines and several Chinese drug companies are banned from selling in the US due to not meeting FDA regulations. This research focuses on the results of a paper analytical device (PAD) used both in the field and in the laboratory to screen for low-quality albendazole. These PADs (Figure 1 below) are around the size of business cards, use colorimetric chemistry to screen for select ingredients, and results can be seen in less than five minutes. A US Pharmacopeia validated method for High Performance Liquid Chromatography (HPLC), as well as an independent UPLC-MS method being developed at Saint Mary's College, are being used to validate the PADs data. All results will be presented.

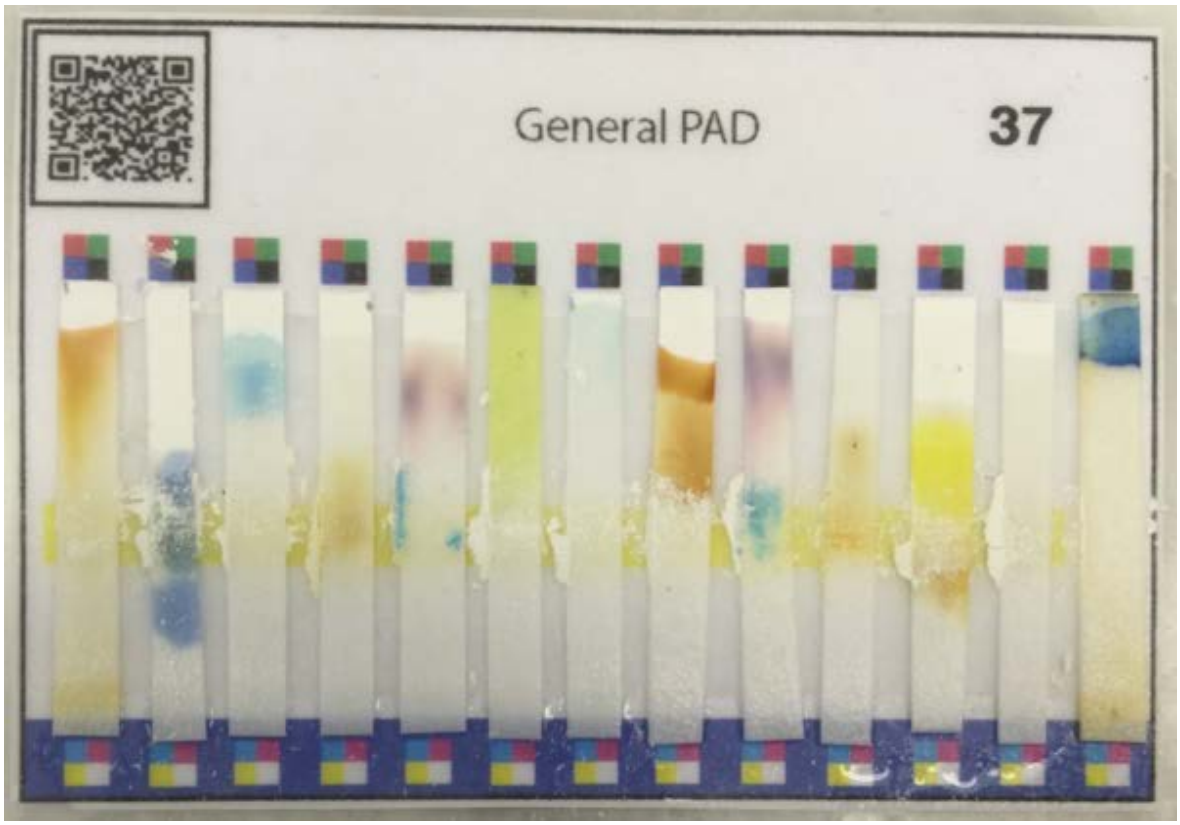

Figure 1: General PAD run with albendazole US standard powder

Keep the Lead Away: Understanding the Problem of Lead in St. Joseph County, Indiana

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Elevated Blood Lead Levels (EBLL), especially in children, have been linked to permanent neurologic defects, resulting in lowered IQ, learning disorders, and increased rates of criminal behavior and incarceration. In late 2015, Flint, Michigan declared a state of emergency due to high levels of lead in the water. According to a recent Reuters report, the rate of EBLLwas nearly 6 times higher in Census Tract 6 in St. Joseph County, Indiana than in Flint. A group of 13 people at the University of Notre Dame has begun working in the community to determine why these EBLL are so high and how community members can reduce exposure to lead.

From our group, teams of 6 researchers collected paint, soil, dust, and water samples from 4 homes with children who had BLL of greater than 3.5 µg/dL. These samples were tested via X-ray Fluorescence (XRF) and Induced Coupled Plasma Optical Emission Spectrometry (ICP-OES). I tested the sample preparation procedures for the ICP experiments and assessed recovery of lead from dust wipe samples, and I carried out most of the analysis of the ICP data. The results from home samples were compared to EPA reference levels, and final reports were given to these families, highlighting the major areas of concern and possible avenues of remediation. In certain homes, children's play areas were found to have high levels of lead in the soil; to remediate this problem, ground cover such as regular mulching or planting of groundcover was recommended. In another home, the level of lead dust in a play cubby was found to be high and total abatement of the cubby was recommended. In the future, the data gathered in this study will be used to inform policymakers in order to spark city, county, and state level action.

Figure 1. In Census Tract 6, 31% of children tested had Elevated Blood Lead Levels, a major Public Health problem.

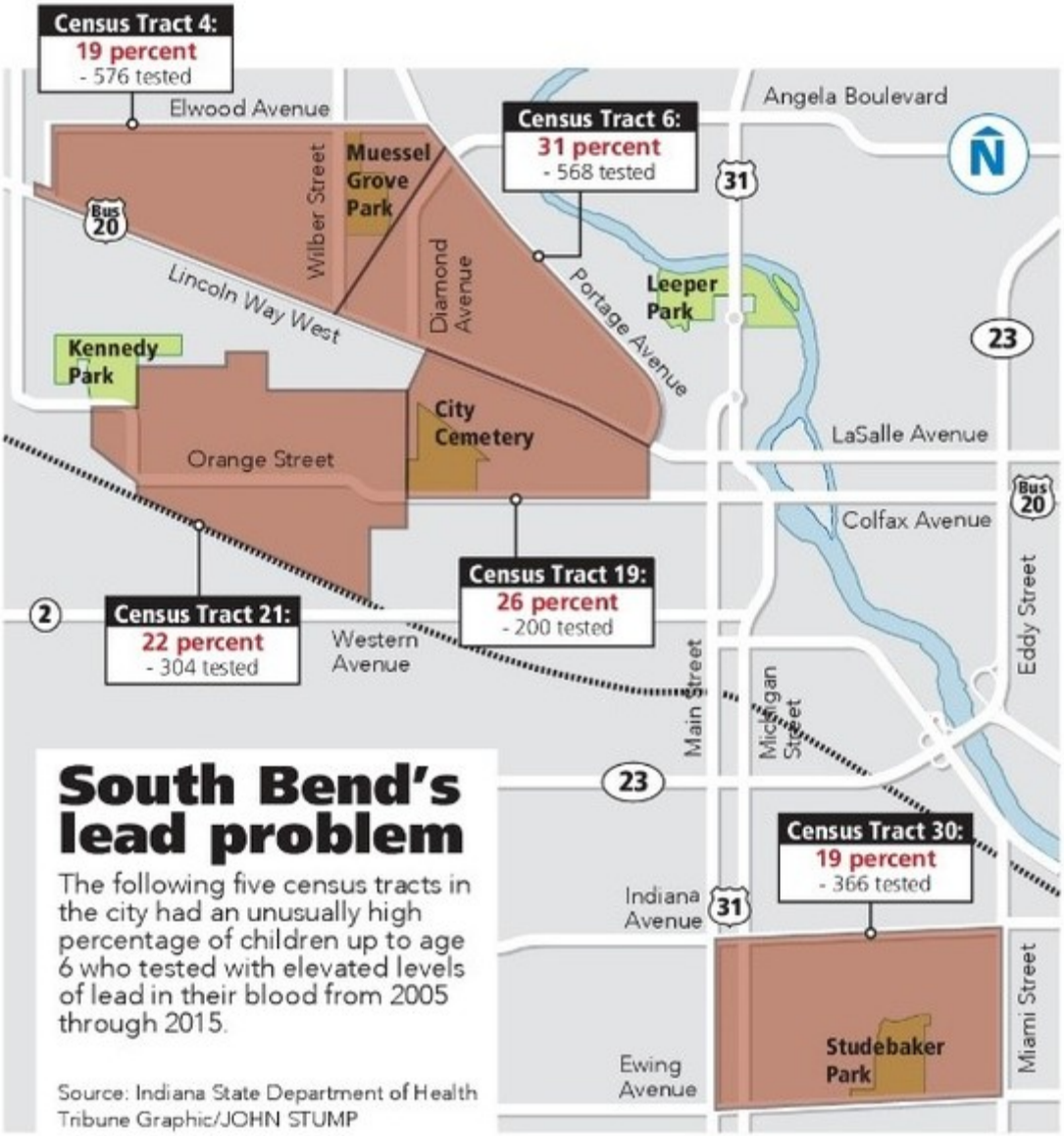

Photo Credit: South Bend Tribune

Development of Luminescent Porous Particle for Two-Color Pressure-Sensitive Paint

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Pressure measurements are essential to the study of fluid dynamics: they can be utilized to identify flow phenomena, the validation of computational fluid dynamics codes, and many engineering applications. Pressure sensitive paint (PSP) is an imaging technique that utilizes a luminescent molecule to relate its luminescent output to the pressure. Compared to the traditional pressure tap or transducer methods, PSP offers surface pressure information with relatively low cost. In PSPresearch, a two-color PSP has been developed by our group to capture unsteady pressures over a moving/vibrating/deforming fluid dynamic objects. It consists of two luminescent dyes: a reference probe and a pressure sensitive probe, porous material, polymer, and solvent. To give quantitative pressure measurements, a uniform distribution in two luminescent dyes is desired. However, the two-color luminophore solution is sprayed over a base layer, and the dyes adsorb onto the layer non-uniformly. To overcome the non-uniformity problem, we developed luminescent particles. These will be mixed with a polymer to create uniformly distributed two-color PSP. In the present study, the concentration of the porous material and luminescent dye, solvent, and drying method were explored to develop the luminescent particles. Fluorescein was selected as the reference probe, while a Ruthenium complex was chosen as the pressure sensitive probe. Silica gel (SiO2) was used as the porous material. We characterized the uniformity qualitatively by illuminating the sample with a constant intensity. The luminescent intensity of the particles was evaluated by using a spectrometer. It was found that a selection of solvent and a filtering as drying method changed the uniformity and intensity. It was shown that, for Fluorescein dye, the best uniformity and the highest intensity were given by dichloromethane as a solvent and a filtering as a drying method. For Ruthenium, the best uniformity and intensity were given by water as a solvent and a boiling process as a drying method. With these processes, Ruthenium particle responded to the change in pressure as a PSP dye.

Development of Novel DNA Extraction Technique for the Detection of Genetically Modified Soy Beans

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In July of 2016, the government of Taiwan enacted strict laws requiring genetically modified (GM) food products to be labeled due to health concerns. The current method of GM detection is polymerase chain reaction (PCR) followed by gel electrophoresis. This technique has numerous drawbacks; it is expensive, requires bulky equipment, and can only be performed by scientifically trained personnel. Consequently, a more practical technique for detection GM food is needed. This lab is contracted to develop a low-cost, polycarbonate device capable of determining whether the soybeans used in the production of soymilk were organic or genetically modified. It will perform three separate steps: isolation of the DNA from the soymilk, amplification of the modified gene, and detection of that amplified DNA segment. This poster focuses on the creation a novel method of isolating DNA that could be incorporated on to the device without the need for expensive laboratory equipment, such as a centrifuge. Passing soymilk through a 0.2uM filter and amplifying using Thermo Scientific's Phire Plant Direct PCR Master Mix allows amplification. Though the DNA using this method does not amplify as much as does our positive control, the band intensity was strengthened by loading more of the amplified product onto the gel. Future research aims to see if the device's novel DNA detection system, which does not utilize gel electrophoresis, can detect the amplified product. If not, the effect of PCR inhibitors present in the soymilk filtrate will need to be reduced. Once optimized, the isolation procedure will be integrated into the device.

Development of a phosphate biosensor using the optical density and pressure of growing yeast

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Eutrophication, a type of water pollution caused by excess nutrients, is rapidly destroying aquatic ecosystems and degrading the quality of water throughout the world. The first step in alleviating the devastating impact of eutrophication is to monitor nutrient levels of vulnerable sources of water. In inland areas, such as the Great Lakes, the major nutrient contributing to the eutrophication of water is phosphorous. Phosphorous monitoring is currently limited to expensive and laborious lab-based approaches. This study explores the possibility of developing a continuous and relatively inexpensive phosphorous biosensor that relates phosphorous levels in potentially eutrophied water to yeast growth. Eutrophication, which occurs around 3 uM, is within the range (1 uM to 100 uM) for which yeast grows linearly with phosphate concentration. As the yeast cells grow, they not only make the sample denser but also release CO2 which increases pressure if the cells are grown in a caped tube. Therefore, in this study yeast growth was measured through optical density and pressure by a spectrophotometer and Vinmetrica SC-55 manometer, respectively. The relationship between optical density and phosphorous concentration, as well as pressure and phosphorous concentration, was determined to be linear. In addition, the phosphorous levels of a 10 uM phosphorous sample, manure sample and Saint Joseph's Lake water sample was determined using yeast growth and compared to the standard method of measuring total phosphorous (TP) and soluble reactive phosphate (SRP). These results illustrate the unique ability of this yeast-based sensor to measure bioavailable phosphorous, defined as the fraction of phosphate that can be assimilated by organisms. The development of this sensor will be critical in understanding the dynamics of biological eutrophication and thus become one step closer to alleviating the devastating effects of eutrophication worldwide.

Linking the Core Oral Microbiome and Gut Parasites in Long-tailed Macaques

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The core oral microbiome is composed of prokaryotic taxa that represent a set of fundamental gene functions found in the majority of hosts. In diseased hosts, the oral microbiome can enter a dysbiotic state usually caused by a change its composition. Moreover, gut parasites can shift the composition of the core oral microbiome by modulating host immunity or by interacting with the microbiota. In this study, I characterize the bacterial and archaeal communities of long-tailed macaques from across Singapore by amplifying and sequencing the 16S rRNA gene from saliva. I relate the parasite load to diversity and composition of the microbiome and compare the core microbiomes of healthy and unhealthy individuals. While it has been shown that there is a great variety in healthy microbiomes, I hypothesize that samples with higher parasite loads represent unhealthy individuals whose microbiomes have decreased diversity and significant changes in composition. The goal of this study is to compare healthy and dysbiotic core communities to shed light on the relationships among parasites, microbiota, and immune function.

Classifying Islamic Terrorism and its effects on US Counterterrorism

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Since 9/11, United States counterterrorism policy has viewed terrorism as a single phenomenon, not allowing for any discrimination in its classification. Under the National Strategy for Combating Terrorism (NSCT), this broad notion of terrorism has resulted in the development of a foreign policy that is ineffective because of its broadness, unable to take the particular measures necessary to combat certain forms of terrorism. Scholarly work to date has examined the existence of different forms of terrorism and debated the utility of such terms as “religious” in academic classifications of terrorism, but little has been done to examine the factors which distinguish one form of terroristic violence from another. To this end, this paper seeks to develop a methodology for classifying different forms of Islamic terrorism. It attempts to develop a taxonomy by examining distinguishing factors such as the stated ends of the group, its political motivation, the religious adherence of leaders and members, and the group’s involvement in running such community involvement programs as hospitals and schools. This paper will then use the Shiite organization Hezbollah as a case study in applying the proposed methodology, and will briefly examine the effects of this methodology on United States counterterrorism policy.

Applying HTC to Economic Innovation Discovery

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The goal of this project is to examine individual output history across a large population using historical census and patent data, in an effort to identify causal mechanisms related to innovative productivity using natural experiments. The challenges associated with matching entities, or individuals, across large census and patent data sets, such as the lack of unique entity identifiers, the inconsistency of formatting within and between data sets, and the volume required by the inclusion of multiple censuses and decades of patent information, introduce significant computational complexity to the project. We adopted a dual approach to respond to these challenges: reduce execution time while preserving and improving match quality. To minimize run time and meet requisite memory demand, entity matching was performed in parallel on a distributed infrastructure, and two algorithms, both applying approximate or “fuzzy” string matching, were employed. The first algorithm incorporates Levenshtein or edit distance, and significantly improved match quality against an original implementation that utilized dynamic regular expressions. The second algorithm, which requires significant pre-processing, attempts to gather all possible fuzzy matches through the generation of a cluster by regular expressions. The Levenshtein algorithm minimizes disk usage, with only a modest improvement in execution period over an original runtime of one week, while the Cluster algorithm offers the benefits of higher quality pairing with a seven fold improvement in execution time compared to both the original and Levenshtein implementation, completing a census-patent merge, while occupying 1,152 cores, in approximately 24 hours. This accelerated execution time will expedite the encompassing research body by significantly reducing data flow bottlenecks and the overall time necessary to process entire census and patent data sets.

Validation by LC-MS of Paper Analytical Devices of Suspect Nepali Antibiotic Pharmaceuticals

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Sheila Lawler
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During the summer of 2016, suspect pharmaceutical drugs were collected from several regions, manufacturers, and pharmacies in Nepal. Over the recent years, the substandard quality of pharmaceutical drugs in developing countries has presented a significant health concern. The World Health Organization recognizes these low quality drugs as substandard, spurious, falsely labelled, falsified and counterfeit (SSFFC) and deems them difficult to detect. Paper Analytical Devices were used to screen the collected Nepali pharmaceuticals. The goal this summer was to validate the findings of the Paper Analytical Devices and to quantitate the active pharmaceutical ingredients (API) of the collected Nepali medicines. To do so, standards of each drug were purchased from Tokyo Chemical Industry and U.S. tablets were donated to develop the sample preparation methods. These methods were further developed using Reverse Phase Liquid Chromatography and Mass Spectrometry with a C18 column. The focus for this presentation is the method development of two antibiotics, azithromycin and amoxicillin clavulanate. Various solvents, crushing techniques, and instrument parameters were tested to determine the optimal method for both pharmaceuticals. Thus far, it was found that azithromycin dissolves best in a 50:40:10 mixture of ammonium acetate buffer (pH 5): acetonitrile: HPLC grade methanol. Due to its film coating, the whole tablet will have to be dissolved and then further diluted. As for amoxicillin clavulanate, all the pills will be prepared in a 0.5 mg/mL solution with HPLC grade water. Future work includes using these method developments to test the Nepali samples that were collected.

Improving the Accessibility of Bioinformatic Workflows Through Cloud Deployment

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The growing field of bioinformatics develops software and workflows that process and help us to understand biology data. One of these programs, the Burrows-Wheeler Alignment Tool (BWA), is used by scientists to discover single base differences, called Single Nucleotide Polymorphisms (SNPs), between samples. Although there are many important applications of the SNP discovery, such as personalized medicine and population genetics, correctly and efficiently running BWA at scale can be challenging for clinicians and scientists who do not specialize in computer science. Here we provide an easier and faster way to execute BWA through the use of Amazon Web Services, Makeflow, and Work Queue. Our framework can reduce the runtime of BWA from several days to only a few hours when applied to a Black Widow Spider (Lactrodectus hesperus) dataset. Using data from both the Black Widow Spider and Yeast (Saccharomyces cerevisiae) datasets, we develop a model for the ideal core usage based on the input data size. Using the optimal number of cores, we then create a workflow script using Make-style syntax to partition the data and process these subsets concurrently. We determined that Work Queue can be effectively used to schedule these smaller BWA jobs produced by Makeflow on Amazon Web Services. Because Amazon can be accessed everywhere, this simple process can be used by scientists worldwide, even those who may not have their own dedicated computing resources, to discover biology breakthroughs faster.

The role of Adenomatous Polyposis Coli (APC) tumor suppressor in intercellular junctions and cell migration

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The Adenomatous Polyposis Coli (APC) tumor suppressor is a paramount figure in the study of tumor progression. This multi-functional protein operates in epithelial cells as a regulator of cell adhesion, cell migration, chromosome segregation, and microtubule/actin organization. Studies in our lab have found that APC plays a significant role in polarity and migration through investigation of Madin Darby Canine Kidney (MDCK) cells. We previously determined that APC does not modulate these processes via secreted factors within the cells. The current study was designed to investigate the way that APC controls these processes by exploring cell-cell communication. We hypothesize that APC's mechanism of action for controlling migration will be mediated through the maintenance of cell-cell contact in its actin/microtubule binding site. These contacts are home to junctional proteins that serve as "glue" for the cells; however, if factors such as calcium, are modified in the cell, the integrity of the intercellular contacts is compromised. Ongoing studies are using calcium switch assays to compare how MDCK cells and knockdown cells differ in their response to decreased calcium. Observing this phenomenon through wound healing assays, we will gain insight on how tight junctions are effected in response to this change. We will also determine junctional proteins essential for controlled cell migration and maintenance of actin/microtubule integrity by western blotting and real-time PCR. The differential expression of Claudins 7 and 8 between normal and knockdown cells will unveil the importance of APC as an intercellular regulator of migration. These findings will uncover novel mechanisms by which APCprotects our cells from disease. Investigation is underway utilizing site-directed mutagenesis of APC's actin/microtubule binding site, to further characterize APC's role in migration. Finally, we are generating APC knockdown cells, using the normal human mammary epithelial cell line (MCF12A), to translate our findings to a human mammary epithelial cell model.

Optical Microbe tection Platform via Low Cost Open Source Electronics

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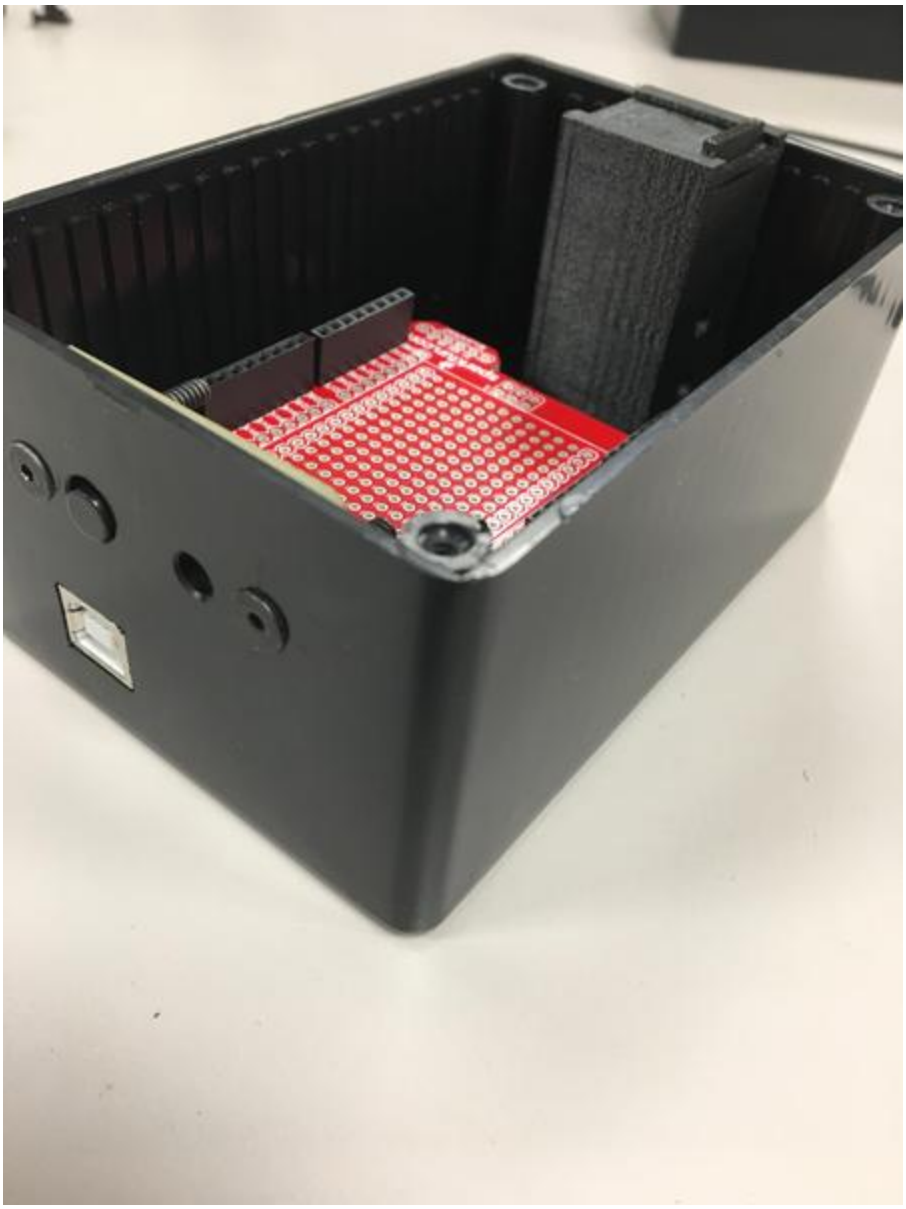
Unsafe drinking water is the estimated cause half a million deaths annually due to diarrheal disease. Contaminated water can cause diseases such as diarrhea, cholera, dysentery, typhoid and polio. To combat waterborne diseases and illness, world health officials need real time data on water quality in the developing world. The goal of our research is to develop an open-source device to help gather data using optical detection of dissolved oxygen concentration via an oxygen sensitive fluorescent probe. The concentration of dissolved oxygen in a water source will determine if microbes and bacteria are present, and whether the source is safe to drink. Our lab designed and fabricated a spectrometer that can detect the florescence from a low-cost oxygen sensitive probe called Ru(dpp). The device is open source, costing approximately $40 to build using commercially available components including an Arduino Uno, visible LEDs, mini photocells, orange acrylic UV filters, and a casing. A code was written to control the device and collect data to measure the oxygen concentration in water samples. We are currently working to determine the sensitivity of the device in measuring dissolved oxygen concentration, preparing for field testing, improving the design of the casing, and comparing the results of our device to commercial devices. Our future plans include licensing this device to allow public health officials to obtain the data needed to reduce the number of lives lost to unsafe drinking water.



Analyzing Resource Metadata from High Throughput Computing in an Opportunistic Environment

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Modern scientific research has an increasing need for parallel and distributed computing resources to process, analyze, and scale ever larger data sets and simulations. Lobster is a dynamic high-level workflow manager developed and used by high energy physicists at Notre Dame participating in the Compact Muon Solenoid (CMS) collaboration to take advantage of distributed opportunistic resources. Opportunistic computing uses non-dedicated and unprivileged computing resources when they would otherwise be idle, but this introduces complexities such as software availability and the risk of eviction. Lobster and the underlying high throughput computing tools it uses, specifically WorkQueue and its Resource Monitor, generate numerous logs and metadata that can be used for troubleshooting, analysis, and inspiration of improvements. An analysis of this metadata, motivated by the goal of reducing the long tail of finishing tasks at the end of a run, leads to insights of the heterogeneity of performance and risks in this opportunistic environment. In order to explore techniques to manage eviction risk and potentials for improvement, a simple simulator was written, and is being validated with parameters taken from real-world metadata.

Longitudinal Effect of Food Insecurity on Academic Outcomes

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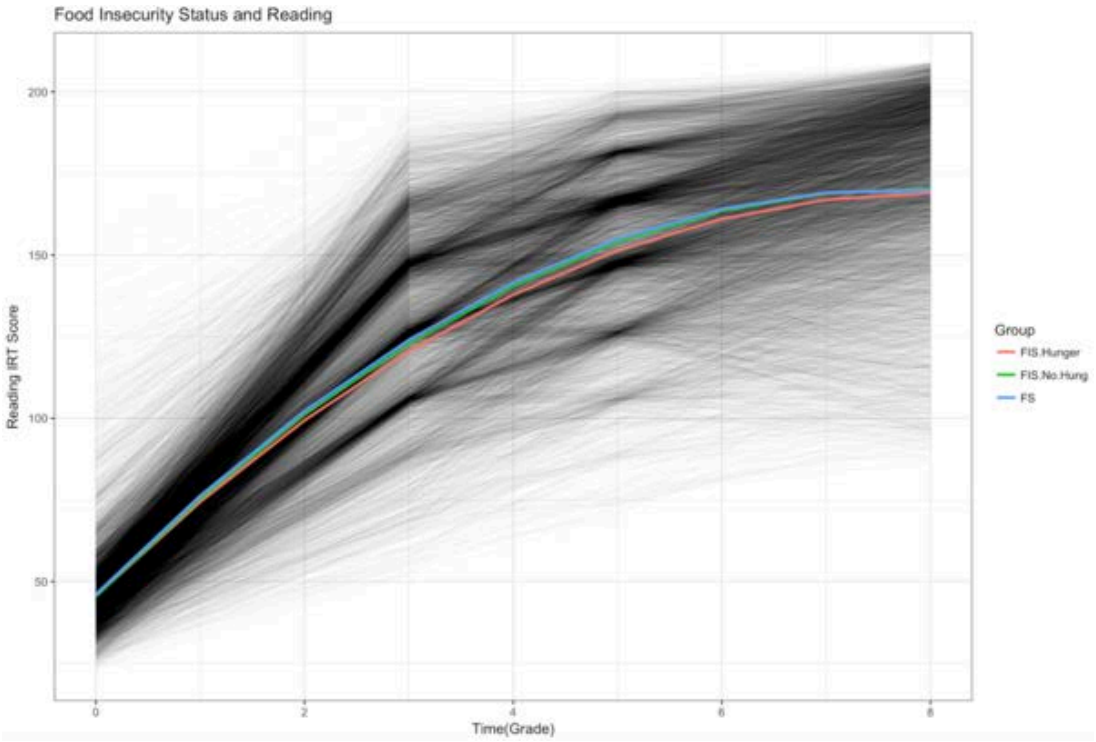
Food insecurity has been associated with adverse developmental outcomes for school-aged children yet remains a problem in households across the United States (Jyoti, Frongillo, & Jones, 2005). Little research has been done to examine how food insecurity affects academic outcomes longitudinally. Data for this analysis was from the Early Childhood Longitudinal Study, Kindergarten Class of 1998-99, a study that followed a cohort of 21,000 students from kindergarten through eighth grade. A multi-level mixed effects model was used to explore how food security relates to academic outcomes in reading and math over the course of four waves of data from kindergarten through eighth grade. Variables controlled for in this model included a composite socioeconomic status measure based on parental income, education and job, gender, race, location of school, and whether the school was public or private. Household Food Insecurity Status (Bickel, Nord, Price, Hamilton, & Cook, 2000) was determined from an 18-item questionnaire and divided participants into three groups: food secure, food insecure without hunger and food insecure with hunger. Results from the analysis supported negative effects on reading Item-Response Theory (IRT) scores but no significant differences were found for math IRT scores between the three groups. Children who are food insecure with hunger had a significant difference in slope when compared to food secure and food insecure without hunger children in that they experience a lower increase in reading scores across the course of the study.


Food Insecurity Status and Reading
Reading IRT Score
200
150
100
50
0
2
4
6
8
Time(Grade)
Group
FIS.Hunger
FIS.No.Hung
FS

Using computational genomics and high-throughput computing to study malaria vector *A. funestus* and parasite *P. falciparum*

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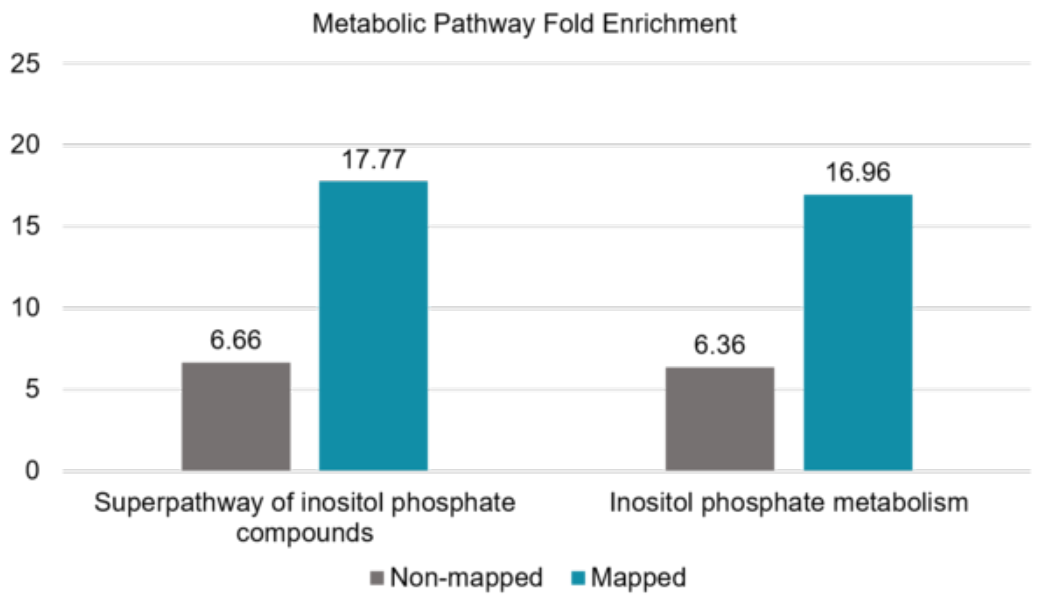
Recent improvements in sequencing technologies have allowed us to study and combat widespread disease agents using genetic and genomic methods. Here at Notre Dame, malaria parasites are a current focus because understanding the genomes of malaria parasites and their mosquito vectors is key to controlling and preventing the spread of this scourge. *Anopheles funestus* is one such vector; however, our current assemblies are significantly lower-quality than desired. HECIL is a new algorithm that has shown promise in increasing assembly continuity by improved correction of errors in low-quality long reads. Here we use an automated workflow and batch system controller called Makeflow to parallelize HECIL and run it on a cluster. This workflow is tested successfully on a smaller yeast assembly, and we hope to apply it to the *A. funestus* assembly in the near future. To better understand how malaria parasites develop resistance to a cutting edge antimalarial medication, a strain of *Plasmodium falciparum* called DD2 was drug-selected over multiple generations in separate experiments, and the resulting child strains were sequenced. An issue when studying malarial parasite strains is that much more data is available for some strains than others, so we developed a bioinformatics method for converting genomic positions from one strain to another using the genome alignment software MUMmer. We show that mapping this experiment data to its DD2 parent, selecting single nucleotide polymorphisms (SNPs) that are present in both child strains, and then mapping them to chromosomes in the widely-studied 3D7 strain provides more significant metabolic pathway enrichment results than mapping to 3D7 directly. This new mapping capability will be used in the future to analyze data from new strains isolated directly from patients for which little data is available.


Metabolic Pathway Fold Enrichment
25
20
15
10
5
0
17.77
16.96
6.66
6.36
Superpathway of inositol phosphate compounds
Inositol phosphate metabolism
Non-mapped
Mapped

Validation by LC-MS of Paper Analytical Devices of Suspect Nepali Omeprazole

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Advisors: Toni Barstis, University of Notre Dame, College of Engineering, Dept. of Electrical Engineering and Christopher Dunlap, St. Mary's College, Dept. of Chemistry Physics

According to the World Health Organization (WHO), substandard, spurious, falsely labeled, falsified, and counterfeit (SSFFC) pharmaceuticals are a prominent issue in developing countries such as Nepal. This led to the development of the Paper Analytical Device (PAD) which screens for the presence, or lack of, the active pharmaceutical ingredient (API) in WHOessential drugs. Omeprazole is responsible for proton pump inhibition and combats the symptoms of acid reflux disease (GERD), an illness common in developing countries. In order to validate and quantify the results from the PADs, 110 samples of omeprazole were collected from various regions in Nepal during Summer 2016. All omeprazole samples were prepared in a 10 mg/mL solution with HPLC grade 2-propanol and analyzed using reverse phase LC-MS, with a Phenomenex Kinetex C-18 column. Data indicated the sample preparation method produced consistent and reproducible results, that every omeprazole pill contained some amount of the API, and that some brands and regions produced data that were consistently lower than the promised amount of API.

The Long Road off the Family Track: The Difficulty of Having it all

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Advisor: Kasey Buckles, University of Notre Dame, College of Arts & Letters, Dept. of Economics

In recent years, men and women have been pressured to attain a career and family life simultaneously. Women in particular have been encouraged “to have it all”. Harvard economist Claudia Goldin looks at family and labor force decisions over time to determine if people can achieve a career and family life. Goldin groups people into birth cohorts of approximately 10 year time spans so those born in the same cohort have the same career and family path. She uses the definition of a career to mean making a wage above the 25th percentile of the male wage distribution. Family is defined as having a child regardless if the person is married. We expand on her research by expanding the definition of having a family. We define a family as having kids and spending at least as much time with them as the 25th percentile of time women spend. In addition we define a career in terms of wage percentile and hours spent at work. We specifically look at college graduates with children under 18 living in their household to see how difficult the goal of balancing both work and family is. Our results show an increase in number of hours women spend with kids and a decline in wages result in less than half of both genders being able to attain both a career and a family life. We also use data regarding changing attitudes about family life to help describe why time with children has been increasing.

Effect of Low Bandgap Metal Oxides and Direct Irradiation on the Degradation of Perovskites

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The excited state and properties of the perovskite material $CsPbBr_3$ material were studied in conjunction with TiO_2 and $ZrO_2$to determine whether exposure to light and air causes degradation of perovskite when adhered to low bandgap metal oxides. Electron-deficient, low bandgap TiO_2 should scavenge electrons from $CsPbBr_3$ and cause its degradation, while ZrO_2 should not affect the degradation of $CsPbBr_3$ due to its high bandgap. Films of $CsPbBr_3$ on TiO_2 and ZrO_2 were prepared by doctor blading the metal oxide onto glass to form a mesoporous layer. The films were soaked in perovskite solution in order to maximize contact between particles. These films were stored in conditions of light, dark, vacuum, and ambient. Absorption spectroscopy, fluorescence spectroscopy, and transient absorption spectroscopy were employed to study the behavior of perovskite in these different conditions and when adhered to the two types of metal oxide. This experiment remains in progress.

ENTROPY improves admixture analyses of low-coverage sequencing data in *Rhagoletis* flies

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The assignment of individuals to discrete populations is of great importance in the study of speciation dynamics. Popular computational methods, such as STRUCTURE (Pritchard *et al.* 2000), analyze genetic differences between individuals to perform this task. However, these programs are best suited for high-coverage sequencing data, which is expensive to produce and may still contain significant error. A new software, ENTROPY (Gompert *et al.* 2014), was recently developed to explicitly account for the uncertainty inherent in low-coverage reads. However, it is still largely unused by the community due to limited resources, which are currently available for only the more traditional approach, and the general difficulty of its execution. Here, we present a series of modules to facilitate ENTROPY runs and their post-analysis via the CLUMPAK tool. This offers an expansion on the supporting scripts already provided by ENTROPY, as it allows users to work with familiar programs contained in the CLUMPAK package. We applied these methods in studying *Rhagoletis* flies, which serve as model organisms for speciation-with-gene-flow. Through our analysis, we found that ENTROPY produces comparable population estimates to those of STRUCTURE. These findings are also consistent with alternative measures of population differentiation, such as differences in allele frequencies and hybridization rates. Specifically, there exists a substantial genetic difference between *R. pomonella* and the closely related undescribed flowering dogwood fly, but no such distinction is present between the apple- and hawthorn-infesting host races of *R. pomonella* itself.

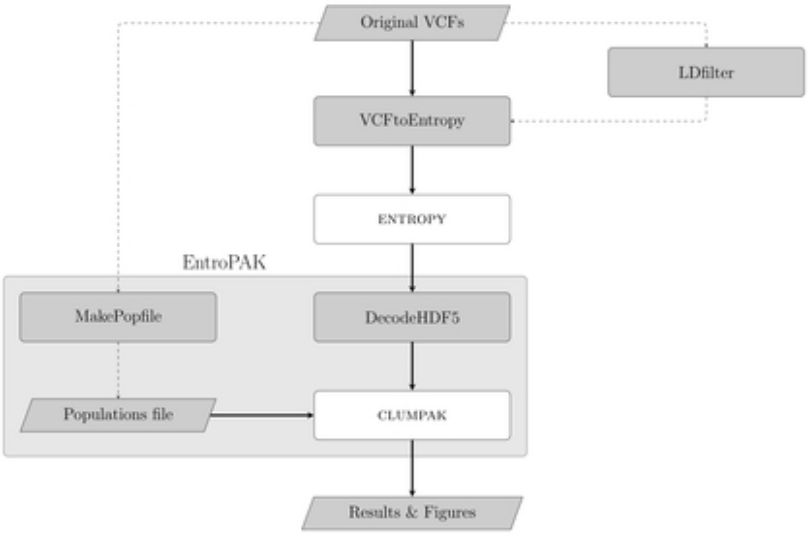

Figure 1: The main ENTROPY and CLUMPAK pipeline. Parallelograms indicate files and rectangles indicate modules; shaded modules represent novel programs; dashed arrows denote optional tasks.

Quantitative Analysis Using Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES) Reveal High Lead Contamination of Soil and Dust in Census Track 6, South Bend, Indiana (IN)

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Lead is a major environmental contaminant in the United States. Before the establishment of the Clean Air Act in 1996 and Consumer Product Safety Act in 1978, lead was introduced into urban soil through car exhaust from leaded gasoline and into homes through leaded paint. Lead poses a great threat to the health and wellbeing of children under seven. Studies have linked high childhood blood lead levels to exposure to lead contaminated soil and dust. Hence, it is critical to gain an understanding of lead level in soil and dust in the communities.

In this study, quantitative analysis of soil and dust collected from homes in census track 6, South Bend, IN were performed using ICP-OES to determine the levels of lead present. Soil and dust samples collected from homes and vacant lots were first qualitatively screened for lead using a portable x-ray fluorimeter. The lead contaminated samples were then prepared using the respective lead extraction assays for each sample type and analyzed using ICP-OES. Two lead extraction methods were derived from documents put out by the Environmental Protection Agency (EPA) and previous research done by Dr. Gabriel Filippelli from Indiana University. For each of the sample types, a comparison experiment was conducted to determine the appropriate extraction assay.

Over 70% of soil samples show lead levels over the 400 ppm EPA action level for lead contaminated soil, some of which show lead levels three to four times over the EPA regulation level. All of the dust samples qualitatively identified with lead have lead levels over the EPA regulation levels for the respective surfaces they were collected from. The results validate soil as a potential major source of lead contributing to childhood lead poisoning. It also shows that dust generated from lead sources at home such as leaded paint still remains a major health hazard for children.


HIGH-PURITY
STANDARDS
CRM-PC-B
0.5% Lead in Paint Chips
1201021
Opened
CRM-PC-A
0.1% Lead in Paint

Analysis of porosity, mineralization, and damage as contributors to fracture risk

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The fracture resistance of human cortical bone can become compromised by aging and metabolic bone diseases e.g., osteoporosis, due to the effects of altered remodeling on tissue composition e.g., mineralization and architecture e.g., porosity.

This study was carried out in order to understand the relative effects of bone tissue composition and architecture on human cortical bone fracture susceptibility. The objective of this study was to construct a computational model capable of predicting the fracture initiation point in human cortical bone based on the cortical porosity and increased levels of bone mineralisation, using finite element analysis. This predictive model may have future implications in the design of preventative medicines relating to bone diseases as well as in the identification of patients whom may be at increased risk of cortical bone fracture.

Physical bone specimens were subjected to micro-CT imaging prior to and after fatigue loading. Following on from a micro-CT based linear finite element modelling of the specimens, this study presents a nonlinear finite element model incorporating a Drucker-Prager yield criterion, linear hardening and element deletion.

A number of high stress specimen sub-volumes were selected on the basis of the linear finite element models for the various specimens. These specimen subsets were subjected to nonlinear finite element analysis. Using 2-point correlation functions it was shown, that for the specimens subjected to nonlinear analysis, there was a greater than random probability that the deleted elements were found to be spatially correlated to the damage volumes in the model.

This study also aims to generate 2-point correlation functions for additional bone specimens in order to further verify the results generated by the model. The experimental specimen fracture paths and the fracture paths predicted by the nonlinear finite element model for the various bone specimens tested will also be compared to ensure the integrity of the results obtained.

Targeted Asparaginase for Improved Treatment of Pediatric Leukemia

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Advisor: Matthew Webber, University of Notre Dame, College of Engineering, Dept. of Chemical and Biomolecular Engineering

Methods to treat acute lymphoblastic leukemia (ALL), the predominant form of pediatric leukemia, are constantly improving. Despite significant developments, ALL remains the leading cause of death for children in the United States. Furthermore, the treatment methods for ALL cause adverse side effects in children due to the toxicity and allergenicity of the therapeutic agents, and this is specifically problematic for a bacterially derived enzyme drug known as L-Asparaginase, a major component in treating ALL. The drug function of this enzyme arises through its catalysis of the reaction of L-Asparagine to ammonia and L-Aspartic Acid. Lymphoblastic leukemia cells lose the ability to synthesize L-Asparagine and thus rely on circulating sources of this amino acid for their survival. The enzyme depletes these circulating resources, contributing to cancer cell death. We have endeavored to endow L-Asparaginase with specific targeting units to improve its therapeutic efficiency and reduce its dose and allergenicity. Targeting the enzyme to cancer cells would localize enzymatic activity to the immediate vicinity of the cell, reducing local L-Asparagine levels without needing to act systemically. This would reduce the dosage needed to observe an effect. Antibodies are the most common method to facilitate biological targeting; however, due to their large size (MW ~150,000 Da), attachment of antibodies to a protein drug is not feasible. High affinity small molecule motifs with affinity comparable to that of an antibody to its antigen, on the other hand, could facilitate the required targeting using a minimal construct. Thus, we have explored routes to modify L-Asparaginase through bioconjugation for attachment of minimal supramolecular affinity motifs. Simultaneously, we are modifying tissue-specific labeling moieties with the complementary portion of these affinity motifs. Thus, a cell or tissue of interest could be labeled with one half of the affinity motif, which would subsequently serve to home the modified enzyme to this site through a supramolecular affinity axis. Ongoing studies will evaluate the potency of this targeting axis in vitro and in vivo.

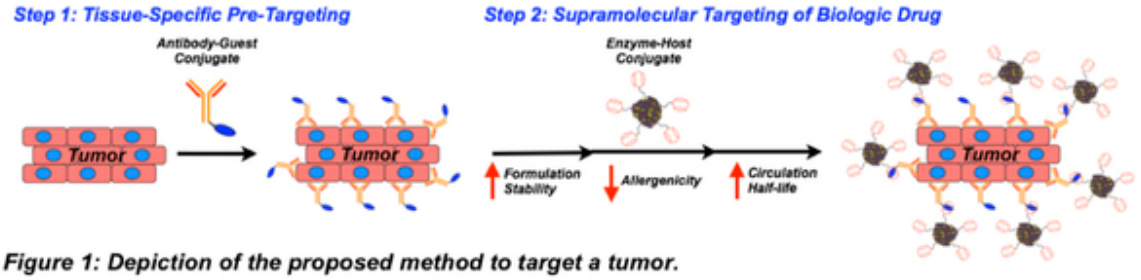

Figure 1: Depiction of the proposed method to target a tumor.

Synthesis of peptidic derivatives of 1,3,5-benzenetricarboxamide and investigation of their supramolecular-assembly

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Advisor: Matthew Webber, University of Notre Dame, College of Engineering, Dept. of Chemical and Biomolecular Engineering

Supramolecular self-assembly describes a process of molecular recognition and organization into defined structures using specific, directional, non-covalent interactions. Although individually the non-covalent interactions that give rise to supramolecular structures are weak, the summation of these inter¬actions can lead to materials with dynamic, responsive and highly tuneable properties. The benefits of supramolecular materials, arising from the versatility and control that these interactions provide, has resulted in a surge in research towards application in drug delivery, tissue engineering and regenerative medicine among many others. We are specifically interested in illustrating the utility of creating supramolecular biomaterials arising from the 1,3,5-benzenetricarboxamide (BTA) hydrogen bonding motif. Specifically, through appendage of peptides to the BTA core, it is our objective to create hydrogels which may be useful as biomaterials, and present bioactive cues to cells of tissues. Our efforts have focused on the development of proof-of-concept materials based on BTAsupramolecular interactions templating assembly of biocompatible peptide materials. BTA is a well-studied supramolecular motif that is proven to form long, helical fibers as a result of hydrogen-bonding between the amide functionalities of adjacent molecules. The directionality and strength of these interactions makes BTA a very reliable core for supramolecular materials. We are exploring crosslinking of these BTA fibers via secondary interactions between the adjacent peptides to form physically entangled hydrogels with tuneable and dynamic properties. The specific sequence of these peptides can be controlled, with the intention of altering both molecular stacking and interfiber crosslinking. We are furthermore probing alterations to the basic supramolecular motif by inclusion of urea (twice the hydrogen-bonding capacity) and triazole (no hydrogen-bonding capacity) in place of the amide in the core motif. Through this bottom-up molecular design, we hope to realize dynamic and tuneable biomaterials with rigid liquid-crystalline cores and pendant bioactive units.

[Re]Evaluating the Cost of Electricity in Hospitals with Unreliable Energy - VSL/E Metric

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Dept. of Physics

Dr. Moses Musaazi
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In the developing world, power outages add another constraint to healthcare facilities seeking to deliver quality healthcare that are already strapped for resources. The results of capacity shortages can range from postponing accurate diagnosis, due to failure of diagnostic equipment like x-rays, to more directly deadly results, due to failures of life-saving equipment such as ventilators. While analysis of such capacity shortages is abundant for regions throughout the developing world, there is, to the knowledge of these authors, currently no analysis that connects capacity shortages to effects on human life. Since what policy makers and health officials alike use as a metric for determining which policies and programs will be effective is morbidity and mortality, elucidating this link between power outages and the direct burden on patients is necessary to demonstrate that policies to minimize power shortages are necessary. We do this by modeling current data and adding in value of a statistical life according to the region the data was taken from. The cost-effectiveness of these programs is then demonstrated by simulating what locally designed and constructed generators would cost and comparing that the amount of money that a government would traditionally spend to save a statistical life. Over Summer 2017, I traveled to Uganda and implemented this analysis at another two health clinics. Preliminary results are additionally included in this presentation.

Development of a yeast biosensor for prednisone detection

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Advisor: Don W. Paetkau, Ph.D., Saint Mary's College, Dept. of Biology, Notre Dame, IN

Substandard, spurious, falsely-labelled, falsified, or counterfeit (SSFFC) drugs are a problem worldwide. Ayurvedic medicines can also be falsified by the addition of allopathic pharmaceuticals, such as steroid hormones, in order to convince consumers of the effectiveness of the ayurvedic medication. Therefore, a cost-effective detection method for the presence of added pharmaceuticals in ayurvedic medications is needed. To address this problem, a *Saccharomyces cerevisiae* biological sensor was designed consisting of an analyte binding receptor, an analyte responsive promoter, and a reporter gene. A tetracycline responsive promoter/*LacZ* reporter gene system (pCM176) was tested with plate and paper X-beta-gal assays. The assays showed limited color production, required long incubation times, and used liquid nitrogen as a reagent. In order to improve on the pCM176 assay, the *Ade2* and *Mel1* reporter genes were tested for their visible color change production when activated by one of three analyte receptors (tetracycline, prednisone, or estrogen). PCR amplified fragments were designed to change the receptor, promoter, and reporter genes of the pCM176 plasmid. The *Mel1* gene showed good color development with a constitutive promoter in both X-alpha-gal plate and paper assays. *Mel1* was cloned into the pCM176 plasmid and successfully transformed into yeast. Cloning of the other systems is currently underway. In the future, these yeast strains will be lab tested in plate and paper assays, and the paper assays will then be field tested in Nepal.

Engineering Multifunctional Nanoparticles for Targeted Drug Delivery in Cancer

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Advisors: David Omstead, University of Notre Dame, College of Engineering, Dept. of Chemical and Biomolecular Engineering, and Basar Bilgicer, University of Notre Dame, College of Engineering, Dept. of Chemical and Biomolecular Engineering; College of Science, Dept. of Chemistry and Biochemistry

Most cancer drugs fail in clinical studies not because they are ineffective in killing cancer cells, but because they cannot be administered in doses high enough to destroy the tumor without dangerously harming the patient. One potential solution to this problem is to encapsulate anticancer drugs in liposomal nanoparticles that selectively target only cancer cells. These nanoparticles can then be attached to various ligands. The conjugation of ligands to liposomes enables active targeting of the tumor through specific binding to tumor-associated receptors. Here, we used a short peptide sequence as the targeting ligand, 'LPAM1pep'. This active targeting decreases the undesirable side effects due to non-specific toxicity, that non-targeted tissue and organs experience. Unlike other lab groups, we design the nanoparticles by synthesizing the targeting ligand as a lipid conjugate before purifying the product for nanoparticle preparation. The liposomal components can then be mixed at desired ratios during nanoparticle preparation. This method provides highly reproducible results with high purity compared to other nanoparticle preparation procedures.

We employed solid phase peptide synthesis to synthesize a lipid conjugate with the targeting ligand 'LPAM1pep'. Studies show that LPAM1 integrin is highly expressed in multiple myeloma cells, and its expression correlates with poor survival. We then employed High Performance Liquid Chromatography to purify the molecule. Prior to nanoparticle preparation, we conducted a binding study using fluorescent labeled LPAM1pep at different concentrations to IM9 blood cancer cells. The results were analyzed using Flow Cytometry. We then prepared the nanoparticles using the same targeting ligand sequence LPAM1pep and delivered it to the cancer cells. These results demonstrate the potential of LPAM1 ligand-targeted liposomes to specifically target multiple myeloma cancer cells and enhance anticancer activity.

Electrochemical Nitrite reduction using Earth abundant based catalysts

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Nitrite is a common drinking water contaminant, especially in areas with significant agriculture. Nitrite has been implicated in methemoglobinemia in infants, a condition wherein cells throughout the body are deprived of sufficient oxygen. Currently, ion exchange is the primary treatment method, however disposal of the waste brine is environmentally and economically expensive. Noble metals based catalysts (e.g. platinum and palladium) are used for electrochemical reduction of nitrite, but they are prohibitively expensive for widespread adoption. The use of Earth abundant based catalysts for nitrite reduction could significantly lower the cost and waste production generated by the treatment processes of drinking water. The purpose of this investigation is to obtain Earth abundant based catalyst with high activity for the removal of nitrite from drinking water. Examples of Earth abundant based catalysts studied in this investigation were molybdenum, iron, nickel, ruthenium and titanium. Thin films of the catalyst were applied to various conductive substrates, like Fluorine-doped tin oxide (FTO), carbon paper and nickel films, by dropcast method using catalyst suspension with varying components ratios of catalyst binder, and solvent. The resulting thin film electrodes were tested for physical stability and analyzed for electrochemical activity for nitrite reduction by cyclic voltammetry. Results of these tests indicate that using carbon paper as a substrate will make the catalyst on the film more stable and more conductive. When using FTO as a substrate only a few catalyst were stable (iron -nickel sulfide and titanium dioxide), but had less conductivity compare to carbon paper as substrate. An anticipated outcome of this project is to obtain electrocatalytic films made of Earth abundant based catalysts with good activity and stability. If the outcome is achieved, this project will contribute to the development of sustainable water treatment technologies. Further studies could expand this technique to nitrate removal, as well as integration as a new technology for drinking water treatment.

Using Optical Character Recognition to Assess Differential Treatment

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Data is an essential input for social science research. However, data is often contained in physical documents that are difficult to analyze. One data collection technique that is becoming more prevalent is optical character recognition, a tool that converts physical documents into electronic text. In this project, we use optical character recognition to build a database that will be used to assess whether certain papers, authors, or topics receive differential treatment at the American Economics Association's annual meetings. To build this data set, we first used software to extract the text from each meeting's program, a physical book that contains meeting times, meeting rooms, presenters, and paper topics. We then manually removed unnecessary text portions from the extracted text. After removing unnecessary text portions, we generated lists of rooms, times, presenters, and topics that can be tabulated and analyzed. Through this application, we find that optical character recognition is a valuable data collection tool for social scientists.

Self-assembly of amphiphilic tripeptides and their peptoid analogues

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College of Engineering
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Advisor: Matthew Webber, University of Notre Dame, College of Engineering, Dept. of Chemical and Biomolecular Engineering

Supramolecular biomaterials enable formation of a variety of nanostructures and properties. Peptides specifically offer an assortment of self-assemblies with numerous biomedical applications. Previously, we have established a library of amphiphilic tripeptides (peptides comprised of three amino acids) that form a diversity of nanostructures and gels. Contrary to most self-assembling hydrogels, near UV circular dichroism and infrared spectroscopy on the peptide gels show minimal signs of common secondary structures (i.e. beta sheets). In order to probe the importance of these interactions to self-assembly, we developed analogous 'tripeptoids' to analyze how peptoid interactions compare to peptide interactions and the importance of hydrogen bonding in the peptide hydrogels. Peptoids are peptidomimetic polymers comprised of N-substituted Glycines that are not found in nature. Though they have a similar structure to peptides, peptoids have a side chain on the nitrogen rather than the alpha carbon. This minimizes hydrogen bonding as well as degradation by proteolytic activity in vivo. Using solid phase sub-monomer synthesis with a sequence of SN2 reactions with bromoacetic acid for the carboxyl group and primary amines for the side chains, we synthesized our family of analogous tripeptoids. These peptoids were are unable to form hydrogels however, they did form nanostructures similar to those of their peptide analogues. This suggests that the minimal amphiphilic tripeptides were able to form self-supporting hydrogels without significant presence of hydrogen bonding.

Synthesis of Novel Oxazoline Compounds for Use as Insecticides and the Evaluation for Mosquitocidal and Larvalcidal Activity

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Dept. of Biological Sciences

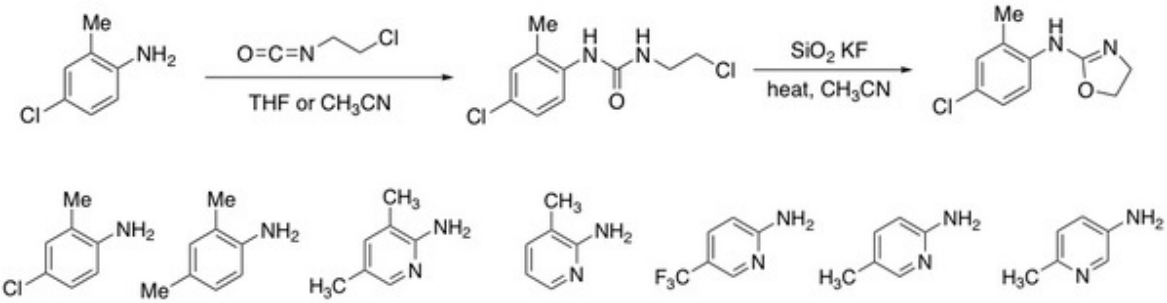
Douglas Shoue
University of Notre Dame
College of Science
Dept. of Biological Sciences

Elizabeth Whidden
College of Science
Dept. of Biological Sciences

Olga Nushtayeva
College of Science
Dept. of Biological Sciences

Advisors: Mary Ann McDowell, University of Notre Dame, College of Science, Dept. of Biological Sciences and Bruce Melancon, University of Notre Dame, College of Science, Dept. of Chemistry and Biochemistry

The extreme rise of vector borne infectious diseases such as the Dengue and Zika viruses have become an increasing threat to global health. While these diseases have been around for quite some time, especially in third world nations, there have been increasing issues with combating these specific diseases. The mosquitoes that carry these diseases have recently become more resistant to the pesticides on the market. Many therapies used to combat the diseases are expensive and may be hard to supply in the field, and some may have some serious side effects. Apart from yellow fever, there are no vaccines on the market for vector transmitted diseases. Ultimately, our goal as a lab is to create insecticides that can combat the resistant misquotes. To do this we are taking known compounds and making analogs them. These compounds specifically target a receptor in the mosquito that is required for movement and reproduction. The receptor targeted is an octopamine receptor, which is a G-protein coupled receptor that in present in invertebrates but not vertebrates. Prior literature proved that the protein had been targeted by oxazoline insecticide molecules which showed effectiveness against aphids and mites. Using the oxazoline synthesis as a framework, we purposely altered the chemical structures we believe that may affect the interaction and conformational change that occurs in the octopamine receptor, and synthesized seven novel oxazoline compounds. The purity of the compounds was assessed using analytical techniques such as, LC-MS, TLC, and 1H-NMR. The newly synthesized compounds will be tested through in vitro and in vivo assays. We believe that since the oxazolines act as an octopamine agonist in aphids and mites, novel derivatives of 2-aminooxazolines could have some mosquitocidal activity through adult contact assays and may also have larvacidal activity.


Me
NH2
Cl
O=C=N
Cl
THF or CH3CN
Me
H
N
H
N
Cl
O
Cl
SiO2 KF
heat, CH3CN
Me
H
N
N
O
Cl
Me
NH2
Cl
Me
NH2
Me
CH3
NH2
H3C
N
CH3
NH2
N
NH2
F3C
N
NH2
H3C
N
NH2
H3C
N

A new approach for alignment-free comparison of temporal networks

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Network comparison (NC) has important applications in many domains. NC can be of two types: alignment-based or alignment-free. Alignment-based NC aims to identify a mapping between nodes of compared networks in a way that maximizes the amount of conserved structure between the networks. Alignment-free NC aims to quantify the topological similarity between compared networks without accounting for any node mapping between the networks. Our focus is on alignment-free NC. Graphlet Correlation Distance (GCD) is a leading method for comparing static networks in alignment-free fashion. However, real-world networks are typically not static, as they evolve with time. So, how to compare evolving (temporal) networks? A straightforward way is to model temporal networks in a static manner and then apply established static NC methods to the resulting static networks. For this, each temporal network is either aggregated into a single static network, or into a series of snapshots, where each snapshot is an aggregated static network corresponding to a specific window of time. In both situations, while GCD could be applied to aggregated versions of the compared temporal networks, valuable temporal information would be lost, and clearly, a better solution is needed. GCD is based on static graphlets (small subgraphs, i.e., basic building blocks of complex networks). Since dynamic graphlets were introduced recently, we generalize static GCD that relies on static graphlets into its dynamic counterpart that relies on dynamic graphlets. Then, we propose the resulting approach, dynamic GCD, as a state-of-the-art method for comparing temporal networks in alignment-free fashion. We evaluate dynamic GCD on different types of synthetic temporal networks from biological and social domains and compare it to static GCD used on aggregated versions of the temporal networks. We measure the ability of the methods to accurately identify networks of the same synthetic network type (i.e., belonging to the same random graph family) as topologically similar and networks of different synthetic network types as dissimilar. We evaluate method accuracy in comprehensive precision-recall and ROC curve frameworks. We find that dynamic GCD outperforms static GCD in all evaluation tests.

Sensitivity and Uncertainty analysis of Ground Water model Replacement TimML

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Surface water and groundwater models have typically been developed separately, and additional approaches for building coupled models at regional scales are needed to assess the effects of climate variability and change, land use change, biogeochemical, and anthropogenic scenarios on water quantity and quality in areas like the Midwest that depend heavily on both surface and groundwater resources. Previous research was focused on the development of a coupled surface water / groundwater hydrology model which integrates groundwater recharge simulated by the macro-scale Variable Infiltration Capacity (VIC) (Liang et al., 1994) hydrologic model into the GFLOW analytic element groundwater model. The spatially explicit hydrologic model is applied to a lake-rich region in northern Wisconsin and Michigan to quantify the groundwater and surface water inputs to the many lakes that are present. The spatially explicit hydrologic model is applied to a lake-rich region in northern Wisconsin and Michigan to quantify the groundwater and surface water inputs to the many lakes that are present. Due to the GFLOW proprietary software being limited to the Window OS, the integrated model is incompatible with the CRC's distributed system, which is native to the Linux OS. The Model's limitation to the Window OS is the cause of the long-time steps required for the model to successfully complete a small number of lake simulations. Our current research is focused on sensitivity and uncertainty analysis of the open-source module TimML, which is also an analytic element groundwater model that is also portable to the Linux OS.

Synthesis of ^{13}C-Labeled Methyl α- and β-D-Arabinofuranosides and Studies of Ring Conformational Equilibria Using Redundant NMR Spin-Couplings and Circular Statistics

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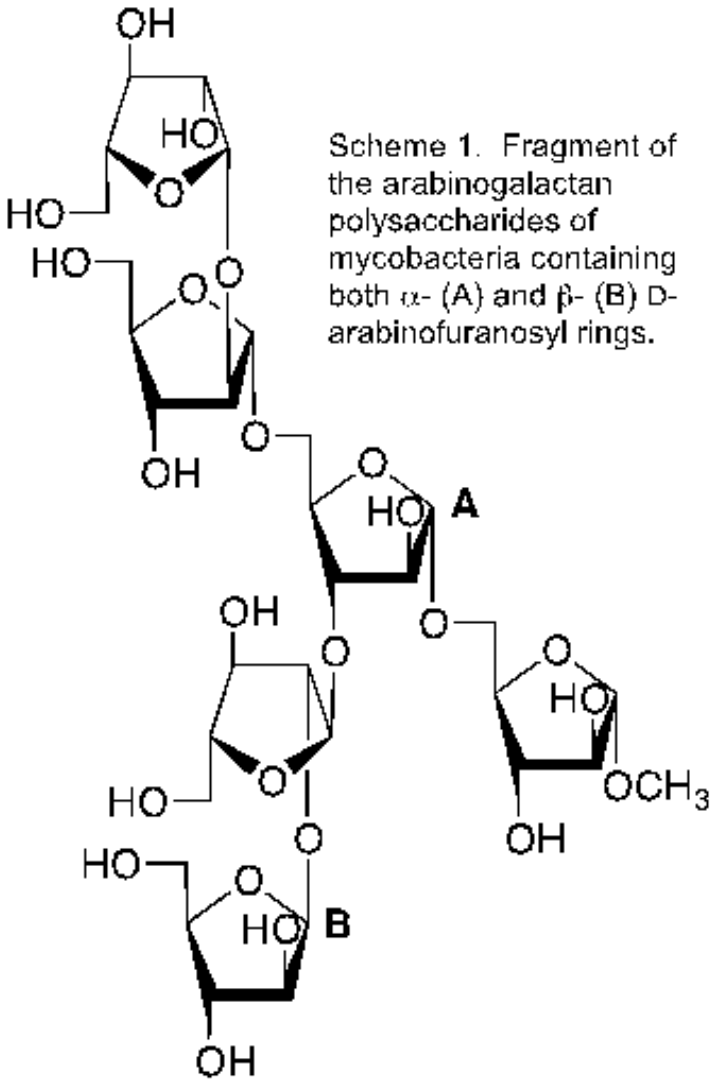
Five-membered ring (furanose) forms of D-arabinose and D-galactose are common constituents of bacterial polysaccharides (Scheme 1), and interfering with their biosynthesis is a potential strategy for antibacterial drug development. Current experimental methods to determine the conformational properties of these furanose constituents are incapable of providing explicit conformational models in solution. However, recent application of circular statistics to redundant NMR spin-coupling analysis by the Serianni lab yields conformational models of flexible carbohydrate domains. This approach will be applied to simple arabino- and galactofuranosyl rings in anticipation of studies of more complex oligosaccharides.

D-Arabinose (200 mg) was dissolved in anhydrous methanol (20 mL), dry Dowex 50-H^+ ion-exchange resin (550 mg) was added, and the reaction mixture was incubated at 80°C. A reaction time of ~1.5 h gave a mixture containing ~53% α-furanoside, ~24% β-furanoside, ~9% α-pyranoside, and ~14% β-pyranoside. Purification on a Dowex 1 × 8 (200–400 mesh) ion-exchange column (2 cm x 15 cm) in the OH- form (~2.5 mL/min, 15 mL fractions) gave the following: α- and β-pyranosides, fractions 3–5; β-furanoside, fractions 9–13; α-furanoside, fractions 26–45. The purified glycosides were analyzed by 1H and 13C NMR to confirm structure and purity (~98% for both furanosides). The procedure was repeated with D-[1-13C]arabinose, D-[2-13C]arabinose, D-[3-13C]arabinose, and D-[5-13C]arabinose, giving pure singly 13C-labeled methyl α- and β-D-arabinofuranosides in 20–50 mg quantities. Efforts are underway to extract $J_{[\sim HH]}$, J_{CH} and J_{CC} values from ^{1}H and ^{13}C{^{1}H} NMR spectra of these products, and to derive equations from density functional theory (DFT) calculations to model the *J*-values. With these results, the *MA'AT* program will be used to model the conformational properties of methyl α- and β-D-arabinofuranosides in solution, and the resulting models will be compared to those derived from aqueous MD simulations. Parallel investigations are also underway for methyl α- and β-galactofuranosides.



Scheme 1. Fragment of the arabinogalactan polysaccharides of mycobacteria containing both α- (A) and β- (B) D-arabinofuranosyl rings.

ZnO and CdSe Dual-Emission Ratiometric Probe for the Detection of Organophosphonates

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Detection of hazardous organic chemicals from air and water remains a major challenge. Chemical warfare agents, toxic industrial chemicals, and explosives such as organophosphonates have received great attention. A ratiometric fluorescence probe based on semiconductor and metal oxide nanoparticles can sense organophosphonates, such as dimethyl methylphosphonate (DMMP), and visibly change to indicate the presence of these molecules. These probes can then be used for real-time, on-site determination of low levels of DMMP. The probe is comprised of a zinc oxide (ZnO) nanoparticle encapsulated in silica ($ZnO@SiO_2$), bound to a cadmium selenide (CdSe) semiconductor quantum dot. Upon detection of DMMP, the $ZnO@SiO_2$ will continue fluorescing, whereas the CdSe quantum dot's fluorescence will be quenched inducing an observed color change. In this way, the change of fluorescence emission due to the quenching of the quantum dot will be visible to the naked eye.

Geochemical and isotopic evolution of carbonatites in Magnet Cove Complex in Arkansas

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Carbonatites are mantle-derived igneous rocks containing more than 50% carbonate minerals (e.g., calcite – CaCO3) often associated with continental rift regions. Carbonatites are known for their high concentrations of Sr (~7000 ppm) and rare earth elements (REEs) which can be directly linked to our understanding of mantle and geochemical processes. Petrogenic investigations using radiogenic isotope systems, such as Sr and Pb, may provide valuable insights with regards to the age and chemical nature of the mantle source giving rise to the carbonatite melts. Moreover, examining the distribution and abundances of REEs can provide critical information relative to the crystallization history of the magma, and degree of enrichment of the mantle source region. Examining the isotope signatures of carbonatites from the Magnet Cove Carbonatite Complex in Arkansas using a variety of micro-analytical techniques. Chemical maps demonstrating the major element composition of the samples were generated using micro-X-ray Fluorescence (μ-XRF), trace elements concentrations were collected using Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS), and isotope ratios were determined by Multi-Collector (MC-ICP-MS). REE signatures and both Sr and Pb isotopic ratios from Magnet Cove were compared to those from previous studies of similar-aged carbonatite from the Oka Complex in Québec, to better understand the scale of mantle processes (regional or continent-wide) . In general, the 87Sr/86Sr ratios (~0.7035 to ~0.7036) from Magnet Cove are higher compared to Oka carbonatites. The Pb isotope ratios from Magnet Cove carbonatites are less radiogenic compared to those from Oka. These results can be attributed to several processes, such as mixing of multiple mantle sources, mantle metasomatic activity, or crustal contamination. Our preferred model involves the participation of multiple mantle sources for the generation of carbonatites at Magnet Cove; however, crustal contamination cannot be ruled out.

Detecting Human Eye Movements from Infrared Cameras

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During the rehabilitation process for people that have undergone neurotrauma, a key assessment clinicians use is the analysis of a subject's balance. Lateral weight shifting is a task done by patients that is more challenging than quiet standing but does not require full walking capability, so it often provides useful data to analyze. This task requires the ability to adjust one's posture to control the position of one's center of gravity (COG). Directly correlated with the COG is the center of pressure, which can be easily measured with force transducers to detect weight shifts. The Locomotion and Biomechanics Lab at the University of Notre Dame uses the transducers in the inexpensive Nintendo Wii Balance Board for this purpose. Using the Balance Board, visual feedback can be adjusted to enhance the speed of learning of subjects who practice weight shifting with the device. Unfortunately, the only measure of how effective the feedback can be is the performance of each subject. The attention of each subject to the feedback is entirely unknown, despite that piece being increasingly important as the amount of feedback manipulation increases. In order to record the attention of someone performing visually guided weight shifting, eye tracking is required, but many methods require a user's head to remain still. To account for this, a wearable headset was developed to allow movement from the user while still recording where the user was looking. A device was built to be worn like glasses that record the general field of vision of the user in addition to the pupil movements of the user to pinpoint an accurate spot where the user is focusing.

Big Data & the Big Five: Computationally Predicting Personality and Psychopathology from Social Media

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The present study is designed to explicate the social media correlates of mental illness—specifically, personality disorders. Using the resources of the Center for Research Computing, an IRB-compliant, web-based data collection framework is being developed and tested to efficiently store structured and unstructured data from social media. Further, recruitment of a large Internet sample through targeted Facebook advertising, crowdsourced online platforms, and the promise of personalized feedback is ongoing. Measures of personality and psychopathology will be evaluated against participants' verbal and nonverbal Facebook and Twitter activity. Emerging computational social science models will be explored to assess personality using closed, open, and nonverbal approaches. Normal personality has been shown to be highly predictive of mental illness and has recently been examined to explicate the structure of personality disorder (Wright & Simms, 2016). Indeed, the hierarchical model of normal personality has been integrated by researchers to form a consensual model for abnormal (i.e., pathological) personality (Watson, Stasik, Ro, & Clark, 2013; Wright & Simms, 2014). Nevertheless, to our knowledge, no study has broadly examined personality pathology in an online context. We argue that the strength of normal and abnormal personality's integration in the literature is indicative of abnormal personality's detectability in online social networks. Further, the assessment of normal personality from social media activity stems from the criterion of personality's persistence over different contexts and one's lifespan—this is how personality can be objectively traced through social media activity instead of personality self-reports. In parallel fashion, the longitudinal nature of social media data is ideal for the detection of pathological personality, which correspondingly persists across varying contexts and time periods.

Utilizing the Cannon to Predict Stellar Parameters

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The Cannon is a data driven analysis tool designed to predict stellar parameters based on a transfer of “stellar labels” from external datasets to large-scale spectral catalogues. The prediction of stellar parameters such as metallicity ([Fe/H]), effective temperature (Teff), carbon abundance ratios ([C/Fe]), and surface gravity (log g) will enable users to focus their attention on interesting stars which meet their criteria. Synthetic normalized spectra were used as the reference set to properly calibrate The Cannon for the test sets. In future work The Cannon will be applied to stellar spectra collected by the Sloan Digital Sky Survey (SDSS), the Large Sky Area Multi-Object Fiber Spectroscopic Telescope (LAMOST), and others. Comparison of the suggested stellar parameters from The Cannon with alternative approaches, such as the non-SEGUE Stellar Parameter Pipeline (n-SSPP) will greatly reduce the time required to obtain confident estimates.

Comparing Tree-Based Models' Variable Predictions for School Crime

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School safety in the United States continues to be of a high-priority for parents, school employees, and government officials. The Department of Education assists in measuring the safety of its students through the bi-annual Crime and Safety Survey (CSS). A large dataset such as this can report unstructured and messy data that is often difficult to interpret when looking for patterns in criminal and problematic activity. Data-mining techniques can be beneficial with organizing these datasets and bringing clarity to important factors that can predict outcomes. This project compares two data-mining models, random forests and multivariate tree-boosting, and their ability to consistently predict variables highly related to two different outcome variables: the frequency of student racial/ethnic tensions and the frequency of student gang activities. Three models, two random forest models and one multivariate tree-boosting model, were constructed to measure the two outcome variables. Each model was run six separate times and the top 25 variables reported to have high importance on the outcome variables were noted. Prediction accuracy was measured by the model's ability to reproduce the same variables that were predicted in the initial trial run. The random forest models resulted in an average of 98% prediction accuracy and the multivariate tree-boosting model resulted in an average of 94.55% prediction accuracy. When the different models' were compared to each other, they shared 69.99% of the same variables related to racial/ethnic tensions and 78.66% of the same variables related to gang activities. These findings reveal that each method is highly reliable with reproducing the same predictor variables that are correlated to the outcome variable.

Field-testing of the MicroBio PAD: Detection of fecal contamination of water in Nepal

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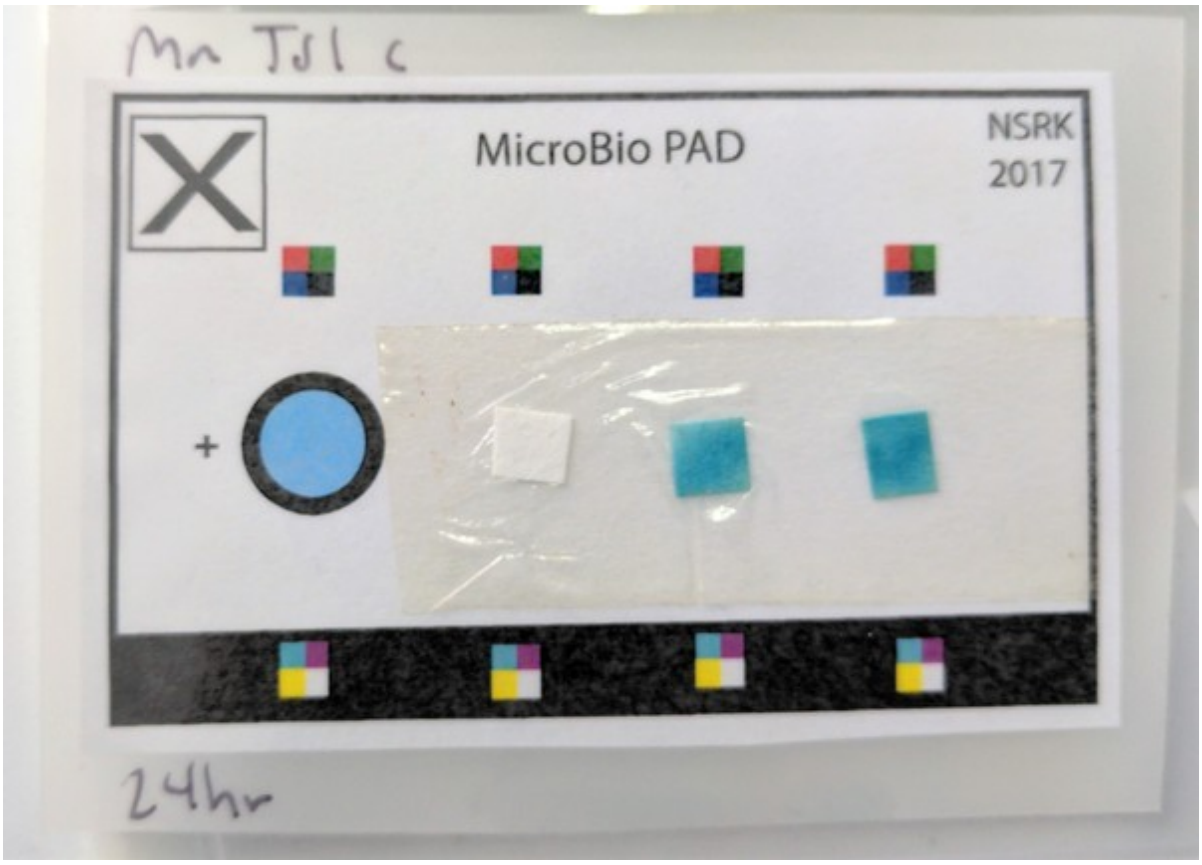
Microbial contamination of water is a significant problem in developing and developed countries causing a serious impediment to public health. In order to develop a user-friendly, rapid, and economical method for detection of indicator bacteria *Escherichia coli* in water, a paper-based microbiological analytical device (MicroBio PAD) was previously created and tested in the laboratory at Saint Mary's College. The purpose of this study was to conduct a field-testing of the device in detecting microbial contamination of water sources in Nepal. Thirty-six water samples were collected from three different locations along four rivers in Nepal (Bagmati, Bishnumati, Manohara, and Rapti) in addition to twenty-four tap/pump water samples. The samples were subjected to the MicroBio PAD test along with the "gold standard" test for the detection of *E. coli* in water, the Most Probable Number (MPN) test. Water samples were enriched in 2X Lauryl Tryptose Broth with vancomycin, then screened on the MicroBio PAD, which consisted of filter paper impregnated with X-Gal. Presence of *E. coli* in the sample was indicated by production of blue/green color on the paper. The MPN test was completed following the standard protocol. Results of the MicroBio PAD test indicated presence of *E. coli* in 31 river water samples and 2 tap/pump water samples. The most probable numbers of *E. coli* ranged from <3.0 to >1100 per mL in the river water samples along with the tap/pump water samples tested. The MicroBio PAD accurately detected *E. coli* in 86.8% of the samples that were shown positive by the MPN method. Further optimization of the MicroBio PAD is needed to increase the sensitivity and quantify the color production.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In Membrane Exploitation of Antigen/Antibody Interaction for Selective Purification and Quantification of Therapeutic Monoclonal Antibodies

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Currently there are almost 40 therapeutic monoclonal antibodies approved for the treatment of a variety of diseases. These drugs are known for their efficiency in treatment due to their high selectivity; however, they are expensive to produce, and their effectiveness varies based on concentration in the patient's bloodstream. Because of these issues, there arises a necessity for technology that provides cheaper and faster purification of antibodies during drug production, as well for technology that rapidly tests antibody concentrations in the bloodstreams of patients. In this lab, these problems are addressed using membranes modified with mimotopes, antigen like peptides, which selectively capture antibodies from solutions. The captured antibodies can be eluted as a purified product, or analyzed to determine the original concentration. While this membrane system has been successfully tested with the antibody Herceptin and its mimotope (K19), the system needs to be extended to additional therapeutic antibodies. Therefore, we tested whether the system successfully extends to the antibody Avastin and its mimotope (A19). However, the conformation of A19 varies greatly depending on small changes in pH which leads to significant amounts of non-specific binding. These conformational issues led to difficulties capturing Avastin, and the leaching of non-specifically bound A19 caused difficulties determining the amount of Avastin capable of being captured. The data collected thus far indicates that a different mimotope for Avastin may be more successful in binding large quantities of Avastin in a membrane.

Deep Neural Networks for Reconstructing Particle Collisions

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In an effort to better understand the fundamental particles of our universe, scientists at the Large Hadron Collider at CERNcollide protons traveling near the speed of light and make observations about their interactions. These collisions occur 40 million times per second and generate petabytes of data annually, making this experiment the quintessential big data problem in terms of velocity and volume. Despite the magnitude of data produced by the accelerator, not all of it is of particular interest to researchers. In fact, the most significant collisions only make up a small fraction of those recorded and are difficult to differentiate from less interesting ones. The challenge of discerning meaningful collisions arises because particles of interest, like the top quark and Higgs boson, decay before they can be detected. Scientists are left to use the daughter particles of a collision to to make inferences about the intermediate particles produced. Ambiguity surrounding the measurement of daughter particles in jets, which parent particle they are attributed to, and the inability to detect neutrinos adds further complexity to the problem. Advancements in using deep neural networks for image recognition and natural language processing have proven their ability to handle complicated problems, thus inspiring their application to particle physics. Using these multilayer neural networks could be helpful in accurately reconstructing collisions and distinguishing exotic ones from trivial ones. This project explores hyperparameters for multilayer networks, in particular the number of layers and the number nodes in each layer, to determine which options work best for reconstructing complex collisions.

Analysis in Energy Systems for Smart Grid Control using Multiple Storage Devices

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A FFT analysis of yearly power loads and sources data results in unexpected key frequencies. These unique frequencies correspond to specific storage devices. This analysis demonstrates the need for hybridization of energy storage devices for optimal control of a smart grid. Furthermore, the juxtaposition of the FFT analysis of energy sources and loads yields a straightforward discussion about the disconnect between loads, storages, and sources. Unlike other research focusing on energy sources and/or power loads with one or two storage devices, this research demonstrates the superiority of an energy systems based approach to storage over a component-based approach. Future smart grids must include hybridization of storage to deal with noise versus vital system behavior and this FFT analysis seems promising moving forward.

Algal Biodiesel Conversion and Characterization for use as Decentralized Electrical Energy in Uganda and Notre Dame

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In Uganda, fewer than 80% of people have access to electricity, and those that do only have access to unreliable electricity that regularly shuts off for hours at a time. We explore the conversion of lipids in algae to useable biodiesel as a source of electrical energy when run through a diesel generator. While previous research focuses on creating industrial-scale models of biodiesel conversion from optimal lipid-producing algal species, this research aims to produce decentralized energy from readily available, on-site resources and indigenous organisms in Uganda and Notre Dame, Indiana. Using various extractions, percent lipid composition of dry biomass from Ugandan algae from Crater Lakes and Lake Victoria and Notre Dame algae from St. Mary's Lake was determined. After esterification of lipids, the fatty acid methyl esters (FAME) produced were run through gas chromatography-mass spectroscopy (GCMS) and compared to marine FAME standards to characterize the potential for their use as biodiesel. This is significant because these strains of algae have never been characterized for use as biodiesel. The conversion of Ugandan algae to biodiesel could be a step towards developing more reliable electricity options in Uganda. Finally, as more US colleges and universities strive to implement sustainable energy options to replace existing coal consumption, characterization of St. Mary's Lake algae as biodiesel could provide a local green energy alternative for the University of Notre Dame to reduce its reliance on coal.

Phase Inversion Membrane System for Heavy Metal Absorption

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As sustainable, reliable sources of fresh water become increasingly valuable, numerous technologies have been developed to abate the harmful effects of heavy metal contamination. Of these technologies, membrane filtration is especially advantageous in its ability to operate continuously on polluted water. This study examines the use of high-permeability, block-copolymer phase inversion membranes for lead(II) and cadmium(II) absorption. Using the non-solvent induced phase separation (NIPS) process, a solution of polysulfone (PSF) and polystyrene-poly(acrylic acid) diblock (PS-PAA) is casted under humidified conditions to yield membranes with permeabilities in the range of 8,000 to 14,000 L m^{-2} h^{-1} bar^{-1}. The carboxylic acid moiety of the PAA block allows quick and efficient “clicking in” of functionally diverse molecules via a carbodiimide coupling reaction. Known for their heavy metal coordination properties, the thiol moiety is introduced to the phase inversion membranes through the coupling of several small thiol containing molecules to the PAA block. FTIR spectra suggest that preliminary attempts at glutathione and cysteamine functionalized membranes are at least partially successful. Indeed, these membranes show Cd^{2+} binding capacities around 0.5 mmol/ g of p each. For the purpose of increasing the heavy metal binding capacity even further, high molecular weight branched poly(ethylenimine) (PEI) is coupled to the PAA block of the membranes via carbodiimide coupling, with the hope that a vast number of primary amines would remain available for further coupling to thiol furnishing reagents such as 2-iminothiolane and N-succinimidyl 3-(2-pyridyldithio) propionate. Current FTIRspectra reveals successful PAA-PEI coupling. If successful, thiol-containing, high-permeability phase inversion membranes would offer an energy efficient solution to the purification of heavy metal contaminated water.

Determination of Crucial Immunogenic Epitopes in Major Peanut Allergy Protein, Ara h2, via Novel Nanoallergen Platform

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Current methods for detection and diagnosis of allergies do not provide epitope specific immunogenic information and thus lack critical information that could aid in the prediction of clinical responses. To address this issue, we developed a nanoparticle based platform, called nanoallergens, that has the ability to multivalently display potential allergy epitopes in order to determine the immunogenicity of each IgE binding epitope. We synthesized nanoallergens that present various epitopes from the major peanut allergen, Ara h2, and directly determined the immunogenicity of each epitope, alone and in combination with other epitopes, using patient sera. This data revealed which epitopes are most critical for physiological responses to Ara h2 and the importance of both thigh and low affinity epitopes for allergic responses. Therefore, this nanoallergen platform can provide more detailed information on patient-specific allergic reactions and potentially aid in more accurate diagnosis and personalized treatment options.

Self-Medication in Long-Tailed Macaques (*Macaca fascicularis*)

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Malaria is the deadliest parasitic disease of humans, and kills more than half a million people annually. The evolution of drug resistance by its causative agents, *Plasmodium* spp., has hindered control of this disease, and created a need for new anti-malarial drugs capable of combatting resistant malarial strains. Medicinal plants have served as a source of such drugs in the past, but the number of potential candidates make promising targets hard to find. Self-medication by non-human primates may help to highlight potential chemotherapeutic agents, however this phenomenon is poorly understood. While non-human primates have been shown to consume a range of plants with pharmacological activity, the relationships between these behaviors and actual disease state remain unexplored. Long-tailed macaques (*Macaca fascicularis*) are infected by a wide range of *Plasmodium* spp, some of which zoonotically infect humans. Here, we utilize a series of molecular approaches to examine the relationships between *Plasmodium* spp. infections and medicinal plant consumption in long-tailed macaques. Macaque diet and *Plasmodium* infection status were assessed using data from an 18S amplicon on DNA from macaque feces. A thorough review of literature on medicinal plants of Southeast Asia led us to identify four botanical genera of interest in these data: *Artemisia, Diospyros, Panari,* and *Psychotria*. We found that *Parinari* spp. were significantly positively associated with *Plasmodium* spp. read count. To facilitate further exploration of this relationship, we began the process of developing diagnostic primers for the presence of this plant and *Plasmodium* spp. infections. If effective, our methods may provide a low-cost tool for the study of self-medication in macaques and other non-human primates.

CNVis: A Web-Based Visual Analytics Tool for Exploring Conference Navigator Data

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Pontificia Universidad Cat´olica de Chile

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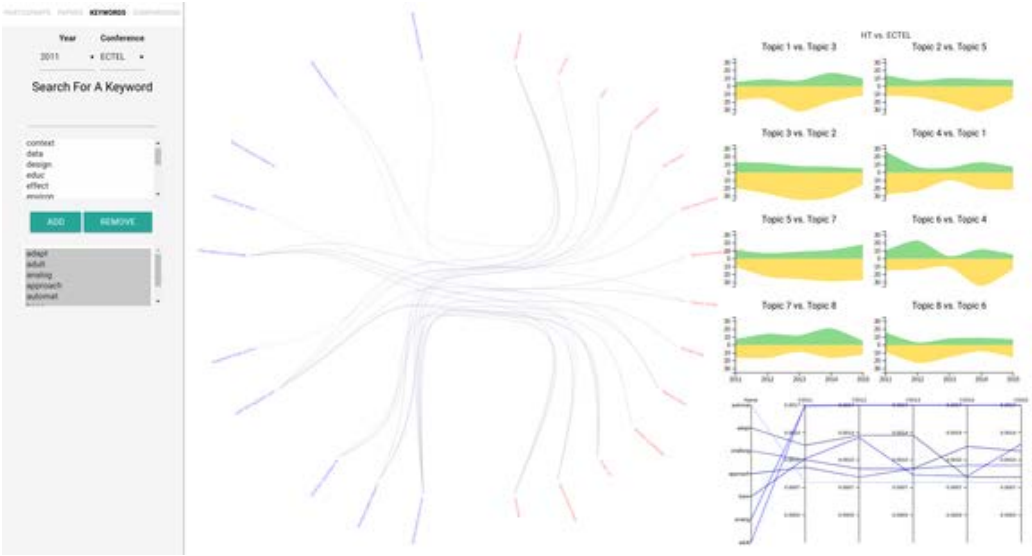
We present CNVis, a visual analytics framework for exploring data from one or more academic conferences, mainly consisting of the papers presented and participants bookmarking papers at said conferences. The framework aims to interpret various conference relationships and trends via comparison and recommendation using three coordinated views (bookmark, keyword, and topic). The bookmark view allows users to view, for a given conference of a year, the relationship between the papers presented at the conference and the participants who bookmarked them. The keyword view enables the viewing of keyword popularity and their trends over the years for a given conference, either by selecting a specified subset of keywords or selecting one or more papers and viewing their associated keywords. The topic view allows for comparison of paper topic areas, either in one or between two different conferences, to reveal the overall conference trends. We demonstrate the effectiveness of this framework using real-world data from three unique conferences over a five year period. Finally, we discuss the areas of expansion and the generalizability for CNVis.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Topic 5 vs. Topic 7
Topic 6 vs. Topic 4
Topic 7 vs. Topic 8
Topic 8 vs. Topic 6

Making the Grade: Change in Social Network Diversity Among First-Year Notre Dame Students

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Encouraging and increasing the diversity of student populations is a goal that many colleges and universities around the United States wish to achieve. To understand overall diversity, it is crucial to examine diversity at an individual network level, and to especially examine how student social networks change during their time in college or university. Do these networks become more diverse throughout a student's four years, or less so? To understand these individual student dynamics more, network surveys taken from a larger study called the NetHealth Project, which concerns the connection between the social ties of University of Notre Dame students and their activity and sleep levels, were analyzed. Students were asked both before they arrived at Notre Dame and then twice after they arrived to list the people with whom they interact and to provide basic demographic information on their contacts. The racial and religious composition of the ego networks of each student are examined at three time points: before arrival, at the end of the first semester and at the end of the second semester. The results show that between high school and college, the composition of a typical student's network became less diverse in terms of both race and religion and that the composition of people's networks is biased towards people of the same race and/or religion Comparing the Fall 2015 and Spring 2016 networks indicates, however, that there is a partial reversal in this trend as students start having more friends who are different than they are. These results imply that with the transition to college, student networks tend to become more homogenous as students choose friends who are similar to them, but that this tendency may dissipate to some extent as students' networks change. More data from more colleges needs to be collected in order to determine whether these processes are unique to Notre Dame or a more general phenomena.

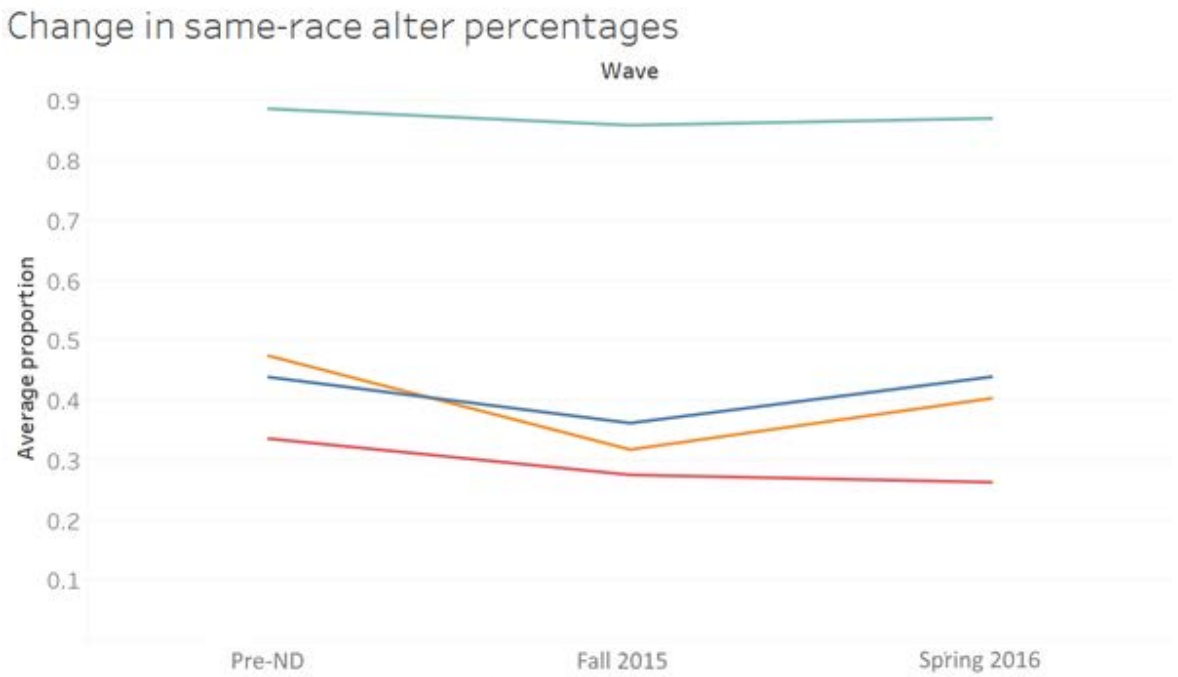

Figure 1: Changes in homophillous racial networks over the three survey waves (Pre-ND, Fall 2015, and Spring 2016)

Measure Names

- Asian - Asian
- Black - Black
- Latino - Latino
- White - White

Syngeneia and Xenoi: The Role of Kinship in the Practice of Hospitality

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The practice of hospitality has been thoroughly studied and considered by scholars in recent decades. Special interest has frequently been given to understanding how shifting worldviews influenced the ancient tradition from Homer's Odyssey, to Abraham's kindness recounted in Genesis 18, and into the letters of Paul and the parables of Jesus. The following paper/presentation will revisit this concept through a historical approach that examines a key similarity, as opposed to the many differences that occurred over centuries: mainly the role of the kinship relationship and familial obligations in extending hospitality to strangers. The intended outcome of this survey is to demonstrate that syngenia (συγγένεια) was foundational to the practice of hospitality. In other words, hosts were obligated to treat strangers/guests as family. This will be demonstrated through the consideration of numerous sources taken from the Greek epics of the Iliad and the Odyssey along with discussions of familial obligations presented by Plato and Aristotle. Inscriptions from the Hellenistic period which focus predominantly on political kinship but demonstrate the importance of "noncontractual role obligations" as fundamental for both familial and political associations will also be considered. In terms of the utilization of Jewish and Christian sources I will look at the story and commentary of Abraham's hospitality towards heavenly strangers in Genesis 18 in addition to the conversation of hospitality and familial obligations found in the writings of Paul and parables of Jesus. This approach will provide further understanding into the interdisciplinary nature of the diverse cultures and faith traditions that played a significant and defining role in the Mediterranean world of Antiquity.

Electrochemical performance of nickel-based electrodes: Improving urea electro-oxidation

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We present electrochemical performance results of nickel-based electrodes for improving urea electro-oxidation for source separated urine treatment. The predominant components of urine are urea, electrolyte salts, and proteins. The nitrogen content of urea presents an obstacle for wastewater treatment due to the complexity and time involved in treating it. Coupling inorganic nickel catalysts and electrochemical methods to treat nitrogen in urine suggests potential energy efficiency improvements and reduced treatment times. This is accomplished by oxidation of urea to inert CO_2 and N_2 gases, subsequently supplying current used to produce water or hydrogen depending on the electrochemical system setup. We synthesized nickel-based catalysts on fluorine doped tin oxide glass, carbon paper, nickel foam, and stainless steel substrates before employing cyclic voltammetry to evaluate urea electro-oxidation. We observed how applied potential affected redox potential, current, and electrode stability for each electrode. We evaluated effects of electrolyte composition and compared nickel electrodes to a platinum electrode, a commonly used but expensive catalyst. Potassium hydroxide (pH 13) was initially used as the electrolyte to provide adequate conductivity and prime nickel for urea oxidation, but a disodium phosphate/dipotassium phosphate electrolyte was later employed as a neutral pH (7) electrolyte for comparison. Cyclic voltammograms showed increased current when urea was added to the potassium hydroxide electrolyte. Substrate selection greatly affected the maximum current produced with nickel foam producing the highest current of all substrates employed. The results using a nickel catalyst differed from results using a nickel cobalt catalyst in that the nickel produced a lower current than nickel cobalt. Nickel produced 1800 μA/cm^2. Neutral pH experiments showed only 100 μA/cm^2, but the experiments with a pH of 13 in the electrolyte solution of potassium hydroxide and urea resulted in a current of about 160 μA/cm^2.

Phase Behavior of Complex Coacervates

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Complex coacervation refers to the complexation of oppositely charged polymer chains in solution. This phenomenon has been used in a variety of ways, including encapsulation, drug delivery, and the creation of coatings and underwater adhesives; such complexes are even in foods for their gelling capabilities. However, the phase behavior and driving forces behind coacervation are still mysterious. There are currently theories in place that accurately describe the behavior, but possibly not out of accuracy of the model. The trials done in this investigation were aimed to build a minimal model capable of understanding the onset of coacervation and the interplay of connectivity in driving the process.

The basis for the simulations used comes from work by Chapela[3], which describes the phase behavior for a charged colloidal system across a range of screened interactions. The system consists of a rectangular box with a slab of atoms at the center and vacuum on either side. From their trials, they were able to obtain critical temperature and density along with surface tension and interfacial width. The current investigation used a similar set up with course-grain chains of N = 1, 2, 4, 5, 10, 20, and 40. Each system consisted of 4,000 molecules. The systems were allowed to equilibrate then density profiles were created to determine the density of the polymer-rich and polymer-poor regions. These densities were fit to a coexistence curve using the law of rectilinear diameter to determine critical temperature and density. The critical properties were compared to the scaling laws proposed by Qin[1] and Voorn-Overbeek[2].

1 Qin, J., de Pablo, J., “Ordering Transitions in Salt-Doped Diblock Copolymers”, Macromolecules, 2016. 9.
2 Overbeek, J. T. G., Voorn, M. T., “Phase Separation in Polyelectrolyte Solutions. Theory of Complex Coacervation”, Journal of Cellular Physiology, 1957.
3 Gustavo A. Chapela, Fernando del Rio, Jose Alejandre, “Liquid-vapor phase diagram and surface properties in oppositely charged colloids represented by a mixture of attractive and repulsive Yukawa potentials”, J. Chem. Phys, 2013

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