SUMMER UNDERGRADUATE RESEARCH SYMPOSIUM

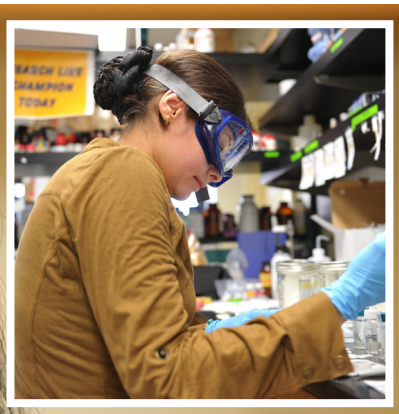
ABSTRACT BOOKLET

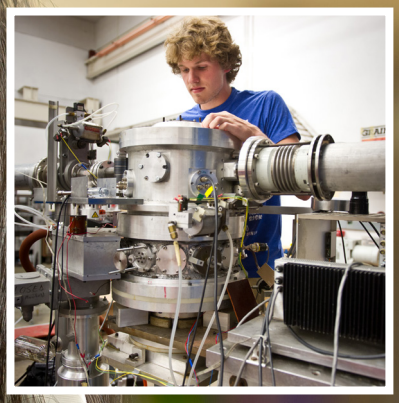
AUG. 2, 2013

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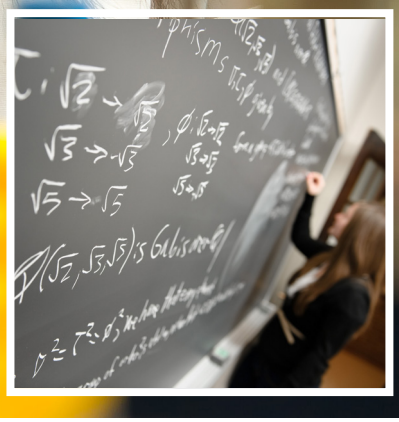
University of Notre Dame:
Biology REU program, Center for Research Computing, Center for Undergraduate Scholarly Engagement, College of Science, Graduate School, and ND*nano*

University of Michigan:
Chemistry REU program and the Interdisciplinary REU Program in the Structure & Function of Proteins









UNIVERSITY OF NOTRE DAME
College of Science

SUMMER UNDERGRADUATE RESEARCH SYMPOSIUM

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Oral Presentations Schedule

Biology, Chemistry, and Engineering — Jordan Room 105

Session I

11:00 am - 12:00 noon

Moderator: Dom Chaloner

11:00 Desiree Garcia-Torres - Probing the determinants of the metal binding specificity of HDAC8

11:15 Sean McGee - Incorporation of Green Design into Field Iodine Deficiency Test

11:30 Clarissa Rogg - Integration of Design and Energy Analysis Tools for Cooperative Energy Efficient Building Design

11:45 Kristin Springer - Delineation of the role for Notch signaling during zebrafish kidney regeneration

Session II

2:00 pm – 3:00 pm

Moderator: Dom Chaloner

2:00 Frances Acevedo Mariani - Polymerized HDLs for vaccine delivery

2:15 Jordan Campbell - Field emission-driven Townsend discharges for silver nanoparticle synthesis

2:30 Bryce Jones - Syntheses and SAR Analysis of Thiophene Aldehyde Derivatives

2:45 Akash Kannegulla - Optical modulation of continuous terahertz waves towards reconfigurable quasi-optical terahertz components

Physics **Jordan Room 322**

Session I

9:00 am - 10:15 am

Moderator: Umesh Garg

9:00 Edward Kielb, Taylor Corpuz, and Michelle Berg - The World's First Diffraction Limited Doppler Spectrometer: iLocater

9:15 Shanel Deal - Using Gamma Ray Burst to Estimate Luminosity Distances

9:30 Sarah Dietz - Detangling the Cosmic Web: Computational Models of Galaxies in Filaments

9:45 María Muñoz López - Analytical model of galactic feedback processes

10:00 Jared Johnson, Aaron Sawyer, and Adrien Saremi - Formation of relativistic jets along the axis of rotation of a black hole

Session II

10:30 am - 12:00 noon

Moderator: Umesh Garg

10:30 Liza Mulder - Electronic Properties of Lead Telluride Quantum Wells

10:45 Kevin Lee - Exploring the Growth Mechanisms of GaAs Nanowires Grown by MBE

11:00 Elissa Canseco - Damage of DNA in DNA-Gold Nanoparticle Mixture by Atmospheric Pressure Plasma Jet

11:15 Diana Gutierrez Zedano - Understanding Strontium's Role in the Stability of SrAu3Ge

11:30 Christine Kuryla - Mathematical Modeling of Dynamic Instability in Microtubules

Physics — Jordan Room 322

Session III

1:30 pm - 2:45 pm

Moderator: Umesh Garg

1:30 Bryce Frentz - New Targets for New accelerators

1:45 Zach Tully - Exploring the Collective Properties of 160-Gd

2:00 Benedict Pinyero - Double Folding Analysis of 6Li Elastic and Inelastic Scattering to low lying states on 208Pb

2:15 Hua Zhang - Constructing and Testing a Beam line for 5U Accelerator and Germanium Gamma Ray Detector Tests

2:30 Trevor Satterfield - Beam Monitor Prototype Using Gas Discharge

Session IV

3:00 pm - 4:30 pm

Moderator: Umesh Garg

3:00 Ruiyang Zhao - Accelerator Mass Spectrometry (AMS) applied in the measurement of 93Zr

3:15 Kirby Hermansen - Carbon 14 AMS: Establishing a Carbon Dating Procedure at Notre Dame

3:30 Alissa Murray - Vaccine Mandates and HPV

3:45 Hanyi Yi - Summary of CMS Minimum Bias Pythia 8 Tunes

4:00 Edward Varty - CMS Upgrade Simulations

4:15 Concluding Remarks

Poster Presentations Schedule Jordan Galleria

Session I

12:00 noon - 1:00 pm

Ephraim Acevedo - EspN and FL-EC7 interact with other proteins in the mycobacterial ESX-1 secretion system

Maria Agostini - Understanding the role of the CCR4-NOT1 complex in the microRNA pathway using single particle techniques

Gregory M Alberding - Combustion Synthesis of Ni and Co catalysts on CeO2, for the production H2 from Ethanol

Jonathan Alvarez - What Does Time Matter? The Impact of Temporal Sampling in Home Range Area Calculations

Megan Baker and Alexander Medvedeff - A first step in evaluating sNLP-12b as an antagonist to red flour beetle sulfakinin signaling

Omari Baruti - Identifying *In Vivo* Coactivator Targets of Transcriptional Activator Gal4 by Photocrosslinking with an Unnatural Amino Acid

Steven Boggess - Ratiometric fluorescent sensors of cysteine sulfenylation

Rachael Bridgman - Determining SERS cross-section of amino acids for protein characterization

Alexa Carollo - Investigating the Photodissociation of Hydroxocobalamin using Steady State and Time Resolved UV-Visible Spectroscopy

Katelyn Carothers - Knockdown of G-protein coupled receptors in adult female *Anopheles gambiae* using RNAi

Gonzalo Cazes-Nasitiqui - Integer Solutions to Diophantine Equations

Rachel Choi - TcpP Diffusion Rate and Concentration in a Chemical Gradient Using Single-Molecule Fluorescence Imaging of *Vibrio cholerae*

Sarah Cox - A New Computational Approach to Gelator Discovery

Randolph David II - Modeling the Formation and Propagation of Thermal Bar in Lake Ontario using Climatological Parameters

Allison Dianis - Inverse Islands: Comparing Matrilineal Structure Using mtDNA Between Singapore and Bali Long-Tailed Macaques

Simone Dozier - Synonymous Codon Usage

Nnamdi Edokobi - Investigation of changes in cardiac innervation in a mouse model of Dravet Syndrome

Nichole Etienne - Mathematical modeling and control of co-transmitting soil-transmitted helminthes

Heather Fick, Jennifer Parra, Kirin Kuar, Stephanie Sesse, Vera Marcello, Arika Haines and James K. Campbell - Design of a Fast-Acting Coliphage Biosensor Device

Amy Fraley - Characterization of Halogenases in the Malbrancheamide Pathway

Burke Gao - Visualizing Mismatch Repair in Live *Bacillus subtilis* using Single-Molecule Fluorescence Microscopy

John Gensic - Making Gasoline from Grass-Using heterogeneous catalysts to convert biomass into biofuel

Daniel Gomez - PrivacyRanger

Andrea Hakaj - Approaches to Identify Novel Phosphorylation Sites in the Checkpoint Protein ZW10

Andrew Hamilton - Exploring Plasmon-Exciton Interactions between Gold Nanoparticles and Gold Nanoclusters

Joel Hlavaty - Biomechanical Engineering and a Model Of Phenotypic Plasticity In Developing Mammals

Peter Hoffman - Polymer-Templated Rainbow Solar Cells & Implementing Photovoltaics into the Chemistry Classroom

Shayna Hu - The Role of GRP78 Expression in Pancreatic Cancer Chemoresistance

Michael Hunckler - Feasibility of gel electrophoresis to determine the permeability properties of tendons

Jonathan Jou - The Role of Fgf Signaling During Regeneration of the Zebrafish Mesonephros

Patrick Jung - Microcontact Printing of DNA Origami onto Silicon Substrates

Akash Kannegulla - Optical modulation of continuous terahertz waves towards reconfigurable quasi-optical terahertz components

Micah Katz - Investigating *In Vivo* Binding Partners of Transcriptional Activator VP16 through the Genetic Incorporation of Unnatural, Photocrosslinking Amino Acids

Taylor Kelson - Thermosensitive acrylamide-based hydrogel nanoparticles as a novel targeted drug delivery vehicle for anti-cancer agents

Kyle Kimler - The Relationship of Vision and Circadian Rhythm in *Aedes aegypti*

Christine Kuryla - Mathematical Modeling of Dynamic Instability in Microtubules

Daniel Kwasnieski - Characterization of Ag SERS-active microelectrodes

Judy Long - Data Git: Provenance Extraction Tool Using Version Control

Rui Yan Ma - Evaluating the Effects of Spatial Scale on the Performance of Climate Envelope Modeling

Aziz Mamur - Synthesis of a Selective Kinase Inhibitor for the M.tb. Ser/Thr Kinase - PknB

Rebecca Marton - Interkinetic Nuclear Migration in the Regenerating Zebrafish Retina

Grace McKenna - An Enantioselective Total Synthesis of Cis-2,5-Disubstituted Pyrrolidines

Christine Mei - Roles and Interaction of MRPP1 and MRPP2 in Reconstitution of Human Mitochondrial RNase P

Max Miller - Performance Evaluation of Amazon EC2 and Google Compute Engine

Ciaran Mooney - Mechanisms Governing Müller Glial Interkinetic Nuclear Migration in the Regenerating Zebrafish Retina

Vaishnav Murthy - Analysis of holes in graphene monolayers

Ansel Nalin - Progress Towards the Total Synthesis of Ambruticin J

Hamim Nigena - Synthesis of IRMOF-3 and Conversion of Dihydroxyacetone to Ethyl Lactate

Joshua Ostrander - The Structure and Dynamics of CORM-3 in Solution Studied Using FTIR and 2D-IR Spectroscopy

Aakash Patel - Determining Heart Rate from Video

Jaqueline-Mae Picache - Characterization of APC-induced microtubule branching

Julian Pilate-Hutcherson - Thiolated gold and silver nanoclusters absorption of visible light

Jessica Rafson - Crystalline InSb from Simple Electrodeposition of Sb onto the Reactive Interface of In Electrodes under Aqueous Benchtop Settings

Julia Resil - Population genetic structure of Balinese long-tailed macaques (*Macaca fascicularis*)

Olaf Rodríguez Gutiérrez - Functional characterization of the carbon dioxide receptor genes in *Culex quinquefasciatus* and *Culex stigmatosoma*

Sarah Semanek - Role of cyclins in Müller glia and neuronal progenitor cell proliferation in the zebrafish retina

Lynda Smith - Hey! Can Someone Turn the Light On? SOS! (Sustainably Off Sunlight)

Jordan Stern - Improved Efficiency of Negative Ion Electron Capture Dissociation (niECD) Through Charge State Reduction and Laser Activation

Daniel Steyer - Analysis of SIRT1 Activity by Capillary Electrophoresis

Donghyuk Suh - Ultrafast 2DIR probe on an organic polymer for a model HFL system.

Joseph Thomaz - Does Visible Light Photolyze Hydroxocobalamin?

Thibault Twahirwa - Experimental Studies on Field Emission-Driven Microdischarges

Valerie Verdun - Analysis of *lunatic fringe* in Renal Progenitor Patterning During Zebrafish Kidney Development

Alyse Volino - Stasis of Saltwater Tolerance in *Anopheles farauti* FAR1 Mosquitoes

Justin Waller - Synthetic processes of gold nano-sphere (NS) & nano-rod (NR) particles for the enhancement of solar cells

Nicholas Weidner - Hurricane and Storm Surge Modeling at Notre Dame

Russell Williams III - Receptor Interacting Protein Mediated Cell Death in ECM-detached Breast Cancer Cells

Nathaniel Wirgau - Synthesis and Characterization of Five- and Six-Coordinate Ferrous Heme-Nitrosyl Complexes

Ying Zhang - Chiral Guest Recognition by Lanthanide Metallacrown Hosts with Threonine-based Ligands

Session II

1:00 - 2:00 pm

Thomas C. Adams - Thermal Rectifiers - The Effects of Thermal Conductivity

Michael Ahlers - Synthesis of a GEX1A Analogue for Niemann-Pick Type C Disease Research

Pauline Alokolaro - Light It Up: High Performance Backside Solar Cell Fabrication

Arnaud Bacye - External modulation of mid-infrared quantum cascade lasers with integrated Mach-Zehnder interferometric modulator

Elijah Barstis - Creating a Device to Detect Substandard Tagamet HB 200® Pills

Omar Beleh - Development of a TR-FRET Assay to Screen for Allosteric Kinase Inhibitors

Buchanan Bourdon - Electrostatic Doping of 2D materials via Polymer Electrolytes: Using COMSOL to Simulate Ion-electron Transport

Krista Briedis - Biological Characterization of Novel Mcl-1 Inhibitors

Sarah Caruso - α3DH3-GSGA-F31A, A *De Novo* Designed Metallopeptide

Brianna Chamberlin - Exploring the polymorphism of piperine

Kasey Clear - A Hybrid Optical Detection Method

Phillip Cook - The New Digital Playground: Applications of 3D Printing within a K-12 Setting

Will Crosby - Synthesis of Nickel Diimine Complexes as Possible Catalysts for the Polymerization of Electron Deficient Monomers

Christine Cuthbertson - Synthesis and Analysis of 2,5,6-trifluoro-3,4-dihydroxybenzoate as a Potential Inhibitor of Wild-type Class 1A Dihydroorotate Dehydrogenase

Williams Dixon - Examining the Conformational Dynamics of Proteins and snRNAs during Splicing using smFRET

Kevin Durand - Plasmon-Enhanced Fluorescence Imaging of the Intrinsic Emission of Single Coenzyme B12 Molecules

Osama El-Sayed - Characterization of J-Binding Protein 1

Taylor Evans - Synthesis of α-$SnWO_4$

Nathan Foje - Non-Invasive Optical Imaging of Near Infrared Electrospun Nanoparticles

Jessica Freeman - An Investigation into the Factors that Affect Compartment Size in *Drosophila* Epidermal Larval Segments during Embryogenesis

Desiree Garcia-Torres - Probing the determinants of the metal binding specificity of HDAC8

Jeremy Gerick - Green's Functions in Chemistry; Optimization and Implementation of PT2 Self-Energy

Brandon Gutierrez - Development of Visually Impaired Transgenic Mosquitoes

Josh Halpern - Enzymatic Synthesis of 3-deoxy-D-manno-octulosonic acid from *in situ* D-Arabinose-5-Arsenate as a Substrate Analogue

John Hargett - Visualizing Imitation Through Motion Capture Technology

Sara Hockney - Role of pax6 in neuronal progenitor cell proliferation during zebrafish photoreceptor regeneration

Gwendolyn Hooley - Identification of a novel gene required for ESX-1 secretion and virulence in *Mycobacterium marinum*

Meghan Hudak - Evolution of *Mycobacterium marinum* for loss of ESX-1 associated hemolytic activity

Elizabeth Huschke - On-Chip Optical Diagnosis Using Capillary Electrophoresis

Nirbhay Jain - A Simple Method of Minimizing Ionic Strength to Reduce Chemical Shift Variance in NMR-based Metabolomics of Urine Specimen

Kipchumba Kaitany - Determining Hepatitis C NS3 Helicase's Active Oligomeric State

Gordon Kane - Assay Development Monitoring VirF Binding to VirB Promoter

Milan Kaushik - Nanomaterial Induced Changes in Cell Membrane Conductivity: A Whole Cell Patch Clamp Study

Daniel Kestell - Simulation of Nanomagnets under Dynamic Conditions

Anthony Krenselewski - Manipulation of Graphene Morphology Compounds via Metal Nanoparticle Mediated Hydroxyl Radical Attack

Christopher Kubitskey - Biosynthetic Production of Novel Substrates

Alexa Kutch - 3D Printing: Rapid Prototyping using Additive Manufacturing

Megan Leander - DMS Ligand-Receptor Interactions Reflect SAR Data

Nevin Longenecker - Possible Student Investigations Related to Engineering a More Sustainable Energy Future

Amber Lott - Membranes with Multiple Porous Crystals for Chemical Separations

Michael Manning - Examining Interprotein Interactions Using Coarse Grained Molecular Dynamics Simulations

Robert Matthews - Raman Spectroscopic Monitoring of Integration of a Tissue-Engineered Oral Mucosa Construct

Jill McNabnay - Changing Climate; Changing Life

Rachel Miceli - Genetic analysis of podocyte development

Alannah Miranda - Low glucose exposure favors the appearance of fast vs. slow oscillations in isolated mouse pancreatic islets

Cameron Moore - Optimizing Paper Tests for Anti-Tuberculosis Medications

Brenda Mueller - Carbon Dioxide Capture in Ionic Liquids

Sarah Neville - Synthesis of New Non-Heme Iron Nitrosyls

Heather M. Nimon - Employing the Energy of Light to Advance Technology

Clarence Pascual - Identifying the significance of the dual Peroxisomal Targeting Signals in *Arabidopsis thaliana* LACS7

Nathaniel Pelz - The Geppetto Project

Samantha Piekos - Generation and characterization of *tnfa* and *nr2e3* transgenic zebrafish lines

Kenneth Poling - Dye Sensitized Solar Cells

Sashary Ramos - Characterization of fluticasone propionate microcrystalline drug product using quantitative polarization microscopy

Grayson Ritch - Structure and Catalytic Activity of Iron 6,6'Dihydroxy Terpyridine Complexes

Ann Rutherford - Development of s-block Organometallic Catalysts for co-polymerization of Polycarbonates

Dillon Skeehan - Opportunistic Grid Computation for High Energy Physics

Emmanuel Sosa - Revolutions of 1848: History of Contingency?

India Stewart - Data Git: Provenance Extraction Tool Using Version Control

Jerone Stoner - Determining the Significance of the ZNF217-PKM2 Interaction in the Metabolic Regulation of Breast Cancer Progression

Joseph Terranova - Effects of pH on Pore Size of poly(isoprene-b-styrene-b-dimethylacrylimade) Membrane

Sara Tweedy - MD Simulations Reveal the Impact of Crystal Packing on the Post-SET Loop of NSD1

Catherine Eve Vogt - Investigation of Small Molecule Binding to the Exon Splicing Silencer in Human Immunodeficiency Virus Type 1 Tat Exon 3

Ian VonWald - *S*-Nitroso-*N*-hexanylpenicillamine (SNHP)-Doped Polymers: Synthesis, Leaching Stability, and Characterization of Nitric Oxide Release

Jiarui Wang - Structure probing of the transcriptionally acting $preQ_1$ riboswitch using single molecule FRET (smFRET)

Milena Westarb - Methods for Cocrystal Synthesis

Mark Wilson - Kinetics of Reaction of (MeClamp)Ti with Hydrazobenzene

Charles Cong Yang Xu - Genetic Differentiation among Populations of *Echinolittorina radiata* across East Asia

ABSTRACTS

Poster Presentation

EspN and FL-EC7 interact with other proteins in the mycobacterial ESX-1 secretion system

Ephraim Acevedo
Marika Kuspa, Dept. of Biological Sciences, University of Notre Dame
Advisor: Patricia Champion, Dept. of Biological Sciences, University of Notre Dame

Tuberculosis is one of the most deadly diseases known, killing 1.4 million people worldwide each year (Who, 2012). The virulence of *Mycobacterium tuberculosis* is dependent upon the ESX-1 secretion system. This system is conserved in pathogenic mycobacteria and certain Gram-positive bacteria. One of the functions of the ESX-1 secretion system is to manipulate the host response to infection. The goal of my project is to study protein-protein interactions within the ESX-1 secretion system. To do so I am focusing on how two ESX-1 associated proteins, EspN and FL-EC7, interact with components of the secretion system. EspN is a novel protein that is involved in the ESX-1 secretion system. FL-EC7 is a construct of the substrates EspC and CFP-10 that shows interactions with two ESX-1 ATPases. We are performing this study by using a yeast two-hybrid screen in order to see which proteins from a *M. tuberculosis* cDNA library interact with EspN and FL-EC7. Using this approach, we found that EspN interacted with proteins that are found in the membrane, cell wall and the cytosol. Some of these proteins are found when M. tuberculosis is under stress. This stress may be associated to the conditions that are found when M. tuberculosis is trapped within the phagosome of the macrophages, where M. tuberculosis resides after infection. This screen will identify novel ESX-1 components, as well as to facilitate studies focused on how these components interact with existing ESX-1 proteins.

Oral Presentation

Polymerized HDLs for vaccine delivery

Frances Acevedo Mariani
Gwangseong Kim, Dept of Pharmaceutical Sciences, University of Michigan
Advisor: Anna Schwendeman, Dept. of Medicinal Chemistry, University of Michigan

High-density lipoprotein (HDL) is a natural nanoparticle composed phospholipid bilayer and Apolipoprotein A-I (ApoA-I). The main functions of HDL are to efflux the excess of cholesterol from endothelial cells and transport it to the liver for elimination. Due to their size (8-10 nm) and long circulation half-life (1-3 days) they could be used for intravenous delivery of peptide antigens covalently bound to HDL phospholipids. Unfortunately HDL undergoes rapid remodeling in plasma by exchanging phospholipids with other membranes, and potentially loosing phospholipid bound surface antigens. Polymerization of HDL lipid bilayer will likely prevent plasma remodeling. ApoAI mimetic peptide (5A) was complexed with polymerizable lipid, 1,2-bis(10,12-tricosadiynoyl)-sn-glycero-3-phosphocholine (Diyne PC), and sphingomyelin (SM) to form sHDL nanoparticles. Diyne PC, SM and 5A were dissolved in organic solvent, combined at 2:0:1, 1:1:1, 0.5:1.5:1 and 0.25:1.75:1 weight ratios and lyophilized. The powders were hydrated to form HDLs and polymerized by UV light exposure for 2 hours. The resulting sHDLs were analyzed to determine size (DLS), purity (gel chromatography – GPC), presence of liposome impurity (turbidity) and stability after cooling to 4°C. Only polymerized HDLs composed exclusively of Diyne PC (2:0:1) remained intact, while the increase in impurities was observed for all other preparations. To increase purity and optimize size, HDL were prepared at 1:0.5, 1:0.75, 1:1, 1:1.5 and 1:2 wt/wt ratios of 5A to Diyne PC. The HDL purity increased with decrease of lipid content and stability was improved by polymerization. The polymerized HDLs were prepared and their composition was optimized to achieve size characteristic size of 8-10 nm and physical stability. The polymerized HDL could be potentially used for vaccine antigen delivery.

Poster Presentation

Thermal Rectifiers – The Effects of Thermal Conductivity

Thomas C. Adams
Ky-Quan Nguyen
Advisor: Tengfei Luo, Dept. of Aerospace and Mechanical Engineering,
University of Notre Dame

While still in progress, a bi-layer junction could be constructed by using the properties of hexadecane to create a thermal rectifier – one-way heat flux transfer mechanism. Interestingly, these predications and calculations are made via simple secondary level algebra and statistics methods with regards to introductory physics applications.

Poster Presentation

Understanding the role of the CCR4-NOT1 complex in the microRNA pathway using single particle techniques

Maria Agostini
Advisor: Nils Walter, Dept. of Chemistry, University of Michigan

MicroRNAs (miRNA) are short, non-coding RNAs approximately 22 nucleotides in length that regulate post-transcriptional gene expression. They function by assembling on mRNA targets and associating with components of the RNA-induced silencing complex (RISC). The major components of RISC are an Argonaute protein (AGO), GW182, and the CCR4-NOT1 complex. This study focuses primarily on the role of the CCR4-NOT1 complex by means of an important subunit involved in deadenylation of the mRNA target transcripts, CNOT1. Here, we verify siRNA knockdown of CNOT1 by Western Blot before analyzing differences in distribution of processing bodies (P bodies) that are often the site of mRNA degradation in U2OS cells stably expressing DCP1a labeled with GFP. In addition to this observation, using a method previously described by members of our group called intracellular single-molecule, high resolution localization and counting (iSHiRLoC), we aim to discover the different localization and diffusion coefficients of let-7-a1 miRNAs that result in CNOT1 knockdown U2OS cells. This process includes microinjecting double-stranded let-7-a1 miRNA labeled with Cy5 on the 3' end of the guide strand. Previously, using this method, members of our group discovered that miRNA exhibit specific localization and diffusion coefficients when microinjected into the cell. Specifically, they observed two kinetically distinct populations. The goal of this study is to determine the effects of the CCR4-NOT1 complex on these values by observing shifts in these behaviors when the cell is depleted of CNOT1. These observations may serve to either verify or alter our current understanding of the role of the CCR4-NOT1 complex in this pathway.

Poster Presentation

Synthesis of a GEX1A Analogue for Niemann-Pick Type C Disease Research

Michael Ahlers
Eve Granatosky and Jarred Pickering, Dept. of Chemistry and Biochemistry,
University of Notre Dame
Advisor: Richard Taylor, Dept. of Chemistry and Biochemistry,
University of Notre Dame

Niemann-Pick Type C disease (NPC) is a rare and fatal lysosomal storage disease that typically presents before the age of 10. Specifically, NPC is characterized by mutations to either the NPC1 or NPC2 proteins that result in defective cholesterol trafficking. Although hydroxypropyl β-cyclodextrin (HPβCD) and histone deacetylase inhibitors (HDACi) such as trichostatin A are current therapeutic candidates for NPC, there is currently no FDA approved treatment. We have recently demonstrated the ability of GEX1A, a type I polyketide natural product isolated from *Streptomyces chromofuscus*, to restore cholesterol trafficking in NPC1 mutant cell lines (Figure 1). Interestingly, herboxidiene is not an HDACi. Given rapid access to GEX1A through fermentation processes, our attention has shifted towards the synthesis of non-natural analogues of the parent compound such as 1. Thus, an efficient route to fragment A has been realized through crotylation chemistry reported by Leighton and co-workers. Once completed, this analogue will be used in NPC1 and NPC2 mutant cell line assays for comparison with GEX1A.

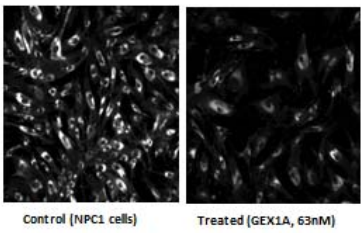
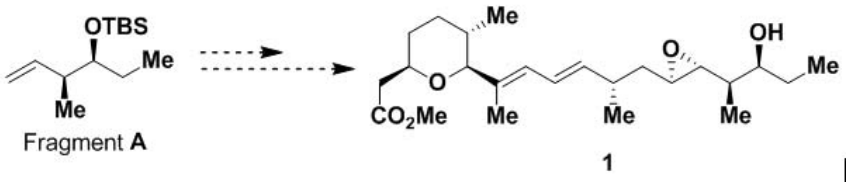


Figure 1. Treatment of NPC1 mutant cell line with GEX1A



Poster Presentation

Combustion Synthesis of Ni and Co catalysts on CeO2, for the production H2 from Ethanol

Gregory M Alberding
Allison Cross, Dept. of Chemical and Biomolecular Engineering
Advisor: Eduardo Wolf, Dept. of Chemical and Biomolecular Engineering,
University of Notre Dame

This research looks at catalysts for the production of hydrogen gas from ethanol. Hydrogen gas production is an important step for the functioning of fuel cells. We created six different CeO2 catalysts, some containing Ni, Co, or both. We are using combustion synthesis techniques to create these different metal-containing catalysts. We then characterized the catalysts, looking at composition, surface area, pore size, and particle size. Finally we used each catalyst in an ethanol reaction to look for selectivity of each catalyst in the production of hydrogen.

Poster Presentation

Light It Up: High Performance Backside Solar Cell Fabrication

Pauline Alokolaro
Yuning Zhao, Dept. of Electrical Engineering, University of Notre Dame
Advisor: Patrick Fay, Dept. of Electrical Engineering, University of Notre Dame

Considerations for meeting future worldwide energy needs must include a serious discussion regarding practical and efficient processes for harnessing solar energy. Although other forms of renewable energy should be a part of a balanced, clean, renewable energy economy, only solar energy offers the quantities of energy that can meet the world's increasing demands. Theoretically, up to 86.7% of sunlight can be harnessed and stored, but current solar technologies cap out at less than half that efficiency. Urban solar power plants will not become viable options until solar cells are small enough and efficient enough to fit within a densely populated area.

Fabrication of compound-semiconductor based multi-junction high-performance solar cells involves the development of "back-side" solar cells in which all of the contacts and interconnections can be made on the back side of the wafer. Multi-junction backside solar cells offer the additional benefit of strong absorption of multiple regions of the solar spectrum. Current work focuses on packaging the solar cells so that they are practical for commercial use. A thin layer of tin will be applied to the bottom of the solar cell for packaging purposes.

The experience will be incorporated into a high school chemistry class during a unit involving the electromagnetic spectrum and quantum chemistry. The unit will include a discussion of the different wavelengths of sunlight and methods of capturing the most energy from the sunlight as well as a laboratory activity involving the construction of a solar cell and measurements of its power.

Poster Presentation

What Does Time Matter? The Impact of Temporal Sampling in Home Range Area Calculations

Jonathan Alvarez
Amy Klegarth, Dept. of Biological Sciences, University of Notre Dame
Advisors: Hope Hollocher, Dept. of Biological Sciences,
and Agustin Fuentes, Dept. of Anthropology, University of Notre Dame

Global Positioning System (GPS) are currently widely used to study larger mammals, including carnivores and ungulates. Only recently have GPS collars been a viable method to study primates, as size restrictions hindered potential studies. The constant locational updates as well as their noninvasive nature after deployment provide great utility for managers by helping them model future ranging patterns based on past land use. GPS collars remove a potential bias of researches closely following primate groups and provide a simple method of acquiring data from anywhere in the world.

Results from a previous study in Singapore, which used GPS collars to track daily and home ranges for 3 monkeys, show that home range sizes calculated using Minimum Convex Polygons (MCPs) display a significant increasing trend with the iterative addition of sample points. Recent statistical analyses show that when the same home range areas are calculated using Kernel Density Estimations (KDEs), the significance between sample sizes is no longer present. However, linear regressions of the data suggest that the difference between sample sizes becomes significantly smaller as more points are added.

This project aims to apply the methods from the Singapore study to six different monkeys located in Gibraltar. The Gibraltar monkeys have been collared for five months as opposed to two months for the Singapore monkeys. This increased data size allows the project to examine the temporal element of the iterative analysis.

Ultimately, the results from this project will inform future analytic methods for a larger collar project in Singapore. The information about home range size and general movement behavior will be incorporated within a landscape genetic Geographic Information Systems model. Specifically, this project will help parameterize migration ability based on recorded home range areas as well as distance and movement rates.

Poster Presentation

External modulation of mid-infrared quantum cascade lasers with integrated Mach-Zehnder interferometric modulator

Arnaud Bacye
Michael Harter and Galen Harden, Dept. of Electrical Engineering, University of Notre Dame
Advisor: Anthony Hoffman, Dept. of Electrical Engineering, University of Notre Dame

Abstract: We present a quantum cascade laser (QCL) with an integrated Mach-Zehnder interferometer that function as an electro-optic modulator. The laser and interferometer are fabricated from the same QC wafer that consists of two core sections: the active region for providing optical gain and a super-lattice of asymmetric coupled quantum wells (ACQWs) for controlling the phase difference between the arms of the interferometer. Amplitude modulation is achieved by tuning the intersubband absorption of the ACQWs via an applied voltage over the super-lattice. The intersubband absorption of the ACQWs was designed using a two-band solver that includes energy band nonparabolicity. Our design has an intersubband transitional energy that tunes from 78.9 meV at a field of -75 kV/cm to 115.6 meV at 75 kV/cm. The waveguide was designed by including the voltage-dependent index of the ACQWs in a commercial 2-D finite element solver to calculate the propagating mode and the effective modal index. The overlap of the optical mode with the ACQWs, approximately 1%, was engineered to enable sufficient control of the phase for optical modulation while minimizing optical loss from the contact layer. Such a device has application in mid infrared photo-acoustic spectroscopy, a technique used for trace gas detection in the medical, environmental, and homeland defense fields.

Poster Presentation

A first step in evaluating sNLP-12b as an antagonist to red flour beetle sulfakinin signaling

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Alexander Medvedeff
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Advisor: Ruthann Nichols, Dept. of Biological Chemistry, University of Michigan

Sulfakinins (SKs) are insect neuropeptides which regulate gut and heart contractions and inhibit food intake by signaling through family A G protein-coupled receptors. Identifying SK peptide-receptor contact sites is important to understanding how these peptides act. In a previous study, the nematode peptide sNLP-12b behaved as a putative antagonist to SK receptors in red flour beetle as measured by a food intake assay. Docking SK ligands as well as sNLP-12b to red flour beetle SK receptors (TcSKRs) was a first step to determine whether the putative antagonist acts through the beetle SK pathway or through a different signaling pathway. Our work included novel receptor modeling and SK ligand docking to TcSKR1 and to TcSKR2, a protein previously unexplored in the signaling pathway. Our results suggest that sNLP-12b makes contacts with TcSKRs and may act as an antagonist to the SK signaling pathway.

Poster Presentation

Creating a Device to Detect Substandard Tagamet HB 200® Pills

Elijah Barstis
Toni Barstis, Dept of Chemistry & Physics, Saint Mary's College
Advisor: Toni Barstis, Dept of Chemistry & Physics, Saint Mary's College

This research focused on the creation of a Paper Analytical Device (PAD) to screen for substandard Tagamet HB 200® pills. Different colorimetric reagent tests are used on the PAD to detect the API Cimetidine and select excipients found in genuine pills and select substituents found in substandard pills. The colorimetric reagent tests and the results of a small field test will be presented.

1. "Essential Drug List." Web accessed July 22, 2013. www.who.int/selection_medicines/country_lists/phl_edl_2007.pdf
2. "Screening for Counterfeit Drugs Using Near-Infrared Spectroscopy." Web accessed July 22, 2013. http://www.pharmainfo.net/pharmaceutical-packaging-articles/screening-counterfeit-drugs-using-near-infrared-spectroscopy

Poster Presentation

Identifying *In Vivo* Coactivator Targets of Transcriptional Activator Gal4 by Photocrosslinking with an Unnatural Amino Acid

Omari Baruti
Amanda Dugan Rachel Pricer, Cassie Joiner, Dept. of Department of Chemistry, University of Michigan
Advisor: Anna Mapp, Dept. of Department of Chemistry, University of Michigan

Transcriptional activators are modular proteins that are required to initiate transcription, the essential cellular process wherein DNA is transcribed into mRNA. Activators have a DNA binding domain (DBD) that specifies localization at a gene, and transcriptional activation domain (TAD) that regulates expression of gene by recruiting the transcriptional machinery, including RNA Polymerase II, to the gene promoter. Although activators are known to recruit multiple coactivator complexes, identifying the individual subunits within these coactivators and the transcriptional machinery, and thus understanding their individual role in transcription, has proven challenging. Here we use in vivo photocrosslinking with a genetically incorporated photo-crosslinker amino acid, p-benzoyl-L-phenylalanine (Bpa) to capture the direct targets of the model yeast activator Gal4 in *Saccharomyces cerevisiae*. Specifically, we examine its interactions with the chromatin modifying complex SAGA. To do this, we used molecular cloning techniques to generate myc-tagged constructs of SAGA subunits, Tra1, Ada2, and Taf12, believed to be putative targets of Gal4. We co-transform these tagged coactivator proteins alongside a Gal4 construct that bears a LexA DBD and the Gal4 TAD and then grow the yeast in the presence of Bpa. Live yeast are then irradiated with UV light to form a covalent crosslink between the Bpa in the Gal4 TAD and its protein binding partners. We then immunoprecipitate the crosslinked activator complexes from yeast lysate and probe for the presence of covalently bound tagged co activator using Western blotting techniques. In this way, we can identify the coactivators that are directly recruited by Gal4 in living cells.

Poster Presentation

Development of a TR-FRET Assay to Screen for Allosteric Kinase Inhibitors

Omar Beleh
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Protein kinases have become important drug targets due to their involvement in many biological processes, including cell division, motility, and overall survival. Dysregulation of these signaling molecules has been shown to lead to disease, particularly in a number of different cancers. Previous research has led to the development of ATP-competitive inhibitors that target multiple kinases to achieve their desired effect. However, since there are over 500 protein kinases in the human body with similar ATP-binding domains, selectivity and characterization of specific signaling pathways can be difficult when designing an inhibitor. One approach to increase selectivity and limit potential toxicity is to develop allosteric kinase inhibitors; that is, an inhibitor that targets a nonconserved binding site specific to a given kinase. One such allosteric inhibitor of c-Abl kinase is GNF-2, which binds to its myristate binding pocket. Here we report the synthesis of a derivative of GNF-2 labeled with the fluorescent dye Cy5. This GNF-2 Cy5 derivative is used in the development of a TR-FRET assay to screen for allosteric inhibitors of c-Abl. Initial hits resulting from the screen will be subjected to further optimization.

Poster Presentation

Ratiometric fluorescent sensors of cysteine sulfenylation

Steven Boggess
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Advisor: Brent Martin, Dept. of Chemistry, University of Michigan

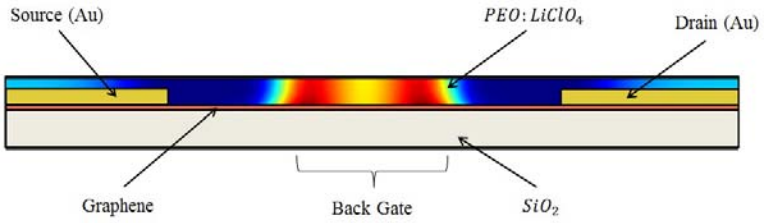
Oxidation of cysteine is an important post-translational modification that regulates many important signaling pathways in cells by blocking the activity of protein phosphatases and enhancing growth factor receptor activation. Upon epidermal growth factor stimulation, NADPH oxidase is stimulated to produce hydrogen peroxide (H2O2), which acts as a second messenger by oxidizing reactive cysteines to the sulfenic acids. Recently, functionalized derivatives of the active methylene compound dimedone have been used to capture sites of sulfenylation for biochemical and proteomic analysis. Dimedone exists in its enolate form at physiological pH (pKa 4.3), where the α-carbon reactivity is tuned to selectively react with weakly electrophilic sulfenic acids. While these probes are valuable for biochemical studies, fluorophore conjugates are useless for live cell imaging. In order to overcome this limitation, we present the synthesis and activity of a family of small-molecule probes that combines dimedone with a fluorescent naphthalene, linking the fluorescent properties to the reactive α-carbon.. These DiNaps (Dimedone Napthalene) retain the reactivity and selectivity of dimedone, and conjugate to numerous known sulfenylated proteins. In order to induce a fluorescence change, we substituted a single α-proton with a methyl or fluorine blocking group. Blocking the α-position prevents a second deprotonation of the dimedone upon conjugation to protein which locks it into its diketone form, thereby changing the electronics of the ring in order to provide a change in the excitation spectrum of the probe. Ratiometric imaging of H2O2 stimulated immature B-cells demonstrates the first presentation of dynamic sulfenylation in live cells.

Poster Presentation

Electrostatic Doping of 2D materials via Polymer Electrolytes: Using COMSOL to Simulate Ion-electron Transport

Buchanan Bourdon
Joshua Vahala, Electrical Engineering, University of Notre Dame
Advisors: Alan Seabaugh, Dept. of Electrical Engineering, University of Notre Dame and Susan Fullerton, Dept. of Electrical Engineering, University of Notre Dame

To reduce power dissipation in electronics, we must reduce the operating voltages of the individual components, including memory. Recent ion-based memory concepts have focused on the formation and destruction of a conductive filament formed by the migration of ions; however, one drawback to this approach is that it requires a high-voltage forming-step. The long-term goal of this project is to develop a low-voltage nanoionic memory based on electrostatic doping that implements graphene and a solid polymer-electrolyte. Graphene is used because it has a high electrical conductivity in which electrons move at 1/300th the speed of light, a surface at which ions will not react, and it is a two-dimensional material that is only one atomic layer thick, allowing us to approach the limits of scaling. The memory will operate by moving ions in the polymer towards and away from the graphene surface, thereby modulating its conductivity, which will be sensed to indicate the memory state. The goal of this summer's research was to use COMSOL Multiphysics software to simulate ion transport in a simplified architecture comprising a source, drain, and backgate to model how the ions respond to an electric potential. We simulated systems with a continuous graphene channel and ones that had a gap. The backgate controls the channel electric potential between the source and drain. Using materials properties derived from experimentation, we determined that the ions require five seconds to reach a homogeneous concentration profile for a backgate voltage of -5V – a timescale longer than preconceived. Specifically, a p-n-p junction is formed in the channel when the backgate voltage is positive, and an n-p-n junction is formed when it is negative. When relaxing the system by switching the backgate voltage from -5V to 0V, we determined that it can take up to 20 and 35 seconds for the anions and cations, respectively, to return to a homogeneous concentration profile. These results will inform decisions on how to gate the device experimentally. Future work will include adding a topgate to generate a uniform electric potential, and accounting for non-idealities such as electrochemistry to more accurately represent the experimental system.

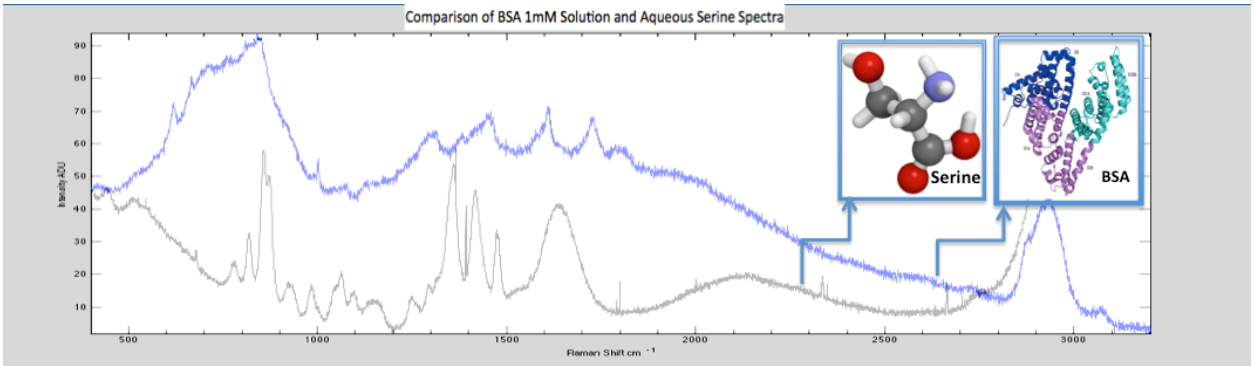


Poster Presentation

Determining SERS cross-section of amino acids for protein characterization

Rachael Bridgman
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Advisor: Zachary Schultz, Dept. of Chemistry and Biochemistry, University of Notre Dame

Proteins are the building blocks of all life forms and are composed of amino acids. The chemical structure of proteins is important for understanding their function. The amino acid sequence dictates protein structure. Raman is a chemically specific method that can be used to identify the amino acids in a protein. Raman is a low signal experiment; however, the signals can be enhanced using gold and silver nanostructures, commonly referred to as surface enhanced Raman spectroscopy (SERS). The signal intensities observed in SERS are often different than regular Raman. Determining each amino acid's SERS cross-section provides a measure of how likely an amino acid will scatter compared to another. However, it has been difficult to develop a reliable process for determining the SERS cross-section of molecules. The goal of this project was to determine the SERS cross-section of all 22 amino acids and to use this information to specify amino acid contributions to the SERS spectrum of proteins like Bovine Serum Albumin (BSA). Toward this goal, we quantified the regular Raman cross section of each amino acid as a solid and in aqueous solution. These results serve as a reference upon which to analyze the bands observed in SERS. The empirical data was used to dissect BSA's spectra and determine which amino acids were detected in the protein. This analysis suggested that the amino acid residues histidine, serine and phenylalanine are present in BSA. Future work quantifying the SERS response of each amino acid will help understand differences in the conventional Raman and SERS spectrum of proteins.



Poster Presentation

Biological Characterization of Novel Mcl-1 Inhibitors

Krista Briedis
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Advisor: Zaneta Nikolovska-Coleska, Dept. of Pathology, University of Michigan

Mcl-1, myeloid cell leukemia protein, is an anti-apoptotic member of the Bcl-2 protein family that regulates the intrinsic pathway of apoptosis. Mcl-1 binds and sequesters activators of pro-apoptotic proteins, thereby blocking apoptosis. Mcl-1 is overexpressed in many human cancers causing disease progression and resistance to chemotherapies. Previous studies indicate that specific down-regulation of Mcl-1 induces apoptosis and overcomes Mcl-1-mediated resistance to apoptosis, emerging Mcl-1 as an attractive molecular target for developing small molecule inhibitors as novel anticancer therapies. The goal of this study was to accomplish biochemical and cell-based characterization of several small molecule inhibitors of Mcl-1. Competitive fluorescence polarization based assay was used to determine the binding affinity of tested compounds using a fluorescein-labeled 21mer Bid BH3 peptide and recombinant Mcl-1 protein. Using CellTiter-Glo luminescent cell viability assay, the potency of the small-molecule Mcl-1 inhibitors to inhibit the growth of cancer cells was determined in a panel of acute myeloid leukemia (AML) cell lines. Furthermore, the compounds were tested in murine embryonic fibroblasts (MEFs), wild type and deficient in both Bax and Bak (double knock-out). These model cell lines were used to determine if the mechanism of cell death induced by the tested compounds was through the Bak/Bax-dependent intrinsic apoptotic pathway. The results obtained from this study will provide useful information for design of novel small molecule inhibitors with improved potency, as well as for further understanding the role of Mcl-1 protein in AML.

Oral Presentation

Field emission-driven Townsend discharges for silver nanoparticle synthesis

Jordan Campbell
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Advisor: David Go, Dept. of Aerospace and Mechanical Engineering, University of Notre Dame

Electron driven reactions have motivated research into alternatives to lithographic processes. Our focus has been to scale down discharges to lower potential differences by increasing the electric field by using smaller gap sizes between electrodes, still maintaining a comparable magnitude of current. Field emission-driven Townsend discharges were identified as a viable type of discharge and proof of concept experiments were conducted to demonstrate atmospheric – pressure synthesis of silver nanoparticles in polymer films. Polymer films were spincoated onto SiO2 wafers sputtered with tungsten and were made from an aqueous mixture of 0.1 – 0.001 M AgNO3 and 0.5 – 1 wt % polyvinyl alcohol. A tungsten needle with a tip radius of either 1 or 5 μm was positioned 2 μm above PVA/AgNO3 film and an electric potential of 300 V was applied yielding field emission currents on the order of 1 nA. The field emitted electrons from the needle were used to electrochemically reduce silver ions to produce silver nanoparticles. SEM and EDX analysis was conducted on each sample before and after field emission trials and confirmed the formation of nanoparticles on the order of 5 – 50 nm silver metal nanoparticles. Future work will focus on repeatability and parametric studies to fully understand and control the synthesis process.

Oral Presentation

Damage of DNA in DNA-Gold Nanoparticle Mixture by Atmospheric Pressure Plasma Jet

Elissa Canseco
Sylwia Ptasinska, Dept. of Physics, University of Notre Dame
Advisor: Sylwia Ptasinska, Dept. of Physics, University of Notre Dame

Plasma healthcare has made pronounced scientific encounters that are revealed clearly in many areas such as medicine, food safely, environmental hygiene, and cosmetics [1]. In medicine, the plasma synergy with gold nanoparticles (GNPs) can possibly yield in greater DNA damage in tumor cells than that inflicted solely by the plasma. Our previous research that utilized Atmospheric Pressure Plasma Jet (APPJ) showed a high increase of strand breaks in DNA treated by APPJ [2]. It is well known that the addition of GNPs, which can penetrate biological tissue, has a significant potential as a treatment for infectious diseases and cancers. In the present work our attention is on the use of APPJ and GNP, we compare qualitatively and quantitatively damage to DNA during APPJ exposure with and without GNPs in samples. The conclusion came through qualitative analyses via a standard gel electrophoresis technique for identifying damage in DNA samples. We are focused on the effects of the APPJ with the addition of gold nanoparticles at different times of plasma exposure, GNP concentrations, and distances from the plasma source. We have found that using both technologies, i.e., plasma and GNPs, the DNA molecule experiences more breaks in its sugar-phosphate backbone.
References:
[1] G E Morfill et al 2009 New J. Phys. 11 115011 DOI:10.1088/1367-2630/11/11/115011
[2] S Ptasinska et al. 2010 Phys Chem Chem Phys. 12 7779 DOI: 10.1039/C001188F

Poster Presentation

Investigating the Photodissociation of Hydroxocobalamin using Steady State and Time Resolved UV-Visible Spectroscopy

Alexa Carollo
Joseph Thomaz
Brenden Arruda and Theodore Wiley, Dept. of Chemistry, University of Michigan
Advisor: Roseanne Sension, Dept. of Chemistry, University of Michigan

It is known that alkylcobalamins, such as methylcobalamin, photolyze and produce cob(II)alamin and an alkyl ligand radical. The photochemistry of hydroxocobalamin (HOCbl), a non-alkylcobalamin, is of interest since theoretical calculations simulating photolysis have suggested that photodissociation of the cobalt-oxygen (Co-OH) bond does occur with excitement at the correct wavelength. The photophysics of HOCbl is also of interest due to its suggested use in the temporal control of DNA cleavage. Previous experimental data suggests that the hydroxyl radical formed from the photolysis of HOCbl causes significant DNA cleavage that can be controlled by visible light illumination with a mercury lamp. In the work presented, we studied the photochemistry of HOCbl using steady state UV-visible and ultrafast transient absorption spectroscopy. In an attempt to reproduce past experiments, steady state spectroscopy was used to characterize the photoproducts following the illumination of HOCbl in solvents of different pH measurements and with different radical scavengers. UV-visible absorption spectra were obtained for illumination times up to ninety minutes. Difference spectra from the initial scan prior to illumination showed no significant change in absorption, giving inconclusive information about the photoproducts of HOCbl. Femtosecond transient absorption spectroscopy was used to study the excited state intermediate of HOCbl following excitation at 266 nm. Average difference spectra were obtained, and the excited state lifetime of HOCbl in solution was determined to be 2.9 ps. The total ground state recovery suggests a low quantum yield of cob(II)alamin. Further research includes studying the wavelength dependence of the photoproducts by exciting HOCbl at additional wavelengths.

Poster Presentation

Knockdown of G-protein coupled receptors in adult female *Anopheles gambiae* using RNAi

Katelyn Carothers
Douglas Shoue, Mary McDowell Dept. of Biological Sciences, University of Notre Dame
Advisor: Mary McDowell, Dept. of Biological Sciences, University of Notre Dame

Malaria, yellow fever, and other insect transmitted diseases are a growing worldwide concern, responsible for millions of human deaths every year. Increased human population and urbanization of tropical areas contribute to the continued spread of the diseases, as well as growing insect resistance to current insecticides and concerns of their effect on the environment and on human health. G-protein coupled receptors, already a common drug target in humans, contribute to a variety of physiological processes in eukaryotes, and are under consideration as novel targets for insecticides. The targets of this study included AgOAR45B, an octopamine receptor, and AgNPF10626 and AgNPF2733, the respective receptor and ligand of neuropeptide F in *Anopheles gambiae*. We attempted to knock down the production of AgOAR45B in adult female *Anopheles gambiae* via infection with a recombinant Sindbis virus containing the antisense sequence to the AgOAR45B, in order to induce RNA interference in the cells. We also transcribed dsRNA for AgNPF10626 and AgNPF2733 for direct injection into the mosquito as an alternative to the viral pathway of gene knockdown. We then quantified the expression of the genes in infected and control mosquitoes using qRT-PCR. Knockdown of gene expression by RNAi can contribute to greater knowledge of the target gene's role in the organism. Future studies may include screening of agonists and antagonists for AgOAR45B and AgNPF10626, and their development as components in future insecticides.

Poster Presentation

α3DH3-GSGA-F31A, A *De Novo* Designed Metallopeptide

Sarah Caruso
Virginia Cangelosi, Dept. of Chemistry, University of Michigan
Advisor: Vincent Pecoraro, Dept. of Chemistry, University of Michigan

De novo protein design is a powerful method for modeling biological systems. Using this technique, it should be possible to design receptors, enzymes, and ion channels from scratch. However, there are many challenges to using this technique, and the field of de novo protein design is just reaching the point where researchers can model natural enzymes with rates that are within several orders of magnitude. The Pecoraro lab recently published a carbonic anhydrase model (CAII) with rates of CO2 hydration that are only 550-fold slower than the natural enzyme. One drawback to this current model is that it has been constructed in a highly symmetric environment, making substitutions to further improve catalysis difficult. Using de novo protein design, my goal is to model CAII within a single-stranded three-helix construct, α3DH3, which contains three histidine residues at the c-terminus for binding Zn(II) and will allow easy point mutations.

Poster Presentation

Integer Solutions to Diophantine Equations

Gonzalo Cazes-Nasitiqui
Advisor: Samuel Evens, Dept. of Mathematics, University of Notre Dame

Diophantine equations are polynomial equations with integer coefficients, whose solutions are given in integers. Among the many Diophantine equations are the ones known as Bachet's equations. These are equations of the form y[^2^]= x[^3^] + k, where k is some integer. For any integer, k, there are only finitely many solutions to the equation, if any exist at all. There are many conditions on k that determine whether or not a solution exists, and how to find it. I will discuss certain conditions that guarantee no solutions, as well as some that do give solutions, as well as proving a general formula for finding the solutions for certain values of k.

Poster Presentation

Exploring the polymorphism of piperine

Brianna Chamberlin
Advisor: Adam Matzger, Dept. of Department of Chemistry, University of Michigan

Piperine, a component of *Piper Longum*, was studied to determine if the compound exhibited polymorphism, the ability of a crystalline material to form multiple unique packing structures. The discovery of novel crystalline forms is of great importance to the pharmaceutical industry due to the effects unique molecular packing can have on the physiochemical properties of a compound. In addition, each form is a unique composition of matter leading to intellectual property implications. Polymorphic studies of piperine are especially intriguing because it exhibits low solubility in water and also qualities of a biomodulator. Therefore piperine can vary the bioavailability of another compound when administered simultaneously. Using polymer-induced heteronucleation (PIHn) and other crystallization techniques, three novel polymorphs have been discovered and one crystal structure has been determined. The crystal forms of piperine have been characterized by Raman spectroscopy, X-ray diffraction, and differential scanning calorimetry.

Poster Presentation

TcpP Diffusion Rate and Concentration in a Chemical Gradient Using Single-Molecule Fluorescence Imaging of *Vibrio cholerae*

Rachel Choi
David Rowland, Dept of Biophysics, University of Michigan
Advisor: Julie Biteen, Dept. of Chemistry, University of Michigan

The bacterium, *Vibrio cholerae*, is responsible for the disease cholera that afflicts many people who lack access to good sanitation and clean water. Since this bacterium has a polar flagellum, it is very motile. Cholera toxin (CT) is a protein complex that causes water and chloride to be secreted in the intestines, leading to the dehydration affiliated with the disease. TcpP, a transcription activator of *toxT*, regulates the production of CT. TcpP works with ToxR to activate *toxT* transcription while the pathway of *V. cholerae* regulating ToxT expression is turned on; during transcription, TcpP should move slowly. When the transcription pathway is turned off, TcpP should move more quickly. We therefore propose to study the motion of TcpP under the effects of chemicals that can turn the pathways on and off, and to use gradients of these inducers to access multiple concentration points. In the experiment, an agar pad is used as a medium for immobilized cells and a concentration gradient of auto-inducer, pH, or spent media. To observe the cells, the agar is put on a microscope slide and imaged by single-molecule super-resolution microscopy. From a few recent experiments, a dye, fluorescein, was used to trace the movement of the gradient. Through the microscope, a heavy flow of cells could be seen moving, which was reduced by the addition of M9 solution. This imaging will show with nanometer-resolution how TcpP moves in the cells when they are at different concentration levels in the chemical gradient. Single-molecule fluorescence imaging of *V. cholerae* cells should show a direct correlation between the TcpP diffusion rate and the concentration in a chemical gradient.

Poster Presentation

A Hybrid Optical Detection Method

Kasey Clear
Sarah Stroud
Advisor: Bradley Smith, Dept. of Chemistry and Biochemistry, University of Notre Dame

Sensing of biologically relevant anions is an important theme in supramolecular and analytical chemistry. Both 'naked-eye' and luminescence methods are commonly used in sensor design. While easy to use and interpret, naked-eye sensing methods are limited by relatively low sensitivity and detection limit for analytes. Conversely, fluorescent and other luminescent sensors have far better sensitivity, but require special instrumentation to detect. The present study demonstrates a method for simultaneous determination of anions by incorporation of both naked-eye detection and turn-on luminescence strategies, allowing rapid qualitative and quantitative analyte detection. In the system, a complexometric indicator is bound to a lanthanide in aqueous solution. Upon addition of the analyte, the indicator is displaced, leading to a detectable color change and a concomitant increase in luminescence by energy transfer from the analyte.

Poster Presentation

The New Digital Playground: Applications of 3D Printing within a K-12 Setting

Phillip Cook
Alexa Kutch
Advisor: Paul McGinn, Dept. of Chemical and Biomolecular Engineering,
University of Notre Dame

3D printing offers novel means by which to design and fabricate custom prototypes out of a variety of materials. As the cost of entry into 3D printing continues to decrease, the technology becomes increasingly accessible to K-12 schools. 3D printers offer a myriad of uses within a K-12 educational framework; from the creation of "maker" spaces to integration within existing science, mathematics and engineering courses. Over the course of a seven-week Research Experience for Teachers program, a locally manufactured and sourced 3D printer was constructed from scratch. The printer was then calibrated and utilized to develop curriculum in mathematics and science. The culminating experience from this project sheds insight on what it takes to create a "maker" environment within a school setting, as well as raises challenges to ensuring the thoughtful and careful integration of the printer into existing educational environments.

Poster Presentation

A New Computational Approach to Gelator Discovery

Sarah Cox
Kesley King, Dept. of Chemistry, University of Michigan,
Advisor: Anne McNeil, Dept. of Chemistry, University of Michigan

Molecular gels are materials that exhibit solid-like properties despite being comprised of mostly liquid. Gelators can be applied to a variety of different uses such as sensing, tissue regeneration, and drug delivery. Small molecule gels self-assemble into long entangled cross linking fibers that can entrap solvent. To predict gelators, which are normally found by chance, a method was developed to examine the solid-state packing structures of lead-containing compounds through the use of crystal morphology prediction software. Compounds with needle-like predicted morphologies were specifically targeted due to their similarity to the fibers in a gel network. Lead-containing compounds were selected for initial screening to develop a gel-based sensor to detect lead in paint. From the total compounds screened through the software, 5% of the largest predicted aspect ratios were scrutinized for possible synthesis and gel screening. After synthesizing 7 derivatives of the first selected compound, a new molecular gel was found! This presentation will describe the efforts to predict new gelators using computational methods and the efforts that lead to synthesizing a new lead containing gelator.

Poster Presentation

Synthesis of Nickel Diimine Complexes as Possible Catalysts for the Polymerization of Electron Deficient Monomers

Will Crosby
Ed Palermo and Mitchell Smith, Dept. of Chemistry, University of Michigan
Advisor: Anne McNeil, Dept. of Chemistry, University of Michigan

Conjugated polymers are promising materials for optical and electronic devices such as solar cells and organic light emitting diodes due their ability to absorb/emit light and conduct charge along the π-backbone. These properties are different from most organic polymers, which are colorless insulators. In the past, synthesis of conjugated polymers was only done through step-growth polymerization, which produces polymers of various molecular weights giving some undesirable properties. This technique has changed within the last 10 years with the discovery of living chain-growth polymerization techniques leading to more regular and easily controlled structures and, therefore, properties, leading conjugated polymers to be more useful and efficient in their applications. To date, one limitation of chain-growth synthesis of π-conjugated polymers is that only electron rich monomers can be polymerized with the current catalysts. Nickel diimine catalysts have been used in the chain-growth polymerization of olefins and 3-hexylthiophene, so their possible use as catalysts for electron deficient conjugated monomers, such as thiazoles, was investigated. Two diimine ligands and their resulting nickel complexes were successfully synthesized. These catalysts were then used in the attempted polymerization of (5-bromo-4-hexylthiazol-2-yl)magnesium chloride. No high molecular weight polymer was obtained, only oligomers, similar to the behavior of more traditional catalysts for chain-growth polymerizations of 4-hexylthiazole, so it does not appear to be a suitable candidate for a catalyst for the polymerization of (5-bromo-4-hexylthiazol-2-yl)magnesium chloride.

Poster Presentation

Synthesis of a Hydroxybenzoate Ligand for a Class 1A Dihydroorotate Dehydrogenase

Christine Cuthbertson
Advisor: Bruce Palfey, Dept. of Biological Chemistry, University of Michigan

Dihydroorotate dehydrogenases (DHODs) catalyze the only redox reaction in pyrimidine biosynthesis—the oxidation of dihydroorotate to orotate. Class 1A DHODs are found in some disease-causing protozoans, which make them possible drug targets in the treatment of Leishmaniasis, Chagas' disease, and African sleeping sickness. An enzymatic route for synthesizing ligands has been established utilizing the enzyme p-hydroxybenzoate hydroxylase (PHBH). PHBH was overexpressed using the plasmid pIE-130 in *Escherichia coli* strain JM105 and purified by salting-out some impurities with ammonium sulfate, dialyzing, treating with heat, followed by affinity chromatography using a Red-Dye column. A ligand was made by the hydroxylation of hydroxybenzoate-precursor by PHBH. Purification was completed by HPLC and the ligand was verified by UV-vis spectrophotometry and NMR spectroscopy.

Poster Presentation

Modeling the Formation and Propagation of Thermal Bar in Lake Ontario using Climatological Parameters

Randolph David II
Rumana Reaz Arifin, Dept. of Civil, Environmental Engineering and Earth Sciences, University of Notre Dame
Dilkushi Pitts, Center for Research Computing, University of Notre Dame
Ashish Sharma, Dept. of Civil, Environmental Engineering and Earth Sciences, University of Notre Dame
Scott C. James, Exponent, Los Angeles, CA
Harindra J. Fernando, Dept. of Civil, Environmental Engineering and Earth Sciences, University of Notre Dame
Andika Suhardjo, Center for Research Computing, University of Notre Dame
Advisor: Dilkushi Pitts, Center for Research Computing, University of Notre Dame

The formation of thermal bars during Spring turnover is an important phenomenon in large temperate lakes. This study is motivated by concerns on nearshore lake health caused by downwelling of dense water at the thermal bar, which acts as a barrier to horizontal mixing. Decreased horizontal mixing reduces the exchange of nutrients, alters habitats of aquatic species, and may intensify eutrophication (algal blooms). Thermal bar formation and their propagation through Lake Ontario are simulated using hourly climatological input parameters from weather stations around Lake Ontario: wind speed and direction, atmospheric pressure, air temperature, water temperature, relative humidity, precipitation, solar radiation and cloud cover factor. The 3D hydrodynamic model – Environmental Fluid Dynamics Code (EFDC) – is used to simulate year 2011, February to August, on a curvilinear grid at ~2-km resolution. Simulation of the thermal bar formation will be continued for subsequent years 2010-2005 and results will be compared with remotely sensed surface-temperature data to help understand the climatic impact on thermal stratification in Lake Ontario.
The mission for the summer REU project was to find an efficient way to gather the weather data for the years 2012-2005, format, and critically analyze the data sheets for the hydrodynamic model. In order to format the weather station data efficiently, python programming was used to format and do data analyze by using plotting python libraries and examining any possible outliers.

Oral Presentation

Using Gamma Ray Burst to Estimate Luminosity Distances

Shanel Deal
Advisor: Peter Garnavich, Dept. of Physics, University of Notre Dame

Gamma ray bursts (GRBs) are short flashes of gamma-rays that occur in star forming regions of galaxies. In the early 2000s, a correlation between the isotropic equivalent energy radiated by the gamma ray burst and the spectral peak energy was found. This is now known as the Amati Relation. With this correlation GRBs could be used as cosmic standard candles. GRBs distances can be estimated by using the calculated isotropic energy and the observed fluence with the inverse-square law. We used the NASA Swift database to identify approximately 150 gamma ray bursts with known redshifts. From the database, we collected the duration, fluence, and the Band Function parameters such as alpha, beta, and the peak energy. We fitted a linear relation between the spectral peak energy and the isotropic energy to test the Amati Relation. We see a rough correlation with scatter and many GRBs fall far from the Amati Relation. We also applied the inverse-square law test. Our results suggest that the Amati Relation will not provide reliable distances to GRBs but other methods of estimating luminosity distance merit further research.

Poster Presentation

Inverse Islands: Comparing Matrilineal Structure Using mtDNA Between Singapore and Bali Long-Tailed Macaques

Allison Dianis
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Advisors: Hope Hollocher, Dept. of Biological Sciences, University of Notre Dame and Agustin Fuentes, Dept. of Anthropology, University of Notre Dame

Landscapes genetically structure populations by restricting gene flow between groups. Long-tailed macaques, *Macaca fascicularis*, have an overall range spanning mainland Asia down through Indonesia, which presents numerous opportunities for populations to be shaped by human altered landscapes. In previous analyses of mitochondrial DNA (mtDNA) of the long-tailed macaque, two distinct monophyletic lineages are observed – the 'insular' and 'continental.' It has been found that individuals sampled from Bali are grouped within a single 'insular' clade of *M. fascicularis*. A preliminary haplotype network constructed using the mtDNA D-LOOP hypervariable region I revealed structure indicative of high site fidelity - leading to the belief that the matrilineal structure of *M. fascicularis* populations has fostered this structure and maintained variation between groups in Bali. In contrast, a preliminary haplotype network constructed using mtDNA D-LOOP hypervariable region I and II from individuals sampled across Singapore indicated minimal population structure across the island. Here I propose a research plan for determining how matrilines vary across *M. fascicularis* populations in Singapore because of the landscape differences between Singapore and Bali. While Bali is a large island with an agricultural landscape and a population who provisions macaques, Singapore is a small island with an urban landscape where macaques are less revered by the local culture. This difference in landscape could reflect in the difference in mitochondrial DNA in Singapore and Bali populations. I also seek to answer how landscape influences the number of matrilines present in a population because long-tailed macaques live in matrilineal based groups; therefore, the matrilines present could be linked to the relative isolation of particular populations. Likewise, this information could correlate to the presence of specific haplotypes within matrilines, showing dispersal trends, or to the landscape of the island, indicating the influence on the maintenance of matrilines.

Oral Presentation

Detangling the Cosmic Web: Computational Models of Galaxies in Filaments

Sarah Dietz
Advisor: Lara Arielle Phillips, Dept. of Physics, University of Notre Dame

Sheets, filaments, and voids are Large Scale Structures (LSS) that describe patterns of galaxy organization in what is known as the Cosmic Web. Filaments contain galaxies, gas and dark matter, and it is of interest to study how galaxies interact with the filaments they are embedded in. We modify an existing fluid dynamics program to create a two-dimensional computational model of a galaxy in a filament. We studied both galaxies with spins parallel to the flow of their host filaments and galaxies with spins perpendicular to their filaments, in order to observe how the exchange of material between galaxy and filament differed for each case. The program solves the incompressible Navier-Stokes Equation allowing us to model the exchange of energy between galaxies and filaments. However it does not allow for variable density and the modeling matter exchange between galaxies and filaments. We therefore turn to programs that provided solutions to the compressible Navier-Stokes Equation to study the models.

Poster Presentation

Examining the Conformational Dynamics of Proteins and snRNAs during Splicing using smFRET

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Advisor: Nils Walter, Dept. of Chemistry, University of Michigan

The spliceosome is a complex cellular machine responsible for catalyzing the two step process in which noncoding introns are removed from precursor messenger RNA (pre-mRNA) transcripts followed by ligation of the flanking coding exon sequences to produce mature messenger RNA (mRNA) through a process termed splicing. Spliceosome assembly upon a pre-mRNA substrate requires the stepwise coordination of five small nuclear RNAs (snRNAs) and numerous proteins with the purpose of creating mRNA that can be correctly transcribed by the ribosome. Given the highly dynamic nature of the spliceosome and the lack of ideal tools available to study splicing, many specific steps of splicing and spliceosome assembly are not well understood. Single-molecule fluorescence microscopy tools have recently been developed in the Walter Laboratory that allow for a more comprehensive study of splicing. In an effort to expand on these techniques, this study has two components. The first objective was to investigate whether a vital heat resistant first step protein, Cwc25, undergoes conformational changes prior to or during the first step of chemistry. This required recombinant expression and purification of a modified Cwc25 protein containing cysteine residues at the N and C-termini for incorporation of FRET-pair fluorescent dyes onto the protein. The second objective was to observe the relationship between the U6 and U2 snRNA during catalysis. Endogenous U6 and U2 snRNAs were depleted from yeast cell extract using DNA oligonucleotides D1 and SRU2 which anneal to U6 and U2, respectively, allowing for recognition and digestion by RNaseH. This depleted extract can then be reconstituted with in vitro transcribed, 3' labeled (Cy3) U6 snRNA and 5' labeled (Cy5) U2 snRNA. Using a spliceosome stalled immediately prior to the first step of splicing, the relationship between the U6 and U2 snRNA can be monitored using single-molecule FRET.

Poster Presentation

Synonymous Codon Usage

Simone Dozier
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Codons are nucleotide triplets that code for amino acids. A set of codons that correspond to the same amino acid are “synonymous”. Surprisingly, which synonym is used can have an effect on translation speed and the final structure of the folded protein. I generated visuals for existing projects, and investigated whether codon functionality extended to viruses.

Poster Presentation

Plasmon-Enhanced Fluorescence Imaging of the Intrinsic Emission of Single Coenzyme B12 Molecules

Kevin Durand
Mou-Chi Cheng, Dept. of Chemistry, University of Michigan
Advisor: Julie Biteen, Dept. of Chemistry, University of Michigan

The inability of traditional optical microscopy to visualize biomolecular events has hindered the ability of researchers to further comprehend biological processes. The benefits of fluorescence microscopy are two-fold: biomolecular activity can be studied in vivo and specific biomolecules can be labeled, but this method is limited to the standard diffraction limit of light, approximately 0.5 μm. With the introduction of single-molecule fluorescence (SMF) microscopy, however, resolutions far below the standard diffraction limit can now be attained. [1,2] Unfortunately, SMF requires bright emission. As such, SMF does not typically resolve intrinsic emission; rather, biomolecules are generally tagged with artificial markers such as fluorescent proteins or organic dyes. [3]

In the hope of eradicating false reporting by extrinsic markers, here we utilize intrinsic fluorescent reporters to study B12-dependent enzymes. Our goal was to use a cofactor directly involved with the biomolecule's function, allowing us to avoid artifacts from artificial labels. For these SMF experiments, the compound hydroxocobalamin, a derivative of coenzyme B12, has been studied *in vitro*. Coenzyme B12 is a valuable reporter molecule because of its intrinsic fluorescence. Furthermore, the activity of coenzyme B12 has been extensively studied. Using a reporter molecule for which thorough information is readily available makes this cofactor-enzyme pair the perfect springboard for the advancement of the study of B12-dependent coenzymes.

Although using hydroxocobalamin to assess enzymatic activity has clear and significant advantages over reporter-engineered molecules, its inherent fluorescence is very weak. In order to enhance its fluorescence, this compound was coupled to silver nanoparticles, which can support a localized plasmon (charge-oscillation) mode and generate electromagnetic fields to enhance fluorescence. We aim to achieve plasmonic enhancement of hydroxocobalamin on the silver nanoparticles. We have grown silver nanoparticles via the rapid deposition techniques developed by the Geddes group [4] and immobilized coenzyme B12 in a network of polyelectrolyte layers constructed on top of the silver nanofilm. [5] In the future, we hope to study adenosylcobalamin in vivo to report on the activity of glutamate mutase. As coenzyme B12 in glutamate mutase approaches the nanoparticles, the protein-coenzyme complex should reside at the optimal distance corresponding to maximum fluorescent enhancement.

Poster Presentation

Investigation of changes in cardiac innervation in a mouse model of Dravet Syndrome

Nnamdi Edokobi
Charles Anumonwo, David Auerbach, and Heather O'Malley, Dept. of Pharmacology, University of Michigan
Advisor: Lori Isom, Depts. of Pharmacology and Molecular and Integrative Physiology, University of Michigan

Dravet Syndrome (DS, also known as Severe Myoclonic Epilepsy of Infancy) is a catastrophic pediatric epileptic encephalopathy caused by heterozygous loss of function mutations in *SCN1A*, encoding the α subunit of the voltage-gated sodium channel **$Na_v1.1$**, which is expressed in brain and heart. Individuals with DS experience severe seizures, behavioral and developmental delays, ataxia, growth and nutrition issues, chronic infections, sensory integration disorder, and disruptions of the autonomic nervous system. They also face higher incidences of Sudden Unexpected Death in Epilepsy (SUDEP) than individuals with general forms of epilepsy. The mechanism(s) underlying SUDEP are not understood, however, cardiac arrhythmias and autonomic imbalance are thought to play a major role. For example, aberrant cardiac innervation by autonomic neurons during development may lead to fatal cardiac arrhythmias. We are using a DS mouse model expressing a human *SCN1A* DS mutation to test for differences in cardiac innervation. We prepared cardiac whole mounts from wild-type and DS mice to compare the localization of cholinergic, adrenergic, and peptidergic neural components using immunohistochemical labeling followed by fluorescence microscopy. We propose that, through understanding the mechanism of SUDEP in mouse models, we may be able to translate our results to the future development of novel therapeutic agents to treat this devastating disease in children.

Poster Presentation

Characterization of J-Binding Protein 1

Osama El-Sayed
Advisor: Raymond Trievel, Dept. of Biological Chemistry, University of Michigan

β-D-glucopyranosylomethyluracil, or base J, is the first hypermodified base found in eukaryotic DNA. It is used in organisms to switch nucleotide sequences in DNA in order to change the variant surface glycoprotein that is expressed. As a result, the expressed glycoproteins are able to change the amino acid sequence as well as the attached sugar. This unique ability is used by these organisms to avoid being destroyed by the adaptive immune system. Very little is still known about the exact function of base J.

JBP1 is a protein involved in the propagation of base J. It has two main domains: J-Binding (JBD) domain and thymidine hydroxylase (TH) domain. The JBD domain is the domain involved in binding the base J while the TH domain is the catalytic domain involved in the reaction. In my project we looked into characterizing the TH domain via x-ray crystallography and limited proteolysis to learn more about its structure and function.

Poster Presentation

Mathematical modeling and control of co-transmitting soil-transmitted helminthes

Nichole Etienne
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University of Notre Dame

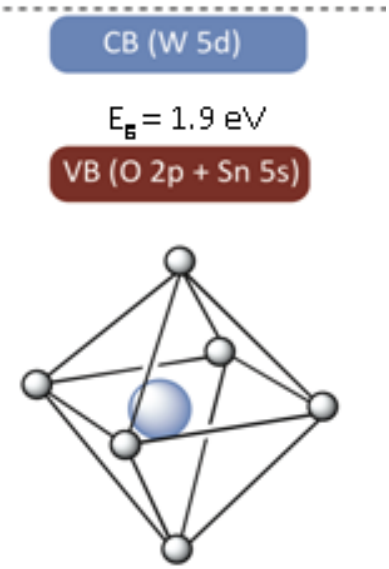
Soil Transmitted Helminthes (STH) refers to a group of nematode worms causing human infection through the contact of parasite eggs or larvae which usually thrive in tropical or subtropical areas of the world. These worms usually enter the human body via direct or indirect transmission, sometimes even via skin penetration. Infection by such worms may result in impairment in physical, intellectual or cognitive development. Over the past few years the numbers for individuals being infected by such parasite has greatly increased, raising awareness worldwide. With this in mind there is a need for a system that controls the number of infection in order to reduce morbidity, hence the use of mathematical modeling. Mathematical modeling refers to a system of concept and languages. This research mainly looks mainly at elimination and control. Mathematical modeling has the ability to help in the understanding of the parasite population biology and the effects of control intervention as well as the exploration of different parameters and the likely outcomes. The STH model used in this research is based on a basic model derived from Anderson and Medley. In this, the host population is taken into consideration as well as worm population and the different parameters of transmission and contact. All of which are based on differential equations and all tested.

Poster Presentation

Synthesis of α-$SnWO_4$

Taylor Evans
Kayla Pyper, Dept. of Chemistry, University of Michigan
Advisors: Bart Bartlett and Kayla Pyper, Dept. of Chemistry, University of Michigan

If we look at the energy consumption today in terms of the amount consumed in one year we are using 13 TW. This number is projected to increase to 30 TW by the year 2050. Using the sun to split water by converting solar energy into chemical energy in order to produce hydrogen as an alternative fuel is the goal. There are many challenges in trying to produce a material that will be efficient in producing both hydrogen and oxygen. The rate limiting step of this reaction is the four electron redox process needed for water oxidation and is the focus of my research. α-$SnWO_4$ is projected to be a promising photocatalyst for the purpose of water oxidation based on the experimental and theoretical calculations of its band structure and absorption properties. The material α-$SnWO_4$ if synthesized in air. Common syntheses utilize vacuum or inert atmospheric conditions, which make it difficult to produce a thin film or uniform powder samples. We have employed a new low temperature hydrothermal method to convert thin crystalline WO_3 films and nanopowders to α-$SnWO_4$, which will be used to study the photoelectrochemical properties.



Poster Presentation

Design of a Fast-Acting Coliphage Biosensor Device

Heather Fick, Jennifer Parra, Kirin Kuar, Stephanie Sesse, Vera Marcello,
Arika Haines, and James K. Campbell
Advisor: George Twaddle, Dept. of Biotechnology, Ivy Tech Community College of Indiana

The American Public Health Assay (APHA) for human waste contaminated water is hampered by a dependency on culturing coliform bacteria with a turn-around time exceeding one day. An assay for coliphage detection, as surrogate for coliforms, has been developed which employs the release of the host indicator cell β-galactosidase enzyme (β-gal) activity by lytic coliphage and the conversion of a colorimetric substrate. While significantly shortening the APHA time to 3 hrs., this assay requires a laboratory equipment to separate phage-induced released β-gal enzyme from intact cells before addition of the substrate. To optimize this assay we have taken advantage of the α-complementation feature of β-gal. We are engineering cell lines containing either the gene fragments of LacZα or LacZΩ of β-gal on separate plasmids. We predict upon lysis of a mix population of cells by coliphage in the presence of substrate, the gene products will complement in trans reconstituting the β-gal activity thus eliminating a separation step in the assay. In addition we are testing the introduction of a cassette of coliphage cell lysis genes on both plasmids under the control of a coliphage promoter to accelerate the enzyme fragment release thus further reducing test time. Our goal is to design a fast-acting hand-held coliphage biosensor device that can be used by someone without any special technical expertise. We anticipate our device being useful in rapidly reporting the contamination of recreational waters in the U.S. or assuring potable water in the water sources in the developing World.

Poster Presentation

Non-Invasive Optical Imaging of Near Infrared Electrospun Nanoparticles

Nathan Foje
Raghuraman Kannan, University of Missouri-Columbia
Sarah Chapman and W. Matthew Leevy, Dept. of Chemistry and Biochemistry, University of Notre Dame
Advisor: W Matthew Leevy, Dept. of Chemistry and Biochemistry, University of Notre Dame

Nanoparticles are part of a growing, powerful wave of new technology that focuses on the special properties that come from extremely small size. Nanoparticles possess great potential in medicine and biology due to their unique properties that allow them to be selectively taken up by specific organs based on their size and chemical properties. Electrospun nanoparticles are made by creating an electric field between the tip of a syringe containing liquid nanoparticle material and a pool of water. As the syringe is depressed small droplets of charged nanoparticle material are expelled and follow the electric field into the water where they are collected. These nanoparticles are especially important in that they can be tuned to selectively collect in specific organs for imaging or potential drug delivery. Near infrared nanoparticles emit light when excited at a certain wavelength which allows researchers to determine the location of the nanoparticles within the animal using high-tech optical imaging equipment. Due to their non-invasive nature nanoparticles show great promise for use in longitudinal imaging studies. Here we discuss the methodology behind the testing of near infrared electrospun nanoparticles, the importance of these nanoparticles, and the results of several pilot studies.

Poster Presentation

Characterization of Halogenases in the Malbrancheamide Pathway

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Advisor: David Sherman, Dept. of Medicinal Chemistry, University of Michigan

Malbrancheamide is a compound isolated from a fungus, *Malbranchea aurantiaca*, that has demonstrated chemotherapeutic potential through its use as a calmodulin antagonist. The halogen substituents located on the indole ring differentiate Malbrancheamide from the rest of the bicyclo[2.2.2]diazaoctane family, and they are critical to its biological activity. Consequently, this investigation was aimed at determining and characterizing the enzymes involved in the halogenation step of the Malbrancheamide biosynthetic pathway. It has been hypothesized that a flavin-dependent halogenase, as well as a flavin-reductase are required for the dichlorination of Premalbrancheamide in two sequential steps to form Malbrancheamide. MalA, a halogenase from the fungal gene cluster consisting of seven genes that are responsible for the production of Malbrancheamide, was expressed alongside previously identified putative halogenase, MalHal, and reductase, MalRed. Additionally, phaC, which codes for a known flavin-reductase from *Pseudomonas aeruginosa*, was also expressed and tested in these reactions in order to determine the halogenase specificity for the reductase that it interacts with. Through testing the isolated enzymes on various substrates (Tryptophan, Premalbrancheamide, Malbrancheamide B, and Isomalbrancheamide B), the details behind the chlorinations in the pathway may be revealed. The product formation was monitored through LC-MS analysis of the reaction solution and further studies will be performed to elucidate the identities of potential products being formed.

Poster Presentation

An Investigation into the Factors that Affect Compartment Size in *Drosophila* Epidermal Larval Segments during Embryogenesis

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University of Notre Dame
Advisor: Jeremiah Zartman, Dept. of Chemical and Biomolecular Engineering,
University of Notre Dame

The epidermal growth factor receptor (EGFR) signaling pathway is a prominent signaling pathway involved in cell proliferation that has been linked to tumor development. This project uses *Drosophila melanogaster*, the common fruit fly, as a model organism to study the effect EGFR has on the patterning of apoptosis during Drosophila embryogenesis. In Joseph Parker's paper, *Control of Compartment Size by an EGF Ligand from Neighboring Cells*, he proposes the primary EGFR signaling ligand, Spitz, is the main control of compartment size within the developing *Drosophila* embryo. Parker found that Spitz, a ligand secreted from the neighboring anterior (A) compartment, regulates the posterior (P) compartment size in the *Drosophila* embryo through a balance of cell proliferation and apoptosis. The aim of this project is to further test his conclusions as well as quantify a concentration gradient across the developing epidermal segments for several main ligands associated with the EGFR signaling pathway. Apoptotic activity in *Drosophila* embryos between stages 10-12 is examined to investigate links between EGFR signaling and apoptotic activity. A long-term goal of this project is to monitor the stages of development using live imaging techniques to visualize the patterns of apoptosis. These patterns can be compared to concentration gradient data to determine whether there are correlations between which cells undergo apoptosis and their relative concentrations of important morphogens. Immunohistochemical techniques on genetically modified *Drosophila* embryos are used to visualize and quantify morphogen concentrations. Staining for TUNEL and cleaved-Caspase-3 mark apoptotic cells. This project is particularly important to cancer research as the EGFR signaling pathway is one of the main pathways implicated in tumor development. Some cancer treatments are specifically targeting this pathway in cancer cells to stop proliferation. Understanding the main ligands involved and their effect on cellular decision-making is a crucial step toward better understanding tumor development.

Oral Presentation

New Targets for New Accelerators

Bryce Frentz
Advisors: Khachatur Manukyan and Ani Aprahamian, Dept. of Physics,
University of Notre Dame

New accelerators, such as the 5MV St. ANA accelerator, at the University of Notre Dame, will produce more powerful beams up to 100's of μAmps. These accelerators require a complete rethinking of target preparation since the high intensity of such beams would melt conventional targets. Traditionally, accelerator targets are made with a tantalum backing. Tantalum, while being a successful material to stop hadron beams, is also brittle, a poor conductor, and, if produced commercially, often contains impurities (e.g. fluorine) that produce undesirable background signals and reaction products. Despite tungsten's brittle structure and poor conductivity, its high proton number, allowing it to stop hadron beams, and lack of impurities make tungsten a more desirable backing than tantalum. In conjunction with tungsten's properties, copper is robust and a far superior conductor of heat. We describe a new method of reactive joining, which we developed for creating targets by using the advantageous properties of both tungsten and copper. This process involved placing a reactive mixture (thermite, Ti+C+Ni, or Ti+C+Si) between tungsten and copper and applying a load force. The mixture is then ignited, and while under pressure, the system produces conditions to join the materials. We present our investigation to optimize the process of reactive joining, as well as some of the final target's properties.

Poster Presentation

Visualizing Mismatch Repair in Live *Bacillus subtilis* using Single-Molecule Fluorescence Microscopy

Burke Gao
Yi Liao, Dept. of Chemistry, University of Michigan
Advisor: Julie Biteen, Dept. of Chemistry, University of Michigan

During DNA replication, the mismatch repair (MMR) system corrects base-paring errors made by DNA polymerase, and increases the fidelity of DNA replication several thousand-fold. The fidelity of DNA replication is important as the consequences of replication errors include the development of cancer in humans and antibiotic resistance in bacteria. Of particular importance to MMR machinery is the highly conserved protein MutS, which exists in both prokaryotes and eukaryotes, and which is responsible for mismatch detection and recruitment of downstream MMR proteins. However, the exact mechanisms by which MutS initiates MMR remains highly debated. A number of studies have shown that MutS can slide along DNA strands until encountering a mismatch-containing site. These findings support the "scanning-model," which argues that MutS binds to DNA and scans it independently in search for mismatched base pairs. Meanwhile, however, a second competing model known as the "replisome-associated model," proposes that MutS proteins are positioned near the replisomes subunit DnaN prior to mismatch binding, which increases the efficiency of mismatch detection in comparison to the scanning-model by allowing MutS to stay near the replication fork where it can target newly formed DNA, rather than having to scan the entire DNA for mismatches.

In order to discover exactly how MutS detects mismatches, we used single-molecule fluorescence microscopy to directly monitor how MutS and DnaN move and interact with each other in live cells of the model organism *Bacillus subtilis*. Because it has superior genetic competence and MMR repair pathways that are highly homologous with corresponding pathways in humans, B. subtilis serves as an ideal platform to carry out such an investigation. Our results have shown enrichment of MutS in the vicinities of DnaN, and have identified three sub-populations of MutS, each with its distinct diffusivity, and thus provide preliminary support for the replisome-associated model.

Oral and Poster Presentation

Probing the determinants of the metal binding specificity of HDAC8

Desiree Garcia-Torres
Byung Chul Kim, Dept. of Chemistry, University of Michigan
Advisor: Carol Fierke, Depts. of Chemistry and Biological Chemistry, University of Michigan

Histone deacetylases (HDAC) play a key role in regulating transcription and other cellular processes by catalyzing the hydrolysis of ε-acetyl-lysine residues. Class I, II and IV HDACs and many other enzymes incorporate a metal cofactor that directly participates in the chemical reaction catalyzed by the enzyme. Under in vitro conditions HDAC8 is activated by Co(II), Zn(II) and Fe(II) while the metal ion that activates the enzyme in vivo is likely Zn(II) or Fe(II). Determination of the metal-dependent activity and metal affinity in vitro provides insight into the selective metal incorporation in the cell. The ability of this enzyme to selectively bind Zn(II) or Fe(II) depends on both the relative free metal ion concentrations in cells and the relative K_D values for the metal-enzyme complexes. Metal binding sites typically contain amino acids that directly coordinate the metal ion and amino acids that form hydrogen bonds with the direct metal ligands, called "second shell ligands", that orient the ligands. However, in HDAC8 the second shell ligands are mainly hydrophobic and this may contribute to the relaxed metal selectivity. The goal of this project is to understand the functional role of the second shell ligands of HDAC8 by determining the effects of varying the structure of the second shell ligand at position 273 (Met substituted with Glu) on metal binding affinity and catalysis. The M273E mutation decreases the Co(II) affinity by 5-fold and may have similar effects on Zn(II) and Fe(II) affinity. However, the metal dissociation rate constants, k_{off}, for the mutant enzyme is comparable to that for the wild type, suggesting an alteration in the apparent association rate constant. Additionally, this mutation decreases the catalytic efficiency of HDAC8; the k_{cat} / K_M value decreases 1000-fold compared to the wild-type enzyme. These experiments provide insight into the determinants of metal selectivity of HDAC8 *in vitro* and *in vivo*.

Poster Presentation

Making Gasoline from Grass-Using heterogeneous catalysts to convert biomass into biofuel

John Gensic
Gregory Neumann, Dept. of Chemical and Biomolecular Engineering,
University of Notre Dame
Advisor: Jason Hicks, Dept. of Chemical and Biomolecular Engineering,
University of Notre Dame

Current use patterns and evidence lead us to the inevitable depletion of fossil fuels. While plant-based alternatives to fossil fuels can slow this depletion, it would be ideal to use non-food biomass for fuel. Lignin, a highly oxygenated and indigestible energy containing plant molecule, provides a possible starting point to make gasoline range hydrocarbon chains. In order to convert biomass into gasoline range hydrocarbon chains, special catalysts are needed to reduce coke and deoxygenate the biomass molecules. Catalysts widely used for various applications are zeolites. Zeolites have pores and surfaces that led to high surface are area to allow more reactions to happen. This catalyst also has solid acidic properties due to the way Al-O-Si bond with each other in the zeolite crystal. The Hicks lab is experimenting with different metals and the zeolite surfaces. There are a large variety of zeolite architectures and the Hicks group is looking at MFI (mordenite framework inverted), BEA and FAU. The goal of the lab I worked in is to use and characterize zeolite catalysts that can be used in reactions related to the conversion of biomass into biofuels. Zeolites are porous minerals (predominately Aluminum, Silicon, and Oxygen) that can hold various cations. These zeolites can act as solid acids and have unique mesoporous and reactive properties.

Poster Presentation

Green's Functions in Chemistry; Optimization and Implementation of PT2 Self-Energy

Jeremy Gerick
Advisor: Dominika Zgid, Dept. of Chemistry, University of Michigan

There are many materials that merit study in the field of solid-state physics, but often these are composed of layers of metals and other solids which can be prohibitively expensive to produce. It is our goal to develop and improve upon theoretical methods to study the properties of so-called "strongly-correlated" materials, materials that display high degrees of electron correlation. Our methods make use of a Green's function, a mathematical object analogous to a wavefunction or density matrix. The advantage of a Green's function, however, is that it gives direct access to the material's photoelectron spectrum, which is an important quantity that relates theoretical results to experimental data. The Green's function is a function of the self-energy, a measure of the interaction between particles and the surrounding system. It is calculation of this self-energy that limits Green's function theory; a first approximation (using second-order perturbation theory) has K^5 computational scaling, where K is the number of spatial orbitals. Our lab has adapted and optimized a method that reduces the cost of using perturbation theory to calculate this quantity, and implemented it into our base code. On top of basic Green's function calculations, our lab is working on adapting Dynamical Mean Field Theory (DMFT) for use on strongly-correlated materials. It is our main goal to use these methods to calculate the temperature of the Kondo effect, an experimentally-discovered phenomenon in metals with magnetic impurities. The knowledge of the Kondo temperature may have interesting uses in molecular electronics and nanotechnology.

Poster Presentation

PrivacyRanger

Daniel Gomez
Advisor: Timothy Wright, Dept. of Computer Science and Engineering,
University of Notre Dame

PrivacyRanger aims to enhance the security of mobile devices, such as iPhones and Android phones, by visualizing privacy risks in an ongoing manner for the user. Security for mobile devices has been somewhat limited until now because user interaction with the underlying system is greatly limited and the devices themselves do not have quite as much processing power as standard desktops and laptops. Therefore, ordinary security measures that work on desktops and laptops, such as firewalls, are not always readily ported to mobile devices. Likewise, a large number of the people who use mobile devices do not have a good deal of technical knowledge, creating a need for easily understood security solutions. In order to satisfy both of these needs, the PrivacyRanger app takes a passive approach to securing mobile devices and protecting users' data. PrivacyRanger monitors the mobile device and alerts users when privacy risks exceed a user-defined threshold. As a result of this process, PrivacyRanger calculates a near-real time risk rating in three different areas pertaining to a device's data: confidentiality, integrity, and availability. These ratings can then be presented to the user in a format that even those without a technical background will be able to understand. In addition, PrivacyRanger offers suggestions to the user as to how he can mitigate the risk of data disclosure and other potential threats. The final decision, however, is left up to the user. After all, the user knows best the value of his personal information. Therefore, the app takes no action of its own, other than to alert the user so an informed decision can be made to better protect the data on the mobile device.

Poster Presentation

Development of Visually Impaired Transgenic Mosquitoes

Brandon Gutierrez
Advisors: Joseph O'Tousa and Michelle Whaley, Dept. of Biological Sciences,
University of Notre Dame

Aedes aegypti is the primary vector for transmission of yellow fever and dengue fever. Treatment of these diseases is costly and not effective, causing vector control to become a promising method for disease prevention. The visual systems of mosquitoes likely provides sensory input driving behavioral responses. This study is designed to further understand the role of visual systems in vector behaviors such as blood-feeding, oviposition, flying, and mating. Rhodopsins are a protein family responsible for initiation of the phototransduction cascade. The role of a major rhodopsin, Aaop1, as well as vision as a whole in vector behavior will be evaluated by developing visually impaired mosquitoes. Two transgenic strategies are being utilized to create these animals. The first strategy is to develop a transgenic line of mosquito in which Aaop1 will be knocked out through the use of transcription activator-like effector nucleases (TALENs). The second transgenic approach is targeted ablation of photoreceptor cells by using the Aaop1 promoter to drive retinal expression of *michelob_x*, a cell death gene. A construct containing the promoter-driven death gene will then be inserted into the genome of *Ae. aegypti* through utilization of a transgenic line containing a recombination site, or through use of the *piggyBac* method to insert the construct into the genome at a random location. The construct will be flanked by a *gypsy* insulator sequence which will serve to prevent any repression caused by the localization of the insert. Upon successful generation of these transgenic lines, behavioral assays will be used to determine the effect of visual impairment on vector behaviors using wild type mosquitoes as a control group.

Oral Presentation

Understanding Strontium's Role in the Stability of $SrAu_3Ge$

Diana Gutierrez-Zedano
Advisors: Kathie Newman and Danielle McDermott, Dept. of Physics, University of Notre Dame

We study the effect of valence charge on the material properties in compounds with the geometry of experimentally synthesized $SrAu_3Ge$. By replacing strontium with barium, calcium, sodium, and magnesium, we examine the geometry and bonding of a compound formed of gold-germanium octahedra. Using Density Functional Theory (DFT), we calculate the energy, geometry, and electronic structure for each compound. Initial calculations show the structure of $BaAu_3Ge$, $CaAu_3Ge$ and $MgAu_3Ge$ are similar to that of $SrAu_3Ge$ while cerium and sodium, which have a different valence charge than strontium, undergo structural rearrangements. A comparison between the compounds can help us understand the bonds between gold and germanium. These bonds call tell us whether the number of valence electrons contributes to the stability of gold-germanium bonds.

Poster Presentation

Approaches to Identify Novel Phosphorylation Sites in the Checkpoint Protein ZW10

Andrea Hakaj
Advisor: Kevin Vaughan, Dept. of Biological Sciences, University of Notre Dame

Mitosis is a highly regulated process where cells duplicate their chromosomes and then segregate these duplicated chromosomes into two new daughter cells. Because each stage of mitosis requires the completion of specific molecular events, an elaborate series of "checkpoints" has evolved to couple completion of critical events with transition to the next stage of mitosis. One of these checkpoints is mediated by the Rod-Zw10-Zwilch (RZZ) complex, a highly-conserved protein complex that recruits and regulates multiple essential proteins at the kinetochores of mitotic chromosomes. At least five distinct kinetochore proteins are dependent on the RZZ complex, including dynein, dynactin, spindly, Mad1/2 and BubR1. How RZZ recruits and regulates these proteins is not known. One possibility, suggested by previous work in the Vaughan lab, is that phospho-regulation of RZZ proteins controls recruitment and regulation of the other components. Zw10, in particular, is a likely target for this phospho-regulation because it has been shown to bind dynein, spindly and Mad1/2. However, Zw10 has been difficult to analyze because it is bound tightly to kinetochores and because limited reagents are available to isolate the protein. In this project, we propose to use novel protocols to: 1) release Zw10 into cytosolic extracts thereby making it more accessible, and 2) to evaluate methods to purify this released Zw10. Building on previous work in the Vaughan lab that identifies Zwint-1 as a novel substrate for AurB (Kasuboski et al., 2011), we will treat NRK2 cells with ZM447439 to block recruitment of the RZZ complex to kinetochores thereby enhancing the cytoplasmic pool of Zw10. After evaluating the impact of ZM treatment, we will test immunoprecipitation with anti-Zw10 antibodies and purification with recombinant zwint-1 as methods to isolate Zw10. Using which ever method provides biochemical quantities of Zw10, we will subject purified Zw10 to MS/MS analysis to identify phosphorylation sites. These sites will be evaluated using mutagenesis and transfection assays. Together this work will test the hypothesis that Zw10 phosphorylation is crucial to regulation of progression through mitosis.

Poster Presentation

Enzymatic Synthesis of 3-deoxy-D-manno-octulosonic acid from in situ D-Arabinose-5-Arsenate as a Substrate Analogue

Josh Halpern
Andrew Pratt and Christopher Holt, David Cech, Dept. of Medicinal Chemistry, University of Michigan
Advisor: Ronald Woodard, Dept. of Medicinal Chemistry, University of Michigan

Kdo (3-deoxy-D-manno-octulosonic acid) is an acidic monosaccharide found in the inner core of lipopolysaccharide (LPS), the main component of the outer leaflet of the outer membrane critical for survival and growth of Gram-negative bacteria. These bacteria are human and plant pathogens that are responsible for many bacterial infections and understanding the biological roles Kdo can help us create novel antibiotics. Kdo serves as a linker between the core oligosaccharides and lipid A of LPS. Absence of Kdo in WT E. coli results in stagnant bacterial growth and increased sensitivity to antibiotics. The synthesis of Kdo using in situ D-arabinose-5-arsenate as a substrate mimic in place of the endogenous substrate, D-arabinose-5-phosphate, is a more facile, direct, and inexpensive in vitro synthesis that requires the enzyme, KdsA (3-deoxy-D-manno-octulosonate 8-phosphate synthase) which further lacks the need for the phosphatase activity of KdsB due to water mediated hydrolysis of the arsenate linkage. Large quantities of Kdo are needed in order to prepare analogues that will provide a deeper understanding of the chemical and biophysical properties of the enzymes involved in Kdo biosynthesis and incorporation into LPS with potential to discover novel inhibitors. KdsA from three species were overexpressed and purified with the KdsA from *Acintobacter baumanii* being found to provide the maximal amount of Kdo. The concentrations of starting materials, D-arabinose, phosphoenolpyruvate, sodium arsenate, and protein concentrations were optimized to provide us with the highest yield of Kdo. Further optimization occurred by varying the reaction time and volumes. Kdo produced in these reactions was quantified via the Aminoff assay. Various purification methods of the Kdo produced via this method are currently being explored.

Poster Presentation

Exploring Plasmon-Exciton Interactions between Gold Nanoparticles and Gold Nanoclusters

Andrew Hamilton
Yong Siou Chen, Dept. of Chemistry and Biochemistry, University of Notre Dame
Advisor: Prashant Kamat, Dept. of Chemistry and Biochemistry, University of Notre Dame

Nanoparticles (NPs) are structures of materials whose size is below 100 nm that have distinct physical and optical properties. These NPs interact with a specific frequency of incoming radiation (depending on size) by the collective oscillation of conduction band electrons on their surface, an effect known as localized surface plasmon resonance (LSPR). When the size of particles falls below approximately 2 nm, different properties are observed, and we term define the substances as nanoclusters (NCs). A discrete electronic structure is found due to quantum confinement effects, resulting in molecular-like properties. The optical transition between these discrete electronic levels leads to bound electron-hole pairs (excitons), resulting in unique photoluminescence (PL) properties. When two such structures are brought into close proximity, interactions can occur between the LSPR and excitons, resulting in well-known phenomena such as increased absorption and photoluminescence of the nanoclusters, increased radiative rates, and exciton-plasmon energy transfer, all of which can be controlled due to their distance-dependence. This research intended to investigate the existence of plasmon-exciton interaction between Au NPs and Au NCs by linking the two structures. To do so, we synthesized gold nanoclusters and gold nanoparticle solutions by known method. Additionally, we capped some of the particles with a silica case – that was functionalized later – of varying thickness in order to investigate any distance-dependence of the aforementioned plasmon-exciton interaction. To evaluate the success of this experiment, various techniques such as UV-Vis absorption, emission spectroscopy, and transmission electron microscopy (TEM) were used. The characteristic properties of the gold NCs include a broad absorption range that onsets at 525nm and shoulders at approximately 400nm before continuing strongly into the UV region, orange fluorescence with a maximum emission of 610nm, and a diameter around 1.5nm. The synthesized NPs had a particle size around 15nm and a characteristic plasmonic peak at 520nm (that varies with the size of the particles). This experiment is ongoing and we intend to further study any interaction using a variety of other techniques such as fluorescence lifetime and nanosecond flash-photolysis.

Poster Presentation

Visualizing Imitation Through Motion Capture Technology

John Hargett
Advisors: Charles Crowell and Michael Villano, Dept. of Psychology, University of Notre Dame

Motion capture technology has been used over the years for a variety of purposes including studies of how humans execute full body movements, as well as methods to animate non-human motion so that it closely mimics human movement. The latter objective has become a very common means for creating realistic characters in animated movies. The goal of this project was to develop an application that will be able to represent data visually that has been gathered during episodes in which human motion has been captured using the low-cost Microsoft Kinect technology.

I used Visual Studio to develop a visualization and filtering application for the eMotion and eCognition lab. Using code based on the Kinect SDK that was developed by Benjamin Bockstege from the Computer Science department for data collection, I am able to capture and store a multimodal data stream over time derived from how the Kinect's joint-based anatomical model represents gross body movements.

The application I developed accesses this stored multimodal data for visual playback and filtering. My application supports visualization of two separate data streams recorded from Kinect as skeletal stick-figure images that reproduce the original recorded movements. For each data stream, my application also produces a graph of joint location in time or a graph of the height of a joint over time. Filtering is supported in the application by allowing users to select a joint to visualize from among all those the recorded in the multimodal input stream. The application also writes information to a text file, specifically the time the movement was started and at what time a joint reaches a certain specified location.

One use of the application developed in this project will be in the study of imitation. This type of study commonly involves an "actor" who executes a movement (e.g., an arm motion) that an "imitator" is them asked to observe and reproduce. If both the actor's and imitator's actions are recorded with Kinect, they both can be visualized simultaneously using my application. This will greatly facilitate efforts to compare the motions of actor and imitator.

Oral Presentation

Carbon 14 AMS: Establishing a Carbon Dating Procedure at Notre Dame

Kirby Hermansen
Advisor: Philippe Collon, Dept. of Physics, University of Notre Dame

Accelerator mass spectrometry (AMS) is a method of separating isotopes and isobars of a certain element through a variety of beam-analysis techniques. One of the applications of this tool is in radiocarbon dating. By determining the isotopic ratio 14C/C in a specific sample, it is possible to determine the age of the sample. In this way, AMS is similar to standard mass spectrometry, but the inclusion of an accelerator allows for analysis of the particles at a higher energy, which for a number of reasons affords smaller sample sizes and shorter experiment times. However, 14C AMS is complicated by the presence of many contaminants, notably (7Li)2 and 14N, which maintain the same mass-to-charge ratio as 14C and thus swamp the detector, clouding out the wanted 14C. Data collected in a short July run on the 10 MV FN Tandem accelerator in the Nuclear Science Laboratory (NSL) confirm these problem-ions, but a lack of sufficient beam time prevented the application of solutions. Noting the past problems and their possible solutions, new settings will be ready for full experimentation in the fall. Optimizing this procedure will then allow for the NSL to work in conjunction with other departments at Notre Dame on precise dating of artifacts and samples.

Poster Presentation

Biomechanical Engineering and a Model Of Phenotypic Plasticity In Developing Mammals

Joel Hlavaty
Advisor: Matthew Ravosa, Dept. of Biological Sciences, University of Notre Dame

Adaptive plasticity is an organism's ability to respond to its environment during ontogenesis. While the evolutionary significance of mammalian craniofacial form can be attributed to natural selection, adaptive plasticity also plays an unappreciated role. Employing a naturalistic approach to studying plasticity in an experimental setting, the Ravosa lab (Biological Sciences) is exploring craniomandibular development from weaning to adulthood in white rabbits. By dividing 40 subjects into dietary cohorts to model masticatory over use and dietary seasonality, we are examining the fine-tuning effects of adaptive plasticity in the feeding apparatus and other cranial elements. Covering the entire duration of rabbit growth facilitates a novel perspective on musculoskeletal plasticity, especially given the multiple anatomical, behavioral and functional similarities between rabbits and higher primates.

We employed microCT imaging of rabbit postnatal development to document diet-induced changes in skull dimensions. To evaluate the functional significance of such bony variation, I am examining the mechanical properties of rabbit mandibular corpus explants during simulated jaw-loading parameters. Collaborating with the Niebur lab (Aerospace and Mechanical Engineering), we developed a 3-point bending model of the mandible. To be properly loaded using the test system, each dissected hemi-mandible is embedded in epoxy at both ends. Subsequently, the embedded portion is polished, which allows for testing in both mediolateral and superoinferior bending, modeling the same jaw-loading regimes encountered during in vivo postcanine biting and chewing. By utilizing initial tests with relatively smaller loading parameters, the force can be plotted against the displacement to characterize the elastic modulus or stiffness. With subsequent increases in applied forces, we can also determine the load-to-ultimate-failure, both of which assess the mechanical properties of the mandible between dietary cohorts.

We have developed a successful loading protocol for testing jaw strength in opportunistically obtained rabbit samples. We are now collecting preliminary data to test the hypothesis that, versus rabbits raised on a control diet of pellets, rabbits subject to annual dietary overloading (hay feeding) exhibit increased mandibular osteogenesis and correspondingly stiffer and stronger masticatory elements. Such findings will have implications for understanding the biomechanical correlates of morphological variation in closely related mammals that vary in diet.

Poster Presentation

Role of pax6 in neuronal progenitor cell proliferation during zebrafish photoreceptor regeneration

Sara Hockney
Advisor: David Hyde, Dept. of Biological Sciences, University of Notre Dame

Macular degeneration is the leading cause of vision loss in North America (Stell 2012). Zebrafish (*Danio rerio*) are a valuable model for studying retinal degeneration because the zebrafish retina is structurally and functionally similar to the human eye. Unlike humans, however, zebrafish naturally possess the ability to regenerate retinal neurons after injury. Upon damage to the zebrafish retina, an increased number of Müller glial cells reenter the cell cycle and produce neuronal progenitor cells that can replenish any of the lost retinal cell types, restoring the visual response (Vihtelic et al 2006). The mechanism that induces this transformation of Müller glial cells and the subsequent regeneration process is not fully characterized. It has been shown that the two pax6 genes, pax6a and pax6, are likely required for progenitor cells' continued proliferation and localization (Thummel et al 2008). To study the transcriptional regulation of pax6, transgenic constructs were generated using transposon-mediated BAC transgenesis for both pax6a, and pax6b. pax6b was designed to express GFP as a reporter gene, but pax6a will express mCherry so that the two can be differentially visualized in future studies. Although many methods of transgenesis are available, this method is particularly valuable because the BAC can hold a large genomic fragment of over 1000 kb that includes the long-range cis-regulatory elements required for correct cell type–specific and temporal expression of the gene (Suster et al 2011). Microinjection of single-cell embryos with the recombineered BAC constructs allows for the localized expression pattern of the pax6a and pax6b reporter transgenes in the separate lines. To verify that the expression of the pax6a and pax6b reporter transgenes mimics the endogenous spatial and temporal expression, in situ hybridization was performed with DIG-labeled probes specifically designed to localize the RNA expression of pax6a or pax6b mRNA. This allows for verification that the reporter transgene is expressed in the same spatial and temporal pattern as the endogenous gene, signifying that all necessary cis¬-regulatory elements required for normal expression of the protein are present.

Poster Presentation

Polymer-Templated Rainbow Solar Cells & Implementing Photovoltaics into the Chemistry Classroom

Peter Hoffman
Advisor: Ian Lightcap, Center for Sustainable Energy, University of Notre Dame

Quantum dot solar cells promise high efficiency and at relatively low costs. Other advantages to using semiconductor quantum dots are the ability to tune the band gap and generate multiple charge carriers with a single photon. A multi-layer, multi-sized cadmium-sulfide quantum dot solar cell, or a rainbow solar cell, has the promise to capture a wide range of the solar spectrum. However, one reason the theoretical efficiency has not been approached is due to difficulty in fabricating the "rainbow" layering. We propose a method that will successfully deposit each of the three quantum dot layers, each layer with its own unique band gap, using successive ionic layer adsorption and reaction (SILAR) onto the optically transparent electrode (OTE) coated with TiO_2 coupled with a polymethyl methacrylate (PMMA) backfill to control the diffusion and deposition of CdS particles.

Poster Presentation

Identification of a novel gene required for ESX-1 secretion and virulence in *Mycobacterium marinum*

Gwendolyn Hooley
Advisors: Patricia Champion and George Kennedy, Dept. of Biological Sciences,
University of Notre Dame

The bacteria that cause Tuberculosis, *Mycobacterium tuberculosis*, use protein secretion to mediate the response to infection. One system responsible for transporting proteins from the bacterial cell into the host cell during infection is the ESX-1 secretion system. Disruption of the ESX-1 system results in attenuation of *M. tuberculosis* and other pathogenic mycobacteria, including the closely related *M. marinum* species. We identified a strain of *M. marinum* in our transposon insertion library with an altered colony morphology relative to the wild-type strain. We demonstrated that this strain is deficient for ESX-1 export. As such, the strain failed to export ESX-1 substrates, was non-cytotoxic to both red blood cells and amoebae. Using sequencing analysis we determined that the strain bears a transposon between the genes *MMAR_1663* and *MMAR_1664*. The orthologue of the *MMAR_1663* mutation is required for virulence of *M. tuberculosis* in a mouse model. Neither of these genes has previously been shown to be required for ESX-1 function. To demonstrate that the transposon insertion is linked to the loss of ESX-1 function, we attempted to complement the defect by introducing a wild-type copy of *MMAR_1663/1664* into the mutant *M. marinum* strain. The complementation plasmid was able to restore the colony morphology to the wild-type and restore cytolysis of amoebae. Yet, the complemented strain failed to lyse red blood cells, or to secrete ESX-1 substrates. Future experiments will be aimed at further characterizing the characteristics of the complemented strain and how this novel gene promotes ESX-1 export in *Mycobacterium*.

Poster Presentation

The Role of GRP78 Expression in Pancreatic Cancer Chemoresistance

Shayna Hu
Advisor: Reginald Hill, Dept. of Biological Sciences, University of Notre Dame

Pancreatic ductal adenocarcinoma (PDAC) is the fourth leading cause of cancer related deaths in the United States with a 5 year survival rate of 6%. A major contributing factor for the high mortality of PDAC is the chemoresistant nature of the disease. GRP78 is an endoplasmic reticulum (ER) chaperone protein that protects cells from cell death and promotes cell survival. It is highly expressed in many tumor types and may play a significant role in tumor progression and chemoresistance. We found high GRP78 expression in pancreatic tumors from both human patients and a mouse model of PDAC, and this projects aims to investigate GRP78's effect on chemoresistance. We plan to address this question by first overexpressing GRP78 in pancreatic cell lines to investigate its downstream targets. Next, we will examine the effect of inhibition on these targets on cell survival and chemoresistance. We have begun constructing vectors to overexpress GRP78 in stably transfected cell lines and in an inducible manner. We ultimately plan to develop a therapeutic strategy that targets the GRP78 pathway to inhibit tumor progression and increase susceptibility to currently available chemotherapeutics. Overall, this will allow us to significantly increase the survival rate of the people impacted by this disease.

Poster Presentation

Evolution of *Mycobacterium marinum* for loss of ESX-1 associated hemolytic activity

Meghan Hudak
Rachel Schluttenhofer and Patricia Champion, Dept. of Biological Sciences**,**
University of Notre Dame
Advisor: Patricia Champion, Dept. of Biological Sciences**,** University of Notre Dame

The pathogenic bacteria *Mycobacterium tuberculosis* infects human macrophages in the lungs and resists the destructive action of the phagosome by interfering with host-cell signaling through the use of the ESAT-6 System 1 (ESX-1) secretion system. It is thought that the ESX-1 system punctures the phagosomal membrane, allowing pathogenic *Mycobacterium* to communicate with the host. The ESX-1 system is conserved and functional in the fish pathogen, *Mycobacterium marinum*, which lyses sheep red blood cells in a contact dependent, ESX-1 dependent manner. Two known substrates of the ESX-1 system, ESAT-6 and CFP-10, are essential for virulence and have been implicated in hemolysis. It is likely that this hemolytic behavior mimics the function of the ESX-1 system against the phagosomal membrane. We have observed that wild-type *M. marinum* that has been passaged through liquid culture multiple times no longer lyses sheep red blood cells efficiently but may still secrete ESAT-6 and CFP-10, indicating that these substrates may not be sufficient to lyse membranes. This project's aim is to observe the process of attenuation in wild-type *M. marinum* in a controlled manner and to identify mutations that affect loss of activity. In doing so we aim to identify additional factors involved in hemolysis and ESX-1 function. We started five wild-type *M. marinum* cultures from glycerol stocks, performed sheep red blood cell lysis assays using newly grown wild-type as a control, and then passaged the cultures. We perform this routine passaging until the red blood cell lysis assay indicates that a strain has become non-hemolytic. So far, we have two strains that have become non-hemolytic compared to the wild-type control. We intend to repeat the red blood cell lysis assay for each culture, and perform a secretion assay to determine if each strain still secretes ESAT-6 and CFP-10. In attenuated strains, we will sequence the ESX-1 loci to identify potential mutations. Strains will be analyzed for changes in the secreted proteome using quantitative proteomic analysis. This project will provide insight on the evolution and process of attenuation in wild-type *M. marinum* and may also identify novel genes involved in the ESX-1 secretion system.

Poster Presentation

Feasibility of gel electrophoresis to determine the permeability properties of tendons

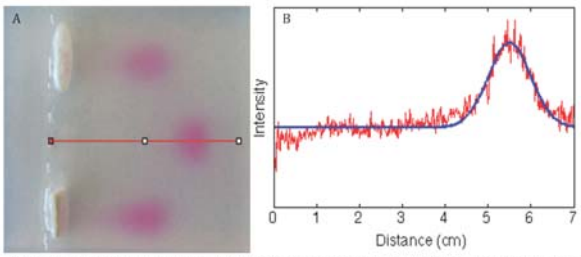
Michael Hunckler
Advisors: Jennifer Tilley and Ryan Roeder, Dept. of Aerospace and Mechanical Engineering, University of Notre Dame

Prevalence of spontaneous tendon rupture has increased dramatically in recent decades, and is typically an end-state manifestation of degenerative changes within tendons. A prominent pathological change associated with tendon degeneration is mucoid degeneration (increased concentrations of proteoglycans (PG) and glycosaminoglycans (GAG)) between the collagen fibers. The ability to non-invasively detect changes in PG and GAG concentrations will therefore facilitate monitoring of disease progression.

Cationic functionalized gold nanoparticles (AuNPs) have been proposed as an X-ray contrast agent that will bind to the negatively charged PGs and GAGs. To be successful, these contrast agents must diffuse throughout the tendon tissue. However, a thorough literature review has revealed that little is known regarding the diffusive properties of tendon. Furthermore, preliminary *in vitro* incubation experiments have failed to observe significant penetration of AuNPs, or other dye molecules, into tendon tissue in the absence of a significant driving force. The objective of this research is to determine the feasibility of gel electrophoresis to determine the permeability properties of tendon.

Slices of bovine foot tendons were embedded in agarose gel. Various samples were cut parallel and perpendicular to the collagen fibers within both the compressive and tensile regions of the tendon. Using gel electrophoresis, the cationic dye Pyronin Y was passed through the agarose gel in the absence and presence of different tendon slices. The intensity profile of the dye path was measured using ImageJ and a Gaussian fit was performed to determine the distance 50% of the dye had traveled. The electrophoretic mobility (cm^2/Vs) of the dye through tendon was then calculated by the following equation: rate of migration/electric field.

The results revealed that in the tensile region of the tendon, the electrophoretic mobility was higher in the parallel direction than in the perpendicular direction ($p<0.05$). However, there was no significant difference between the electrophoretic mobility in the perpendicular and parallel directions within the compressive region ($p>0.05$). These results are in agreement with the structure and composition of the various tendon regions, and suggest that gel electrophoresis may be a feasible method with which to measure the permeability and diffusive properties of tendon tissue.



A) Agarose gel with embedded tendon slices and the Pyronin dye moving through the gel. The intensity of the line in the middle lane is analyzed (B). A Gaussian fit is used to find the distance 50% of the dye traveled.

Poster Presentation

On-Chip Optical Diagnosis Using Capillary Electrophoresis

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Dept. of Electrical Engineering, University of Notre Dame
Paul Bohn, Dept. of Chemistry and Biochemistry, University of Notre Dame
Advisor: Scott Howard, Dept. of Electrical Engineering, University of Notre Dame

Electrophoresis is a common separation method used to identify the components of biological samples. A potential difference is applied to the sample and differences in electrophoretic mobility cause ions to travel at different rates and separate into bands which can be identified through a number of detection techniques. Electrophoresis can also be carried out in microfluidic capillaries, enabling faster separations and smaller sample sizes. Capillary electrophoresis is a common component in microfluidic "lab-on-a-chip" systems.
Optical waveguides coupled with microfluidic channels present the possibility of a novel detection scheme for on-chip capillary electrophoresis. Though the propagation of energy is confined to the waveguide through total internal reflection, an exponentially decaying oscillating electric and magnetic field called the evanescent wave extends beyond the waveguide boundaries. Interaction between this evanescent wave and the surrounding medium affects the intensity profile of light within the waveguide. This property can be used to identify dissolved ions in capillary electrophoresis channels. This project addresses the development of a coupled waveguide and microfluidic system to evaluate the effectiveness of evanescent field detection in cerebrospinal fluid separations important for the study of Alzheimer's disease, Parkinson's disease, and amyotrophic lateral sclerosis.

Poster Presentation

A Simple Method of Minimizing Ionic Strength to Reduce Chemical Shift Variance in NMR-based Metabolomics of Urine Specimen

Nirbhay Jain
Bagganahalli Somashekar and Ayyalusamy Ramamoorthy Depts. of Chemistry and Biophysics
Advisor: Ayyalusamy Ramamoorthy, Dept of Chemistry, University of Michigan

Metabolites are small molecules, such as various amino acids, organic acids, carbohydrates, ketones, and aldehydes, which are the final products of cellular regulatory processes. Metabolite levels profoundly signify the ultimate response of biological systems. The science of metabolomics refers to the identification and quantification of metabolites found in an organism, and is the fastest growing field in relation to biomarker discovery for disease diagnosis. Various biological specimens, such as body fluids, including urine and blood, cells, and tissues are being used for metabolomic analysis, which provides plethora of metabolite rich information. These biological samples are generally analyzed by nuclear magnetic resonance (NMR) spectroscopy. However, subtle physiological changes between urine samples, such as pH variance and salt concentration differences, can cause changes in the chemical shifts of metabolites across the NMR spectra of multiple samples, interfering with multivariate statistical analysis. Therefore, peak alignment, the identification, , and quantification of metabolites are still complex procedures, as there is an inherent lack of consistency across samples. In an effort to overcome this problem, we propose a simple separation procedure, to be used with urine samples, which precipitates salts and proteins in urine samples that can cause chemical shift variance while leaving metabolites unchanged (Figure 1). In this approach (Scheme 1), native urine samples were combined with equal parts methanol and acetone (1:1:1 v/v/v), followed by preservation in -20 °C for an hour, to precipitate proteins and salts. Later, the samples were centrifuged and the supernatant dried under N2 gas. The resulting urine residue was then reconstituted in 500 µL of phosphate buffer of pH 7.2, prepared in D2O. Subsequently, 1D 1H NMR measurements were carried out with water presaturation. The resulting spectra of the various urine samples showed consistent chemical shift values for metabolites in each spectrum. This procedure greatly reduced the chemical shift perturbations across the different urine samples, allowing for more accurate multivariate statistical analysis, identification and quantification of urine metabolites, which can be used routinely in NMR-based metabolomic analysis of urine samples, most importantly biomarker discovery for cancers.

Oral Presentation

Magnetic Fields and the Formation of Relativistic Jets

Jared Johnson
Adrien Saremi
Aaron Sawyer
Advisor: John Poirier, Dept. of Physics, University of Notre Dame

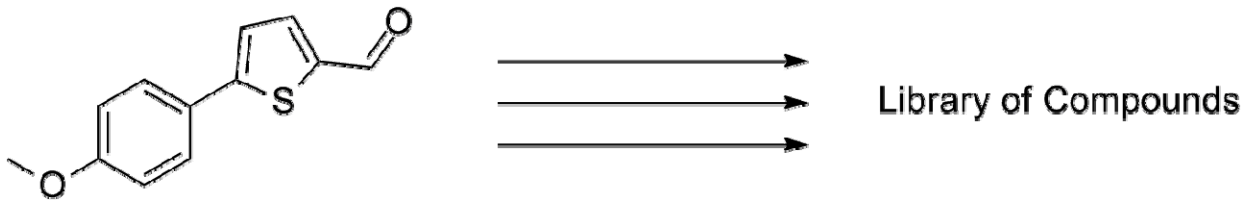
When matter falls towards a black hole, it will form a disk around the black hole known as the accretion disk. Accretion disks give rise to relativistic jets coming from the central object. The hypothesis is that the twisting of the magnetic field produced by the accretion disk collimates the outflow along the rotation axis of the central object, so that when conditions are suitable, a jet will emerge from each face of the accretion disk. Along with the theory that the magnetic field is twisted due to the spin of the black hole, a particles motion in the z direction can be associated with the formation of relativistic jets. We have constructed a model of the magnetic field for an accretion disk formed around a black hole in an active galactic nucleus, and used it to show that a particle's motion is in the z direction. A computer program was created to simulate the motion of a particle in the magnetic field. The particle is shown to leave its circular motion and move in the z direction.

Oral Presentation

Syntheses and SAR Analysis of Thiophene Aldehyde Derivatives

Bryce Jones
Marvin Miller, Dept. of Chemistry and Biochemistry, University of Notre Dame
Advisor: Marvin Miller, Dept. of Chemistry and Biochemistry, University of Notre Dame

The discovery and development of small molecule drugs is a central component of anticancer research. A library of compounds based on a 5-(4-methoxyphenyl)thiophene-2-carbaldehyde lead compound was synthesized and tested *in vitro* for anticancer activity on MCF7, PC-3, and HeLa cell lines. Most compounds exhibit excellent activity against MCF7 cultures but minimal to no activity against PC-3 and HeLa cultures. A structure activity relationship analysis reveals that the starting aldehyde retains activity upon diversification. The specific results are disclosed herein.



Poster Presentation

The Role of Fgf Signaling During Regeneration of the Zebrafish Mesonephros

Jonathan Jou
Kristen McCampbell, Dept. of Biological Sciences, University of Notre Dame
Advisor: Rebecca Wingert, Dept. of Biological Sciences, University of Notre Dame

Nephrons, the functional unit of the kidney, are segmented epithelial tubules that clear the blood of toxins, absorb ions, and maintain water homeostasis. Damage to nephrons lead to renal dysfunction, a condition associated with both acute and chronic kidney diseases. There is a high degree of conservation between zebrafish and human nephrons. Further, zebrafish possess an innate ability to regenerate damaged nephrons and to grow new nephrons continually during adulthood. Thus, zebrafish is a relevant model for investigating the mechanisms of epithelial regeneration and exploring the signaling pathways that control neonephrogenesis. In this project, we are assessing the role of fibroblast growth factor (fgf) signaling. The Fgf family of growth factors is closely associated with nephron growth and branching during mammalian renal ontogeny. Thus, we hypothesized that Fgf signaling may play one or more roles in regulating nephron regeneration and specifically chose the genes fgf2, fgf7, fgf8a and fgf20a and the changes in their expression after acute kidney injury induced by gentamicin exposure. Quantitative real time polymerase chain reaction assays showed an increased expression of fgf mRNA transcripts immediately after injury. Interestingly, we detected localized fgf8a transcripts following injury using whole mount in situ hybridization in clusters of cells that resemble neonephric precursors, thus implicating a role for fgf8a in the regeneration response. Inhibition with SD5402, a robust fibroblast growth factor receptor competitive inhibitor, showed a decreased number of cells expressing the pax2a proliferation marker in preliminary immunohistochemical assays, suggesting that Fgf signaling plays a role in stimulating regeneration in the zebrafish mesonephros. Future experiments will use transgenic and chemical genetic perturbations to modulate Fgf signaling during regeneration.

Poster Presentation

Microcontact Printing of DNA Origami onto Silicon Substrates

Patrick Jung
Marya Lieberman, Dept. of Chemistry and Biochemistry, University of Notre Dame
and Valerie Goss, Dept. of Chemistry and Physics, Chicago State University
Advisor: Marya Lieberman, Dept. of Chemistry and Biochemistry, University of Notre Dame

This paper shows our progress on developing microcontact printing methods to localize DNA nanostructures on modified silicon substrates. With potential applications in optical, electrical, molecular, and chemical sensing, microcontact printing may provide an easy and less costly method of making DNA nanostructured patterned surfaces. We used a poly(dimethylsiloxane) (PDMS) stamp to pattern a self-assembled monolayer onto a silicon substrate followed by a deposition of DNA origami. We chose our stamp to be fabricated from PDMS because of its flexibility, durability, and reproducibility in microcontact printing. Early PDMS stamps were cast off laser-printed masters and then used to make rough patterns on a silver substrate. We prepared well-defined patterns from masters made using photolithography. The design consisted of two micrometer squares formed in an array with two micrometer spacing. SEM images showed correct production of the pattern into a chromium mask. Our PDMS stamps were cast off silanized versions of these masters. Control tests of contact between the PDMS stamps and clean substrates of mica and silicon showed little to no chemical interactions. Monolayers of aminopropyltriethoxysilane (APTES) were successfully transferred to the cleaned silicon substrates by both methods of deposition and microcontact printing. Contact angle testing of the modified surfaces showed a more hydrophobic surface than the unmodified surfaces. DNA origami was chosen as our ideal material for patterning on the silicon because of its mechanical rigidity, self-assembly, and functionality as a binding agent. Atomic Force Microscope (AFM) images have shown our successful deposition of the DNA origami onto freshly cleaved mica and APTES modified silicon. We are currently investigating the potential of DNA origami to be localized and bound to the two micrometer square monolayers produced by the patterned PDMS stamps.

Poster Presentation

Determining Hepatitis C NS3 Helicase's Active Oligomeric State

Kipchumba Kaitany
Advisor: Wei Cheng, Dept. of Pharmaceutical Science, University of Michigan

Helicases are a class of proteins essential to all living organisms. The hepatitis C virus expresses NS3 helicase, an ATPase RNA helicase that is vital for hepatitis C replication. As such, elucidation of the NS3 helicase's molecular mechanism may lead to the development of novel anti-viral strategies and a better general understanding of helicase function. Previous papers have reported differences in activity between bulk assays and single molecule studies. It has been suggested that the variance in reported activity stems from differences in NS3 oligomeric states. In order to monitor NS3 helicase activity and oligomeric state simultaneously, we have designed a fusion protein in which a monomeric teal fluorescence protein (mTFP) is fused to the N-terminus of NS3. We expect this N-terminal fusion to retain helicase activity that can be monitored using optical tweezers, while the presence of mTFP will facilitate the monitoring of NS3's oligomeric state through quantification of mTFP photo bleaching events using simultaneous two-photon fluorescence. Two restriction sites in the wild-type NS3 expression vector were chosen for PCR cloning: BamHI and KasI located between the His-tag and NS3 gene. Following digestion of the wild-type NS3 vector and mTFP insert with BamHI and KasI, ligation of the two components proved unsuccessful. Troubleshooting of the ligation suggests that KasI may have difficulty cleaving the mTFP insert due to restriction site context.

Poster Presentation

Assay Development Monitoring VirF Binding to VirB Promoter

Gordon Kane
Anthony Emanuele, Dept. of Medicinal Chemistry, University of Michigan
Advisor: George Garcia, Dept. of Medicinal Chemistry, University of Michigan

Shigella flexneri is a gram negative, enteropathogen that causes severe dysentery, infecting an estimated 165 million worldwide and taking one million lives annually. *Shigella* is primarily transmitted via a fecal-oral route and therefore considered a problem of developing nations, but it is of major concern due to the low number of bacteria needed for infection (ten to one hundred bacteria) and the recent emergence of single and multi-drug resistant strains in industrial and third world nations. The pathogenesis of *Shigella* is controlled by the virulence regulatory protein VirF. Knockout studies have shown VirF is essential for host infection but not viability, which makes VirF an ideal candidate for novel antibiotic development as a potential virulence target. It is hypothesized that targeting virulence over viability will place less selective pressure towards the emergence of drug resistant strains. Presented is the current progress towards the development of an assay to monitor VirF binding to the VirB promoter region (a known binding region of VirF). In the future, the assay will be used to determine the ability of our lead compounds to block VirF from binding to DNA.

Oral and Poster Presentation

Optical modulation of continuous terahertz waves towards reconfigurable quasi-optical terahertz components

Akash Kannegulla
Advisor: Lei Liu, Dept. of Electrical Engineering, University of Notre Dame

We report the optical modulation of continuous terahertz waves in the frequency range of 570-630 GHz with photo-induced free carriers in semi-insulation silicon illuminated by a commercially available digital light processing projector. A modulation depth of 20 dB and a speed of ~1.3 KHz have been demonstrated. This modulation mechanism is capable of generating optically re-configurable quasi-optical THz components directly on silicon wafer without any micro-fabrication processes. A photo-induced polarizer with tunable polarization angle has been demonstrated showing a 3-dB extinction ratio. Prototype demonstrations of 4 × 4 coded aperture imaging using the Hadamard coding have been performed and this technique has been successfully applied to mapping THz beams with 6 X 6 pixels at 590 GHz. The reported approach provides a simple but powerful means to realize a variety of novel re-configurable THz circuits and components.

Poster Presentation

Investigating *In Vivo* Binding Partners of Transcriptional Activator VP16 through the Genetic Incorporation of Unnatural, Photocrosslinking Amino Acids

Micah Katz
Amanda Dugan, Dept. of Chemistry, University of Michigan
Advisor: Anna Mapp, Dept. of Chemistry, University of Michigan

Transcriptional activators are modular proteins that mediate gene expression through the recruitment of various coactivator complexes and the transcriptional machinery to the promoter of the gene to be transcribed. Aberrations within transcriptional networks are manifested in the pathogenesis of many human diseases, therefore there is a great desire to understand how activators function in cells, with the future goal of targeting activator-coactivator interactions to restore normal cell phenotype. We know that the complex network of activator-coactivator contacts involved in transcriptional activation is comprised of many moderate affinity protein-protein interactions (PPIs). Common in vitro methods such as co-crystallization and GST-pulldowns are most effective for investigating high affinity interactions, thus the limitations of these approaches leaves many important sections of the transcriptional activator interactome unmapped. However, recent studies have shown that unnatural, photoactivatable amino acids such as p-benzoyl-L-phenylalanine (Bpa) can be genetically incorporated via nonsense suppression routes into the surface regions of transcriptional proteins in living cells. Subsequent exposure of these cells to ultraviolet light activates the photo-crosslinking moiety, thus allowing for the in vivo covalent chemical capture of moderate affinity protein interactions. Here we use in vivo photocrosslinking with Bpa to capture the contacts made by the transcriptional activation domain (TAD) of the viral activator VP16 within the RNA Pol II holoenzyme, a complex essential for transcription to occur. We have incorporated pBpa into the VP16 TAD in Saccharomyces cerevisiae and have tested VP16 crosslinking to the PolII subunit Rpb1, the essential TFIID subunit TBP, and the Mediator subunit Med2, and have found that TBP is a direct target of VP16 in cells and additionally that several subunits within the RNA Pol II holoenzyme may act as direct targets of VP16 during assembly and recruitment of the complex. By examining further the specific binding partners of transcriptional activators during initiation, we hope to identify potential sites for therapeutic intervention.

Poster Presentation

Nanomaterial Induced Changes in Cell Membrane Conductivity: A Whole Cell Patch Clamp Study

Milan Kaushik
Sriram Vaidyanathan, Biomedical Engineering
Advisor: Mark Banaszak Holl, Dept. of Chemistry, University of Michigan

The delivery of biomolecules such as nucleic acids and proteins to tissue for therapeutic applications is an area of active research. Materials such as surfactants, cationic polymers (e.g. poly (ethyleneimine)) and cationic lipids (e.g. DOTAP) which are widely used as drug delivery agents are also known to interact with the membrane. However, the relationship between cellular interaction and membrane uptake is poorly understood beyond the context of cytotoxicity. We hypothesize that the membrane – material interactions are important for cellular uptake. We have investigated the effect of sodium dodecyl sulfate (SDS), cetrimonium bromide (CTAB), G5 polyamidoamine (PAMAM) dendrimers, and G5 PAMAM Dendrimers with precisely defined number of dyes on the membrane conductivity of HEK293A cells using an automated whole cell patch clamp technique. Our group has observed that the exposure of cells to surfactants and polymers results in increased membrane conductivity. For the first time, we show that detergents increase the membrane conductivity of cell membranes within a second after exposure. Detergents below the critical micelle concentration (CMC) can increase membrane conductivity even when cells are physically intact. SDS is more efficient at solubilizing cells compared to CTAB. CTAB induces substantial increase in membrane conductivity but does not cause solubilization of the cell membrane, even at concentrations up to 200 times above CMC. We have also observed through fluorescence microscopy that G5 PAMAM dendrimers induce increased membrane conductivity as materials are absorbed onto cells. These results suggest that detergents and polymers are intercalated in the membrane. Future work will focus on determining the role of this membrane intercalated material in drug and gene delivery.

Poster Presentation

Thermosensitive acrylamide-based hydrogel nanoparticles as a novel targeted drug delivery vehicle for anti-cancer agents

Taylor Kelson
Advisor: Raoul Kopelman, Dept. of Chemistry, University of Michigan

Polymer hydrogel nanoparticles have recently been studied as promising drug delivery vehicles for specific targeting of anti-cancer drugs to tumor sites. Biochemically inert nanoparticles have demonstrated biocompatibility and biodegradation, efficient drug loading, and useful drug release kinetics. When targeted with surface modifications, these nanoparticles have shown highly specific binding and cytotoxic activity against tumor cells both *in vitro* and *in vivo*. The swelling response of these nanoparticles to stimuli such as temperature, pH, and presence of other chelating ions has also been investigated. Many types of hydrogel nanoparticles display lower critical solution temperature (LCST) type behavior (rapid deswelling/collapse at elevated temperature). We examine an interpenetrating polymer network (IPN) nanoparticle formulation composed of acrylamide and acrylic acid, which displays upper critical solution temperature (UCST) type behavior (rapid swelling at elevated temperature). UCST behavior is potentially more promising for targeted drug release and delivery. We examine the thermosensitive drug release properties of these IPN particles using the platinum-containing anti-cancer drug cisplatin. Certain formulations of these nanoparticles show promising drug release properties, including correlation with temperature. These properties demonstrate promise for further development as a targeted anti-tumor therapy incorporating thermal or ultrasonic heating of the tumor site to promote targeted drug release.

Poster Presentation

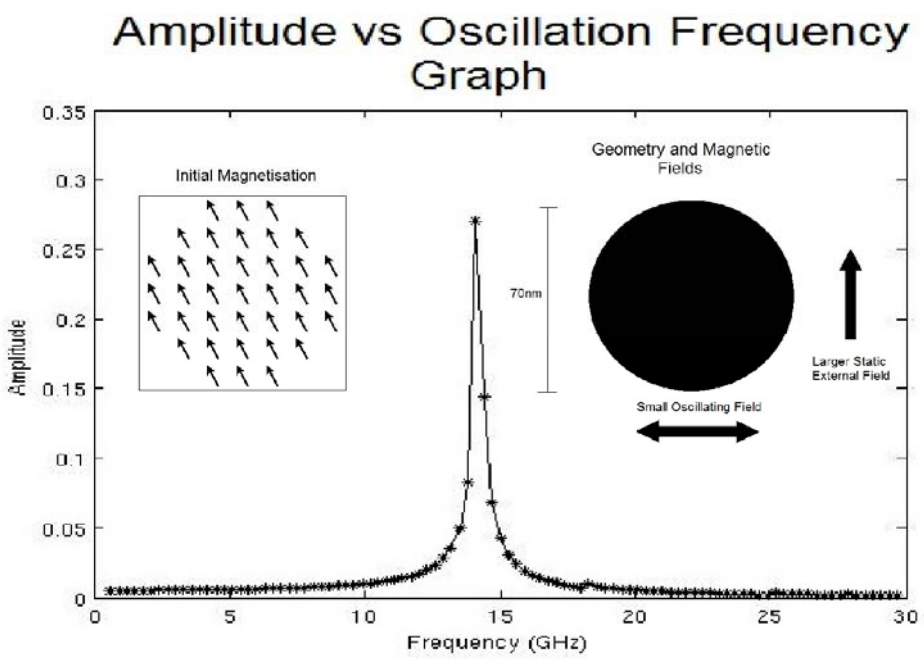
Simulation of Nanomagnets under Dynamic Conditions

Daniel Kestell
Gyorgy Csaba, Himadri Dey, and Wolfgang Porod, Dept. of Electrical Engineering, University of Notre Dame
Advisor: Gyorgy Csaba, Dept. of Electrical Engineering, University of Notre Dame

Nanomagnets can be used for logic in computers instead of CMOS transistors. These Nanomagnets could provide lower power consumption than transistors. However, the dynamic switching properties of the nanomagnets are not yet well understood. In this research, the effect of dynamic conditions on the magnets, i.e. the response to an oscillating external field, were investigated by simulation using the OOMMF micromagnetic package. These simulations could be directly compared to experiments.

The effect of simulation parameters, magnet shape and size, coupling strength of magnets were investigated with respect to dynamic conditions. Some of the results for the 150nm Circle simulation and the 90nm circle simulation could be compared with those of the experiments. For most cases, there was a good agreement between the experiments and the simulations, but for larger magnet sizes a lot has yet to be explained.

Shown in the figure is an example of a Frequency vs. Amplitude plot typical of those simulated in this project. These are used to study the resonance behavior of the magnets. Inset is the Geometry of the magnet and its initial magnetization. This simulation had a quite coarse mesh. This figure is for a 70nm diameter circular nano-magnetic dot with an applied external field of 250mT.



Oral Presentation

The World's First Diffraction Limited Doppler Spectrometer: iLocater

Edward Kielb, Taylor Corpuz, and Michelle Berg
Advisor: Justin Crepp, Dept. of Physics, University of Notre Dame

iLocater is a spectrograph currently being designed and constructed for the Large Binocular Telescope that will search for exoplanets near M-Dwarf stars using the Doppler technique. The adaptive optics system of the LBT will create diffraction-limited observations, which will provide the highest resolution observations possible. Due to the M-Dwarf spectra peaking in the near infrared (NIR), iLocater will operate in that region, and as such the detector needs to be isolated from vibrations, radiation, and thermal changes. In order to test the method by which iLocater will correct for atmospheric and technical perturbations, stellar spectra were simulated via Matlab code to ensure that the method accurately corrects for hot pixels, photon noise, dark current, and dispersion truncation. In addition to M dwarfs, iLocater will also observe binary star systems to add important constrains to existing planet theories.

Poster Presentation

The Relationship of Vision and Circadian Rhythm in *Aedes aegypti*

Kyle Kimler
Advisor: Joseph O'Tousa, Dept. of Biological Sciences, University of Notre Dame,

Vision and the circadian rhythm are closely tied across the animal kingdom. The disease vector *Aedes aegypti* follows this general rule in that its circadian rhythm has been shown to play an important role in its daily activity. While it is known that vision entrains the biological clock through the interaction of clock proteins and the phototransduction cascade, the metabolic pathway that gives the mosquito cognitive vision, it is unknown whether the inverse is true. *Ae. aegypti*'s sensitivity to light changes throughout the day as a result of light/dark adaptation. Upon dark adaptation these animals become more sensitive to light. But how do the clock proteins affect this dark adaptation? To determine if the circadian rhythm has an effect on visual sensitivity, we recorded *Ae. aegypti*'s response to light over a 24 hour time course using an electroretinogram (ERG). An ERG creates a plot of the voltage of mosquito eye nerves while the eye is exposed to flashes of varying intensities of light. First, mosquitoes were tested on a 12h/12h light/dark cycle, to visualize how the mosquito responds to light at different times of the day; second, mosquitoes were tested in 24h constant dark, to see if the mosquito's circadian response to light is conserved. If *Ae. aegypti*'s vision is affected by clock proteins, it would mean that circadian rhythms have a profound physical effect on sensory organs of the animal, an effect that goes beyond behavioral changes.

Poster Presentation

Manipulation of Graphene Morphology Compounds via Metal Nanoparticle Mediated Hydroxyl Radical Attack

Anthony Krenselewski
James Radich, Dept. of Chemistry and Biochemistry, University of Notre Dame
Advisor: Prashant Kamat, Dept. of Chemistry and Biochemistry, University of Notre Dame

Based on previous research, it is known that gold nanoparticles in the presence of hydrogen peroxide and ultraviolet radiation mediate the oxidation of reduced graphene oxide (RGO) via a hydroxyl radical attack. The first goal of this project was to investigate whether other types of nanoparticles resulted in a similar effect. The oxidation of the RGO was monitored by measuring the decrease in its absorption characteristic using a UV-visible spectrophotometer. It was discovered that copper nanoparticles, synthesized through the reduction of copper (II) ions in aqueous solution using sodium borohydride, resulted in the same oxidation of the RGO. Furthermore, the copper caused the reaction to occur even more rapidly than in the presence of the gold nanoparticles. The increased rate of reaction made it possible to fully oxidize the RGO resulting in the formation degradation products from the RGO. Through the use of gas chromatography/mass spectrometry, it was possible to identify one of these products as diethyl phthalate. The investigation is currently attempting to identify whether the morphology of the RGO can be controlled by manipulating the placement of the copper nanoparticles in relation to the RGO sheets as well as manipulating the duration and intensity of the ultraviolet radiation.

Poster Presentation

Biosynthetic Production of Novel Substrates

Christopher Kubitskey
Advisor: David Sherman, Dept. of Chemistry, University of Michigan

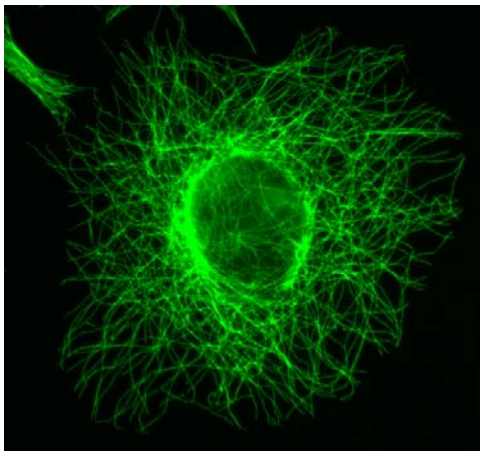
With the emergence of bioenergy alternatives as an environmentally friendly replacement for fossil fuels, research into accessing these high value chemicals has increased dramatically. Recently, the curacin A biosynthetic pathway, which contains a terminal sulfotransferase-thioesterase (ST-TE) enzyme cassette, was observed to produce a natural product with a terminal olefin. Interestingly, when presented with non-native substrates, the same enzymes were able to catalyze the production of olefinated hydrocarbons. With the introduction of novel substrates, the flexibility of the ST-TE can be taken advantage of to produce long, fuel like hydrocarbons with a terminal olefin in vitro. This project seeks to evaluate the ability of an acyl activating enzyme (AAE) from a related natural product pathway (Synechococcus) to directly load an acyl carrier protein (ACP), which precedes the terminal ST-TE in the biosynthetic pathway, with long chain fatty acids in an effort to produce fuel-like molecules with a terminal alkene. To achieve this, proteins were cloned and overexpressed as excised domains. Modifications to the ACP were monitored by detecting increased mass by LC-QTOF-MS as well as by observing mobility shift by HPLC. Initial data results indicated that the CurM ACP had remained in its original form instead of being loaded by the Synechococcus AAE. The selectivity of the AAE as well as domain excision may have contributed to these results. Excised native ACP was then cloned and overexpressed. The native Synechococcus ACP, however, showed an ability to be loaded by the Synechococcus AAE. Fusion Synechococcus AAE-ACP constructs are currently being cloned and its ability to be loaded by non-native substrates will be similarly evaluated.

Oral and Poster Presentation

Mathematical Modeling of Dynamic Instability in Microtubules

Christine Kuryla
Advisors: Mark Alber, Dept. of Applied and Computational Mathematics and Statistics and Holly Goodson, Dept. of Chemistry and Biochemistry, University of Notre Dame

Microtubules are biological polymers that have many functions in cells, such as support and structure in the cytoskeleton, providing avenues and mechanisms for intracellular transportation, and separating chromatids during cell division. Microtubule dynamic instability is an integral part of cell functioning, enabling microtubules to rapidly find and change spatial arrangements and interact with necessary biological components. Due to dynamic instability, microtubule ends switch randomly between phases of growth and depolymerization (subunits are being constantly added and removed from the ends of the various microtubules). The mechanisms of dynamic instability are not well understood, partially due to the complexity of microtubule structure. Experiments have shown that microtubules do not exhibit behavior consistent with the classical model of equilibrium polymer dynamics. Mathematical and computational models have been created to attempt to explore and better understand the phenomenon of dynamic instability. A coarse-grained stochastic model of a system of microtubules from Gregoretti et al (JCS 2006) had previously been extended to simulate free microtubules in solution. To improve the model and make it more biologically realistic, a Monte Carlo algorithm was implemented that allows new microtubules to spontaneously form (nucleate) from the free subunits in the solution. Additional statistical output and analysis was also added to facilitate the investigation of the microtubule behavior. This enables the exploration of the effect of the ease of nucleation on the behavior of the system. The simulations will be compared with experimental results to attempt to better understand dynamic instability. The refinement of the understanding of dynamic instability has implications for the development of cancer treatments and the study of self-organized systems.



Poster Presentation

3D Printing: Rapid Prototyping using Additive Manufacturing

Alexa Kutch
Phillip Cook
Advisor: Paul McGinn, Dept. of Chemical and Biomolecular Engineering,
University of Notre Dame

3D printers provide an opportunity to rapidly print objects using an additive manufacturing process. Currently, a common use of 3D printers is in prototyping. The printer allows a person to prototype an object quickly, efficiently, and at low cost. They use lighter parts, less energy, and put out less waste than traditional methods. 3D printers have been used to create machine parts (the printer can actually create parts for itself), prosthetics, individual products (lamps, jewelry, etc.), food (candies, chocolates, etc.), and countless other items. With the proper material, the possibilities are endless. As a high school mathematics teacher, I am especially excited about the opportunities the printer will provide in my classroom. I hope to incorporate it in several units of my geometry and calculus classes. My goal is to have my students create objects to print as well as provide students with manipulatives to better understand the lessons.

Poster Presentation

Characterization of Ag SERS-active microelectrodes

Daniel Kwasnieski
Advisor: Zachary Schultz, Dept. of Chemistry and Biochemistry, University of Notre Dame

Redox processes occurring on catalytic surfaces are important in many industrial and research applications. However, catalyst poisoning results when molecules or reaction products irreversibly bind to the surface and impede the chemical reaction involving the catalyst. This is a persistent problem affecting the efficiency of these reactions. Understanding the mechanism that leads to the desired redox product or the poisoning phenomenon may be aid by single-molecule studies on catalytic surfaces. Our approach focuses on developing and characterizing Ag microelectrodes as a platform for combined surface-enhanced Raman spectroscopy (SERS)-electrochemical studies with sufficient sensitivity for single-molecule detection. The Ag electrodes are constructed by electrolytically depositing Ag on a Cu electrode, with different Ag morphologies resulting from varied electrolysis times and initial surface topography. By controlling the surface energy electrochemically, we can monitor redox processes occurring on the electrode surface. The SERS enhancement factors (EFs) of these substrates are calculated by comparing the Raman signal intensity of thiophenol adsorbed to the Ag substrates to that of neat thiophenol. The EFs can then be correlated to the various morphologies produced from varying the electrolysis time, and the substrates with the largest reproducible EFs can be selected for use in future SERS-electrochemical studies of single-molecule redox reactions.

Poster Presentation

DMS Ligand-Receptor Interactions Reflect SAR Data

Megan Leander
Kathryn Marchetti, Chloe Bass, Benjamin Maynard, Ruthann Nichols,
Dept. of Biological Chemistry, University of Michigan
Advisor: Ruthann Nichols, Dept. of Biological Chemistry**,** University of Michigan

Myosuppressins (MS) decrease insect cardiac contractility; thus, mimetics to their signaling pathway may disrupt vector physiology. Our hypothesis was myosuppressin ligand-receptor contact sites are consistent with structure-activity relationship (SAR) data. To test our hypothesis, *Drosophila melanogaster* myosuppressin (DMS; TDVDHVFLRF-NH2) was docked to its receptors, DMS-R1 and DMS-R2. The MS receptor (MS-R) of the disease vector *Rhodnius prolixus* was identified and modeled; it shared similarities to DMS-Rs in primary sequence and the binding pocket. *R. prolixus* myosuppressin (RMS; pQDIDHVFMRF-NH2) was docked to RMS-R to identify ligand-receptor contacts. Docking the non-peptidyl MS agonist benzethonium chloride provided additional contact site data. Additionally, an examination of MS-Rs identified a novel feature not shared by other family A rhodopsin-like receptors. Our results proved our hypothesis and provide the basis to design mimetics to influence vector physiology.

Oral Presentation

Exploring the Growth Mechanisms of GaAs Nanowires Grown by MBE

Kevin Lee
Advisors: Jacek Furdyna, Malgorzata Dobrowolska-Furdyna, Xinyu Liu, Richard and Pimpinella, Dept. of Physics, University of Notre Dame

Research dedicated to understanding and controlling the growth of semiconducting nanowires has grown in interest for their potential to advance technology for application in next generation computing, ballistic photonic waveguides, and for interconnecting molecules for molecular computing. We have successfully grown GaAs nanowires by Molecular Beam Epitaxy. In this work, we investigate the principal growth mechanisms underlying nanowire growth by measuring the morphology of the nanowires and comparing them to a simple growth model. From this, we are able to make several conclusions. The findings of this research conclude that Adatom Diffusion contributes more to the overall growth rate than Direct Impingement. From this research, it is evident that in order to gain control of the growth of semiconducting nanowires, more research is required to study the effects of growth conditions on Adatom Diffusion.

Poster Presentation

Data Git: Provenance Extraction Tool Using Version Control

Judy Long
Advisor: Charles Vardeman, Center for Research Computing, University of Notre Dame

Data and software provenance metadata provides the context necessary to understand, trust, and reuse scientific data, a critically important component of curating the massive datasets generated by High Energy Physics (HEP) experiments where data is not reproducible. Data and Software Preservation for Open Science (DASPOS) explores solutions to meaningful documentation and preservation of data to provide a model for HEP and other disciplines. To further this goal, we have prototyped and are testing the viability of Data Git (DGit), a tool for extraction and machine readable documentation of provenance metadata, using W3C standard ontologies. DGit is a Python wrapper for Git distributed version control that utilizes Git's handling of repository contents to extract and document provenance metadata of a repository in machine readable format, for the purposes of later querying. DGit demonstrates a useful model for capturing the state, contents, and changes of a repository, making the metadata accessible and linkable at a later point in time.

Poster Presentation

Possible Student Investigations Related to Engineering a More Sustainable Energy Future

Nevin Longenecker
Advisor: Jay Brockman, Dept. of Computer Science and Engineering, University of Notre Dame

The Science Research Course at John Adams High School began several years ago following repeated requests from students over the years for an additional year of investigative science. The original research course was designed to allow students to become familiar with reading research journals, writing research proposal and performing investigations. This revised and enlarged syllabus incorporates a significant emphasis on STEM education based on the new core standards.

Poster Presentation

Membranes with Multiple Porous Crystals for Chemical Separations

Amber Lott
Jeremy Feldblyum, Dept. of Chemistry, University of Michigan
Advisor: Adam Matzger, Dept. of Chemistry, University of Michigan

Microporous coordination polymers (MCPs) are crystalline porous frameworks of alternating organic ligands and metal clusters. MCPs are highly effective for separating gases from gas mixtures. In particular, single crystal membranes (SCMs) have shown excellent separation factors for light gases such as CO2/ H2. However, there are problems that arise from using SCMs for such separations. SCMs have low permeability, so they can take long amounts of time to separate gases on even modest scales. In addition, SCMs are not ideal for industrial scale operation due to the amount of time needed to manipulate individual crystals for membrane fabrication. To overcome these challenges, we sought to develop membranes containing multiple MCP single crystals embedded in a single membrane. Using the zinc-based MCP MOF-5, we tested a number of approaches to yield pinhole-free membranes. Membranes were fabricated by melting polycaprolactone pellets into thin films and subsequently depositing MOF-5 single crystals onto the polymer. Membranes were initially tested by separating small molecule dyes from solution based on the well-defined pore size (~1 nm) of the embedded MCP single crystals. A dispersion composed of methanol and nanoparticulate copper phthalocayanine dye was tested on the membrane and resulted in methanol being separated from the dye. A solution of astrazon orange dye, copper phthalocayanine dye and methanol was also tested and resulted in the passage of only solvated astrazon orange through the membrane. We are now testing the separation performance of solutions containing large and small molecule dyes to assess separation bases on the molecular-scale pores of embedded single crystals. We hope to extend our study to gas separation experiments in the near future. Our results indicate that membranes with multiple embedded porous crystals are excellent contenders for chemical separation.

Poster Presentation

Evaluating the Effects of Spatial Scale on the Performance of Climate Envelope Modeling

Rui Yan Ma
Jason Dzurisin, Dept. of Biological Sciences, University of Notre Dame
Advisors: Jason Dzurisin and Jessica Hellmann,
Dept. of Biological Sciences, University of Notre Dame

Climate envelope models (CEMs) or species distribution models (SDMs) are computer algorithms that predict species distributions based on occurrence data and bioclimatic environmental data (e.g. temperature and precipitation). These models aim to determine the probability of a species occurrence in a given location based on its calculated environmental niche. The Spatial Portal for Analysis of Climatic Effects on Species (SPACES) is a tool within the Collaboratory for Adaptation to Climate Change site which implements various climate envelope models. This project investigates the effect of spatial scale on the performance of each algorithm. In order to do this, we evaluated various statistical measurements such as the AUROC (area under the receiver operating characteristic curve) and AUPR (area under the precision recall curve) that evaluate the models performance. We tested seven algorithms using openModeller desktop and eight algorithms using a command line openModeller instance. Input data included occurrence records of *Centrocercus urophasianus* and the nineteen bioclimatic variables defined by Worldclim. For each algorithm, we evaluated our models at three different spatial extents: USA, North America and global. We trained the model using current environmental layer sets and projected the model onto both current and 2080 environmental layer sets. We employed an external Python script to evaluate the model performance using the model outputs. AUC, AUPR and correlation coefficient were calculated and compared amongst all algorithms and spatial extents. Results suggest that maximum entropy has the highest AUROC among most instances, and thus has the best model performance in all three spatial extents. GARP Single Run has the lowest AUROC values among most of the instances, and the AUROC values of this algorithm fluctuate between different runs. Therefore, we do not recommend using it to predict species distribution. While maximum entropy performed most optimally across all spatial extents, a suite of multiple algorithms should be employed and the results should be compared among algorithms within the same spatial extent to determine the most suitable algorithm for the projection. Tools such as SPACES allow for such an ensemble approach and thus represent a powerful tool for species distribution modeling approaches.

Poster Presentation

Synthesis of a Selective Kinase Inhibitor for the M.tb. Ser/Thr Kinase – PknB

Aziz Mamur
Michael Steffey, Dept. of Medicinal Chemistry, University of Michigan
Advisor: Matthew Soellner, Depts. of Medicinal Chemistry, Chemistry, Pharmacy, University of Michigan

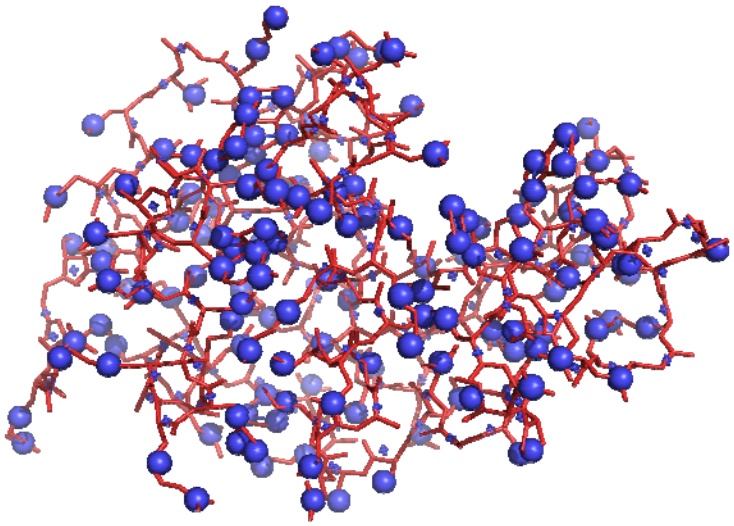
Protein kinases are known for their key role in cell signaling and regulating biological processes such as proliferation, differentiation and apoptosis. One of the methods of developing kinase inhibitors is to mimic the interaction of ATP with the kinase pocket and recognize the so-called active conformation, a conformation otherwise conducive to phosphotransfer. The highly conserved nature of the ATP pocket, however, makes achieving selectivity for a particular kinase difficult. Herein, we are developing a selective inhibitor of a protein kinase PknB from the pathogenic Mycobacterium Tuberculosis (M.tb). PknB is one of the 11 ser/thr protein kinases (STPKs) encoded in M.tb. genome and mediates signal transduction in the mycobacterial cell and is essential for cell growth. We screened a library of kinase inhibitors obtained from GlaxoSmithKline against PknB using a TR-FRET based assay and obtained a hit – GSK690693. This compound was originally optimized by GSK for the inhibition of the human kinase AKT. Based on modeling studies, we hypothesized that N-acetylation of the piperidine group in GSK690693 could result in selective inhibition of PknB while resulting in a steric clash and thereby loss in potency of AKT inhibition. We describe here, our progress toward the synthesis of a selective PknB inhibitor based on the GSK690693 scaffold.

Poster Presentation

Examining Interprotein Interactions Using Coarse Grained Molecular Dynamics Simulations

Michael Manning
Advisor: Kevin Kubarych, Dept. of Chemistry, University of Michigan

There are many chemical phenomena such as interprotein interactions that occur in protein systems that are outside the scope of fully atomistic molecular dynamics simulations. To study these interactions on a longer timescale than that available through fully atomistic simulations, coarse-grained (CG) models can be used. These models combine groups of three or four atoms from amino acids and solvents into beads. Grouping atoms together decreases the computational load, allowing system sizes (or simulation times) that can be several orders of magnitude larger than what is possible using fully atomistic simulations. We will use GROMACS (Groningen Machine for Chemical Simulations) molecular dynamics package along with the MARTINI coarse-grained force field to explore the protein-protein interactions and hydration dynamics of Hen Egg White Lysozyme (HEWL) and polarizable, coarse-grained water as a solvent. To do this, we have created a large system comprised of thirty-two proteins, that we can use to model the effects of biomacromolecular crowding on protein and water dynamics.



Poster Presentation

Interkinetic Nuclear Migration in the Regenerating Zebrafish Retina

Rebecca Marton
Manuela Lahne, Dept. of Biological Sciences, University of Notre Dame
Advisor: David Hyde, Dept. of Biological Sciences, University of Notre Dame

Zebrafish can regenerate lost photoreceptors due to Müller glial cells that reside in the inner nuclear layer of the retina. Müller glia divide in response to light-induced photoreceptor damage to produce neuronal progenitor cells that ultimately differentiate into new photoreceptors. During eye development, neuronal progenitor cells follow a pattern of movement referred to as interkinetic nuclear migration (IKNM). In IKNM, neuronal progenitor cell nuclei migrate from the basal region of the retina, where DNA is replicated, to the apical surface, where they undergo cell division. Recently, the Hyde lab demonstrated a similar Müller glial nuclear migration in the adult zebrafish eye during the regeneration response. While studies implicated actin/myosin interactions as a driving force of IKNM in development, the mechanisms that govern Müller glia nuclear migration during regeneration are not yet understood. Immunohistochemistry experiments that I conducted using phalloidin labeling revealed the presence of filamentous actin in processes in the trailing side of Müller glial nuclei during the regeneration response, suggesting the involvement of actin/myosin interactions in the regenerating retina. To assess the role of actin/myosin interactions in IKNM, I am identifying targets to inhibit actin filament formation. One such class of targets are α-actinins, cross-linking proteins that stabilize actin filaments. Quantitative real time PCR (qRT-PCR) experiments were used to determine what zebrafish α-actinin subforms change in expression during retinal regeneration. Upregulation of α-actinin1 and α-actinin3a beginning prior to the onset of Müller glial nuclear migration suggest that these subforms may be involved in IKNM, while downregulation of α-actinin3b and α-actinin2 suggests that these subforms may be associated with dying photoreceptors. In situ hybridization experiments confirmed α-actinin1 expression in Müller glia at the onset of IKNM but not in the undamaged retina. Together, qRT PCR and in situ experiments provide strong evidence for α-actinin1 as a target to inhibit actin filament formation in Müller glia during IKNM.

Poster Presentation

Raman Spectroscopic Monitoring of Integration of a Tissue-Engineered Oral Mucosa Construct

Robert Matthews
Shiuhyang Kuo, Cynthia L. Marcelo, and Stephen E. Feinberg
Oral and Maxillofacial Surgery, School of Dentistry, University of Michigan
Alexander Khmaladze and Michael D. Morris, Dept. of Chemistry, University of Michigan
Advisor: Michael D. Morris, Dept. of Chemistry, University of Michigan

Raman spectroscopy is a non-invasive tool that can monitor cells development of tissue constructs and their integration into animals and, ultimately, human patients. In oral surgery, there is a need for engineered tissue constructs that can be used to replace damaged oral mucosal tissue. In the animal studies that precede trials in humans, we are using Raman spectroscopy to monitor cell viability and development of normal metabolic function. In this study, Raman spectroscopy is applied to *Ex Vivo* Produced Oral Mucosa Equivalent (EVPOME) constructs. EVPOMEs are made from human oral epithelial cells grown on a commercially available acellular dermis matrix. We performed an *in vivo* study in which the EVPOMEs were grafted into Severe Combined Immunodeficiency (SCID) mice, that do not reject the EVPOME constructs. The constructs were placed in the mice for one week or three weeks. During construct, development abnormalities were introduced into some specimens by maintaining them at 43 ºC for a short period of time. Raman spectra of thermally stressed EVPOMEs show differences in certain bands, because development is slowed from heat-induced denaturing, which changes protein secondary structure. We chose the ratio of the 1445 cm^{-1} (CH_2 bend) band intensity to the 1003 cm^{-1} (phenylalanine ring breathing) band intensity. Comparison with implanted unstressed controls showed that integration of the stressed constructs is slower than integration of the unstressed controls.

Oral Presentation

Incorporation of Green Design into Field Iodine Deficiency Test

Sean McGee
Advisors: Kathleen Eggleson, College of Engineering, and Marya Lieberman, Dept. of Chemistry and Biochemistry, University of Notre Dame

Iodine deficiency has emerged as the number one preventable cause for mental illness in children in developing countries. A test in the form of a paper analytic device (PAD) can detect iodine in urine, which would provide more efficient targeting of aid to those in need. Identification and characterization of potential harms at any stage of the product life cycle is part of green design. Evaluation of the iodine deficiency PAD in this way reveals considerable risk in addition to the potential benefit to human health. Some of the key ingredients in the test, trivalent and pentavalent arsenic, could lead to significant environmental damage if not disposed of properly. In order to combat these risks, this project has explored the usage of iron oxide nanoparticles to adsorb the arsenic, immobilizing it and thus removing its toxicity after disposal. Testing of leach residues from the test via inductively coupled plasma optical emission spectroscopy (ICP-OES) has shown that iron oxides synthesized in situ have a high affinity for arsenic adsorption, lowering the concentrations of arsenic residues to below EPA and WHO standards of 5 ppm. Current testing involves incorporating iron oxide synthesis into the test design to maximize efficiency of use and ease of disposal.

Poster Presentation

An Enantioselective Total Synthesis of Cis-2,5-Disubstituted Pyrrolidines

Grace McKenna
Advisors: John Wolfe and Nicholas Babij, Dept. of Chemistry, University of Michigan

Cis-2,5-Disubstituted pyrrolidines have extensive biological applications including β3 adrenergic receptor antagonist activity. They pyrrolidinyl scaffolds show increased selectivity and metabolic selectivity in comparison to related acyclic amine molecules. As a result, these compounds could improve existing treatment or provide novel biological applications, including the treatment of overactive bladders. This work enumerates the progress made in creating a concise enantioselective synthesis of the cis-2,5-pyrrolidine core scaffold through the use of palladium-catalyzed carboamination reactions to cyclize the substrate, (1R)-2-amino-1-phenylhex-5-en-1-ol. Substrates with different protecting groups have been synthesized in four to five steps and in good yields. Current efforts are focused on finding optimal conditions for the palladium-catalyzed carboamination reaction. Application of these conditions with different substrates and aryl bromides will yield a number of different derivatives.

Poster Presentation

Changing Climate; Changing Life

Jill McNabnay
Advisor: Jessica Hellmann, Dept. of Biological Sciences, University of Notre Dame

Climate change is often thought of merely in terms of the impact it is having on humans. However, thousands of species around the globe are also being affected by our warming climate. Approximately 97% of all animals on Earth are invertebrates, and estimates are that almost 30% of the invertebrate phylum (approximately 10,000 species) are currently at risk of extinction. What role is climate change playing in this massively increased rate of extinction? How are organisms being impacted by changes in temperatures, weather patterns, and precipitation patterns, among other factors that climate change influences? And what can be done about it? The research being conducted in Dr. Hellmann's lab at the University of Notre Dame seeks to answer these questions by using the Karner blue butterfly as a model organism. The Karner blue is an endangered species, so seeking answers to how to help these organisms survive a changing environmental landscape is incredibly important. Every species matters within an ecosystem, and the loss of one species impacts all other species in that environment. Finding strategies to help manage the Karner blue butterfly population can hopefully not only save the Karner blue, but can possibly provide clues as to how to help other species in the wake of climate change as well. The students in my classroom will be doing similar experiments as those being conducted in Dr. Hellmann's lab to see what impact a warming climate has on non-endangered species of butterflies.

Poster Presentation

Roles and Interaction of MRPP1 and MRPP2 in Reconstitution of Human Mitochondrial RNase P

Christine Mei
Advisors: Michael Howard, Dept. of Biological Chemistry and Carol Fierke, Dept. of Chemistry, Biological Chemistry, University of Michigan

Transfer RNAs (tRNAs) are transcribed as precursors that need to be processed, in order to properly function in protein synthesis. One of the first processing steps is removal of extra nucleotides flanking the 5' and 3' ends of the tRNA. The maturation of the 5' end of tRNA is catalyzed by RNase P. RNase P in human mitochondria relies on 3 proteins for tRNA cleavage: MRPP1, MRPP2, MRPP3. MRPP1 is a tRNA methyltransferase that binds to MRPP2, a short chain dehydrogenase/reductase. MRPP3 is the endonuclease, responsible for tRNA cleavage. The requirement of MRPP1 and 2 for tRNA cleavage by MRPP3 remains enigmatic. Thus, I aim to study the relationship between MRPP1 and MRPP2 and their role in human mitochondrial RNase P. Since MRPP1 and 2 form a complex, we sought to characterize MRPP2's activity in the presence and absence of MRPP1. With my work, MRPP1 was shown not to hinder the activity of MRPP2, using acetoacetyl coenzyme A as a substrate. Truncations of MRPP1 were produced in order to investigate the protein-protein interaction of MRPP1 and MRPP2. A truncation encompassing the methyltransferase (MTase) domain was purified to homogeneity and shown to weakly associate with tRNA. Future studies involve using a pull-down assay to determine if the MTase Domain of MRPP1 can associate with MRPP2 and determining if the MTase domain is sufficient enough for human mitochondrial RNase P activity.

Poster Presentation

Genetic analysis of podocyte development

Rachel Miceli
Rebecca Wingert, Dept. of Biological Sciences, University of Notre Dame
Advisor: Rebecca Wingert, Dept. of Biological Sciences, University of Notre Dame

The kidneys are key specialized organs consisting of segmented functional units called nephrons. Development of the kidney in vertebrates includes the formation of up to three increasingly complex kidney structures, the pronephros, mesonephros, and metanephros. Segmentation of the nephrons which make up these structures is highly conserved between humans and zebrafish, making the zebrafish a good model system to study developmental pathways in the human kidney. The zebrafish embryo has a simple pronephros composed of two nephrons sharing a common glomerulus. The glomerulus functions as a blood filter, and the epithelial cells of this apparatus are called podocytes. Mature podocytes are characterized by cellular extensions, called foot processes, from their basal surface. These foot processes interdigitate with the extensions of neighboring podocytes and form cell to cell junctions called the slit diaphragm. Previously, our lab has identified and isolated two mutants: zeppelin (zep) and lightbulb (lib). lib encodes a mutation in aldehyde dehydrogenase 1a2, which is required for retinoic acid (RA) biosynthesis, and disrupts podocyte formation during nephrogenesis. The cloning of zep is ongoing, and further characterization revealed that zep mutants begin to exhibit severe edema at around 4 days post fertilization, and that the embryos exhibit dramatically reduced numbers of podocytes. To gain further insight into podocyte development in the zebrafish pronephros, the RNA transcripts for the podocyte markers such as wt1a, wt1b, nephrin, and podocin were localized in the pronephros at various time points of development in wild type and zep zebrafish embryos using whole mount in situ hybridization. zep mutants displayed reduced wt1b-expressing podocytes at the 15 somite stage, suggesting that podocyte specification is abrogated. Future directions include performing rescue experiments on zep mutants using RA, and further investigation of the role that the Notch pathway plays in podocyte development.

Poster Presentation

Performance Evaluation of Amazon EC2 and Google Compute Engine

Max Miller
Advisors: Jaroslaw Nabrzyski and Maciej Malawski, Center for Research Computing, University of Notre Dame

Analyzing high performance cloud computing infrastructures such as Amazon EC2 and Google Compute Engine will help determine the highest performing and cost effective option that will suit the needs of a large range of workloads. The performance of these two infrastructures will be measured using an assortment of open-source benchmarking tools. Amazon EC2 and Google Compute Engine support a large range of instance types that typically vary in available RAM or CPU resources. Due to this degree of variation, analysis of each instance type must be taken into consideration when measuring the performance of a cloud computing provider as a whole. To begin the analysis, an OS image was created with all benchmarks installed. This proved to be initially problematic due to many compilation and runtime errors that were encountered. These errors were difficult to debug due to lack of documentation on some benchmarking suites, however each were eventually resolved. The same image with all the configured benchmarks was used for all the various instance types. A ruby script that used the cloud service library 'fog' was made that helped to automate collecting all the data from the benchmarks. This Ruby fog script established a connection with Amazon EC2, created a new instance with the pre-configured image, and then sent a command to the new instance to run a script that started all the benchmarks one by one. The benchmarks were run ten times on all five instance types, and then the averages were calculated as a measure to make any outliers insubstantial. Once data was collected for Amazon EC2, it was imported into Microsoft Excel and graphed to visualize the various performance differences among the instance types. Future steps include the benchmarking of Google's Compute Engine. Once the data from Amazon EC2 and Google Compute Engine is collected, the final step will be to compare the two cloud computing providers, establish performance characteristics, and determine the highest performing and cost effective instance type.

Poster Presentation

Low glucose exposure favors the appearance of fast vs. slow oscillations in isolated mouse pancreatic islets

Alannah Miranda
Eric Glynn, Dept. of Pharmacology, University of Michigan
Advisor: Les Satin, Dept. of Pharmacology, University of Michigan

Pancreatic islets respond to elevated levels of glucose in the blood by generating electrical pulses, which in turn stimulate the influx of calcium into the cell and insulin release. The electrical pulses, or oscillations, occur in distinct patterns that are mirrored by fluctuations in free calcium in the cell. Islet oscillations can be classified as either slow (periods; 2 minutes) or fast (periods; 2 minutes); however, the dominant factor that determines whether islets will exhibit a fast or slow oscillation is unknown. We hypothesize that exposure to low glucose prior to a glucose challenge favors the production of faster islets. To test this possibility, isolated mouse islets were incubated overnight in medium containing 11 mM glucose. They were then exposed to low glucose (2.8 mM) for varying durations of time (0, 15, 30 and 60 minutes); after this, islets were challenged with 11 mM glucose. Islets were loaded with fura-2, a fluorescent dye, which changes its fluorescence at 502 nm depending on how Ca-bound it is. Calcium was measured from the ratio of the fluorescence intensity excited by 340 nm (Ca2+-bound) or 380 nm (CA2+-free). In 2.8 mM glucose, no calcium oscillations were observed, as expected. However, in response to elevated glucose (11 mM), faster oscillations tended to occur in islets that were pre-exposed to low glucose. In contrast, islets from the same mouse when continuously exposed to 11 mM glucose tended to exhibit significantly slower oscillations. Longer periods of exposure to low glucose were associated with a higher percentage of fast oscillating islets. These results suggest that switching off glucose metabolism for varying periods of time tends to favor the fast type oscillation over the slower one. This may help explain why faster oscillations were reported in studies using low glucose pretreatment. The results imply that prolonged fasting will tend to enhance faster oscillations, and will facilitate future comparison of the underlying biophysical mechanisms of each type of oscillatory mode.

Poster Presentation

Mechanisms Governing Müller Glial Interkinetic Nuclear Migration in the Regenerating Zebrafish Retina

Ciaran Mooney
Manuela Lahne, Dept. of Biological Sciences**,** University of Notre Dame
Advisor: David Hyde, Dept. of Biological Sciences**,** University of Notre Dame

Inherited retinal diseases, such as retinitis pigmentosa and retinal macular degenerations, result in the irreversible loss of photoreceptor cells leading to blindness. Unlike humans and other mammals, lower vertebrates, such as zebrafish, have the ability to undergo retinal regeneration following injury. Thus, zebrafish are a popular model organism to study retinal regeneration. Following light-induced injury in the zebrafish retina, Müller glial cells undergo dedifferentiation, enter the S phase of the cell cycle and produce neural progenitor cells that ultimately replace the lost or damaged photoreceptor cells. During this process, Müller glia undergo interkinetic nuclear migration (IKNM), where their nuclei migrate along a basal-apical axis in phase with cell cycle progression. While IKNM has been well characterized during neuroepithelia development, our laboratory has only recently observed IKNM in the zebrafish during retinal regeneration. Preliminary data found that actin filaments accumulate at the basal side of Müller glial nuclei that migrated apically during retinal regeneration. Additionally, Müller glial IKNM in regenerating adult zebrafish retinas decreased following inhibition of rho kinases, which phosphorylate and activate the myosin light chain, and facilitate actin-myosin mediated contraction. I am investigating the role of specific myosin isoforms during Müller glial IKNM in the regenerating zebrafish retina. Using in situ hybridization to localize specific RNA expression, I have determined that non-muscle myosin heavy chain myh10 mRNA is upregulated in Müller glia during zebrafish retinal regeneration following the onset of IKNM. This suggests that the non-muscle myosin heavy chain myh10 isoform may be involved in IKNM during zebrafish retinal regeneration.

Poster Presentation

Optimizing Paper Tests for Anti-Tuberculosis Medications

Cameron Moore
Seungyup Sun
Advisors: Marya Lieberman and Abigail Weaver, Dept. of Chemistry and Biochemistry, University of Notre Dame

Low quality drugs are a persistent problem, especially in developing countries where testing is rare. The PAD (Paper Analytical Devices) Project focuses on creating cheap paper tests that allow medicines to be quickly screened in a field setting. However, certain tests on the current Tuberculosis (TB) PAD were found to be functioning differently than expected. Specifically, tests that used 1,2-naphthoquinone-4-sulphonate (NQS), sodium nitroprusside (SNP), and sodium nitroprusside/ferricyanide (Magic SNP) did not work in the field. Our goal was to see how long each test could last on a PAD. After preparing these tests on PADs, we tested some of them fresh and left others to dry for between one to nine days at room temperature or at 37°C. The drugs tested were acetaminophen, streptomycin, ethambutol, isoniazid, and pyrazinamide. The results showed the NQS test to be particularly unstable and unable to give consistent results after a day. The SNP and Magic SNP tests were effective with isoniazid and pyrazinamide and lasted more than 9 days. All three tests gave results with the streptomycin on the day the tests were made, but lost effectiveness almost overnight. The results of our research will help clarify what positive and negative results should look like for these tests as well as how long they can last, which will help improve the TB PAD.
We also designed and prototyped some new forms of the PAD test that would increase the number of lanes on one device while also ensuring that a picture of the results would still be easy and convenient to take. We will present two of the successful designs that double the number of available lanes.

Poster Presentation

Carbon Dioxide Capture in Ionic Liquids

Brenda Mueller
Advisor: Joan Brennecke, Dept. of Chemical and Biomolecular Engineering,
University of Notre Dame

Carbon Dioxide capture is essential to lowering emissions without dramatically lowering energy output. Dr Brennecke's group is researching this by capture through ionic liquids. The ionic liquid needs to be viscous enough to flow well through the system, not degrade with temperature fluctuations, and also not form a precipitate when carbon dioxide reacts with it. The reaction also needs to be reversible in order to release the carbon dioxide for sequestration. This can be done by increasing the temperature as long as precipitates did not form. In the lab I have been synthesizing different ionic liquids and testing their properties. I have looked at the density, viscosity, water content, thermal decomposition, melting point, and carbon dioxide capture. Through all of this the curriculum that has surface is one that will be presented after the air pollution unit. An introduction on carbon capture and its usefulness will be presented along with an article explaining the processes of carbon dioxide capture and why they are important. Then a lab showing that a gas can react with a liquid to form a precipitate will be done by the students. In the same note this will also show a pH change so a universal indicator will also be added to tie that back into previous material. In the lab write up they will have to tie this work back into carbon capture research and why forming precipitates is important. In the last day they will have a performance assessment based on all the components as well as relying on previous background information. This will be done through a carbon dioxide scenario that the students will have to evaluate and critique.

Oral Presentation

Electronic Properties of Lead Telluride Quantum Wells

Elizabeth Mulder
Advisors: Richard Pimpinella, Joseph Hagmann, Xiang Li, Malgorzata Dobrowolska-Furdyna, Jacek Furdyna, and Xinyu Liu, Dept. of Physics, University of Notre Dame

While the properties of semiconductors are well known in the bulk, their less well known surface states have become a focus of recent research. Tied to this research is the prediction and discovery of Topological Insulators (TIs) and Topological Crystalline Insulators (TCIs), materials with novel surface states where an insulator has a highly conducting surface. A topological crystalline insulator has this same characteristic, but only for certain faces of a crystal. Additionally, TIs and TCIs conduct charges via the Quantum Spin Hall Effect, which minimizes scattering and thus improves conduction. Both of these classes of materials have possible applications in spintronics and quantum computing. By studying semiconductors in thin films, quantum wells, nanowires, and quantum dots, researchers hope to better understand semiconductors in this form, to measure the electronic and magnetic properties of their surface states, and to discover new examples of TIs and TCIs. My research this summer has focused on measuring the electronic properties of quantum wells that combine two families of semiconductors, specifically Cadmium Telluride and Lead Telluride (CdTe/PbTe/CdTe), whose interfaces hold promise of TCI surface states. The samples used in my study are grown by Molecular Beam Epitaxy, and measured using Magneto Transport experiments. I have found that samples grown on higher temperature substrates have higher mobility and lower carrier concentration, while the resistivity shows no significant change. These results will be used as a guide toward designing future structures for observing and characterizing TCI surface states.

Oral Presentation

A Parametric Model of Galaxy Feedback Processes

Maria Jesus Munoz Lopez
Advisor: Lara Arielle Phillips, University of Notre Dame, College of Science, Dept. of Physics

Filamentary structures forming the cosmic web have much higher density than the cosmic mean, and provide a continuous flow of matter into galaxies. In this cosmic web, inflow and outflow have been studied both observationally and through simulations to help explain galaxy evolution and metal enrichment in the filamentary environment. Parametric models have been used in the past to help account for the outflow from galaxies in large-scale simulations, but they do not take galaxy orientation, or differing feedback processes into account. In this new model, an attempt is made at identifying not only the amounts of matter and energy feedback from a galaxy but also the direction it takes and thus where it flows over time. This will eventually lead to a better understanding of the distribution of enriched materials in the filamentary cosmic web.

Oral Presentation

Vaccine Mandates and HPV

Alissa Murray
Advisor: Melinda Gormley, University of Notre Dame

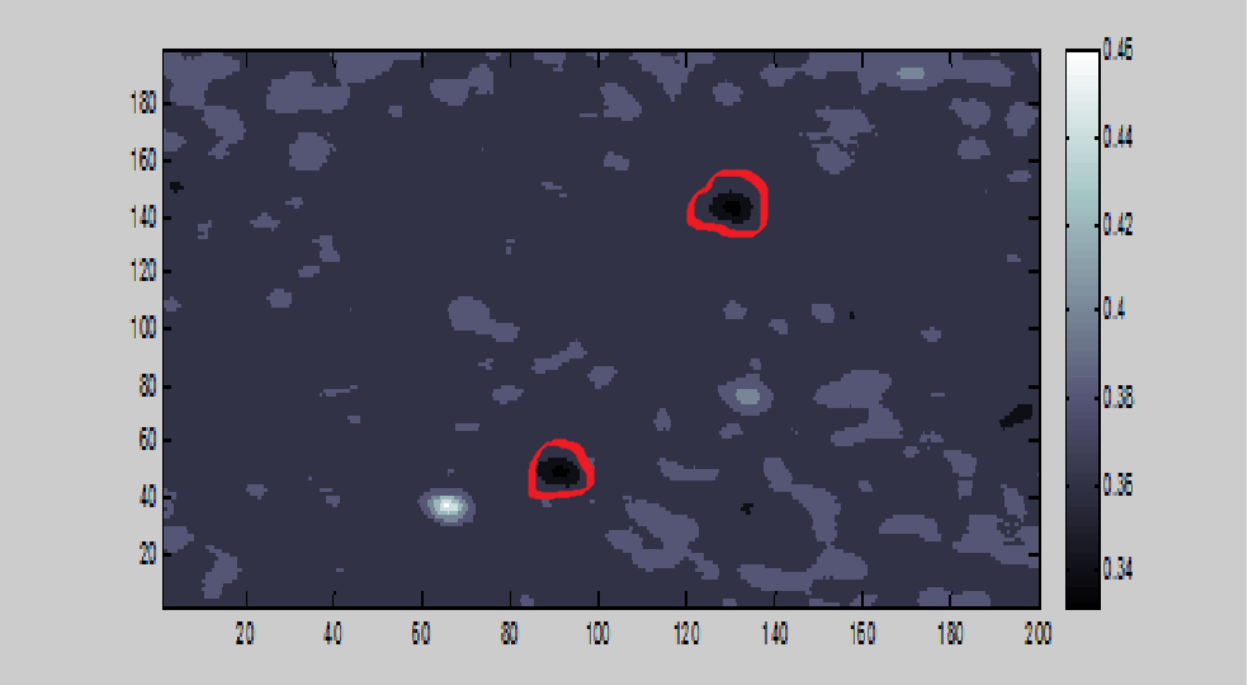
Vaccination has been proven to be the most effective way to control and prevent outbreaks of disease. Many vaccinations that the majority of Americans have received since childhood prevent highly contagious, airborne diseases, for which vaccination is the only truly effective means of protection. However, as technology has advanced and more vaccines have come into development, there exist vaccines for which alternative methods of prevention exist. This is the case with two vaccines recommended by the Immunization Action Coalition, the vaccines for Hepatitis B and for Human Papillomavirus, or HPV. Although both of these diseases can be avoided based on certain lifestyle choices, the vaccine for Hepatitis B is mandated in 47 states and Washington D.C., while a mandate for the HPV vaccine has been the source of much controversy since its approval by the FDA in 2006. In my paper I will consider the ethical questions regarding vaccine mandates, and will extend those questions to the case of the HPV vaccine. I will analyze the claims for and against a mandate of such a vaccine, and will consider what a mandate of the HPV vaccine would mean for the vaccine program in the context of public health as a whole.

Poster Presentation

Analysis of holes in graphene monolayers

Vaishnav Murthy
Zhongming Li and Nicolas Havard, Dept. of Chemistry and Biochemistry,
University of Notre Dame
Advisor: Gregory Hartland, Dept. of Chemistry and Biochemistry, University of Notre Dame

Graphene is an exciting new material due to its mechanical and electronic properties. Due to its high conductivity, it can be used in the future as a supercapacitor. However, when monolayer graphene is deposited on a surface it is common for there to be very small gaps or "holes" in this deposited layer. The goal of this research project is to analyse the properties of these holes present in monolayer graphene. To do this, we use the spatial modulation spectroscopy (SMS) technique on monolayer graphene deposited on an appropriate substrate (glass or silicon wafer) to get its intensity profile. We plan to use this intensity profile to accurately predict the size of the hole. We also plan to repeat the experiment with a laser of a different color to investigate whether the holes exhibit resonance.

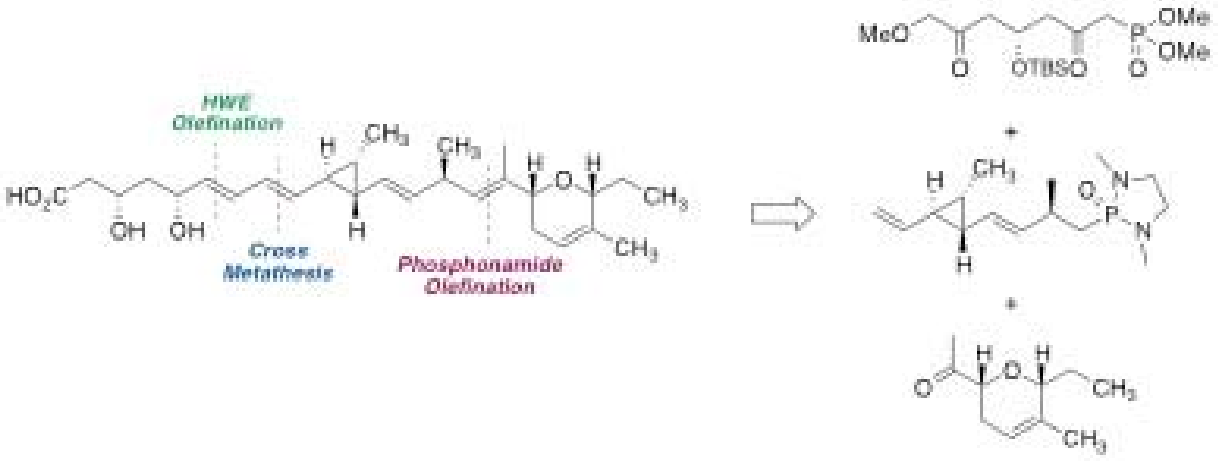


Poster Presentation

Progress Towards the Total Synthesis of Ambruticin J

Ansel Nalin
Advisor: Richard Taylor, Dept. of Chemistry and Biochemistry, University of Notre Dame

The ambruticins are a class of cyclopropane-containing polyketides isolated from myxobacteria fermentation of *Sorangium cellulosum* by Warner-Lambert scientists in 1977. Recently, Reeves and co-workers characterized the polyketide synthase gene cluster responsible for ambruticin production and proposed ambruticin J as a putative biosynthetic intermediate of the natural product. Because the ambruticins have shown interesting antifungal activity, they have been targeted for total synthesis and investigated in medicinal chemistry. Herein, we report our progress toward the total synthesis of ambruticin J. Our highly convergent synthetic route is highlighted by our cationic methodology to generate trisubstituted cyclopropanes. Synthetic production of ambruticin J will enable investigation of downstream biosynthetic transformations including the stereoselective epoxidation and cyclization essential to the generation of the C3-C7-pyran ring.



Poster Presentation

Synthesis of New Non-Heme Iron Nitrosyls

Sarah Neville
Amy Speelman and Nicolai Lehnert, Dept. of Chemistry, University of Michigan
Advisors: Amy Speelman and Nicolai Lehnert, Dept. of Chemistry, University of Michigan

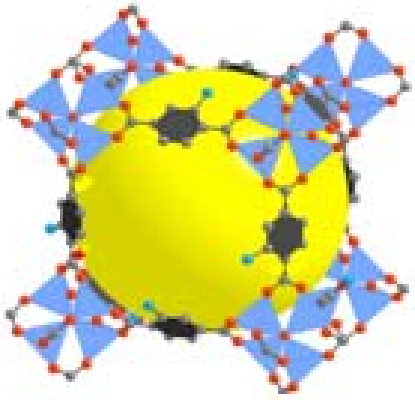
Nitric oxide (NO) has been implicated in numerous signaling and immune defense pathways in mammalian systems. In particular, when invading pathogens are detected in the body, macrophages release toxic NO. Many pathogenic bacteria contain flavodiiron proteins (FNORs), which are able to reduce NO to N_2O. As a result, these pathogens are resistant to the body's immune system, and are thus able to proliferate, resulting in infection and disease. However, the mechanism of the reduction of NO to N_2O by these enzymes is not completely understood. To study the mechanism of the enzyme, the non-heme iron model complex $[Fe_2(BMPA\text{-}PhO)_2(NO)_2](OTf)_2$ (BMPA-PhOH = N-(2-hydroxybenzyl)-N,N-bis(2-pyridylmethyl)amine), which self-assembles into a dimer, was constructed. In addition, the synthesis of a complex with the nitro-substituted derivative BMPA-NO_2PhOH was attempted in order to determine how changes in the electronic structure of the NO complex impacts reactivity. Future work will include further characterization of the model complex using spectroscopic methods, as well as characterization of the reactivity (*i.e.* N_2O production) of the compound upon reduction. In addition, EPR studies will be performed to determine whether the newly synthesized model complex is a monomer or a dimer.

Poster Presentation

Synthesis of IRMOF-3 and Conversion of Dihydroxyacetone to Ethyl Lactate

Hamim Nigena
Jongsik Kim, Dept. of Chemical and Biomolecular Engineering, University of Notre Dame
Advisor: Jason Hicks, Dept. of Chemical and Biomolecular Engineering,
University of Notre Dame

The goal of my research project was two-fold: 1) synthesizing a post-synthetically modified Sn-containing metal organic framework (MOF), Sn-IRMOF-3, and 2) the catalytic conversion of dihydroxyacetone (DHA) to ethyl lactate (EL) with the carbonized MOF (Sn/NC). The synthesis of the MOF, which contained an amine functionality, involved a solvothermal approach, using N,N-dimethylformamide (DMF), Zn(NO3)2• xH2O, and 2-aminoterephthalic acid as a reaction solvent, a precursor for metal oxide cluster, and an organic linker, respectively. The resulting MOF (denoted as IRMOF-3) possessed microporosity with high surface area (BET surface area of 980 m2/g, and a Langmuir surface area of 1370 m2/g) as well as a ~ 100 mm-sized cubic structure (obtained by SEM). The IRMOF-3 was modified by metallation with a Sn-precursur. Subsequently, the Sn-IRMOF-3 was carburized to generate a Sn/NC material. The catalytic conversion of DHA to EL was then studied under relatively mild conditions using the Sn/NC material as a catalyst. The average particle size of Sn on the nanoporous carbon support was ~ 100 nm via TEM, and the Sn was considered highly dispersed on the nanoporous carbon based on the lack of a tin oxide diffraction pattern in X-ray diffraction experiments. Lastly, the Sn/NC was exhibited a high activity toward the catalytic conversion of DHA, and this catalyst can be a promising material for the production of ethyl lactate, a raw material for the synthesis of a bio-degradable polymer. Future studies will involve the catalyst stability under reaction conditions, as Sn leaching was observed in the reaction media.



Poster Presentation

Employing the Energy of Light to Advance Technology

Heather M. Nimon
Advisor: Mark Wistey, Dept. of Electrical Engineering**,** University of Notre Dame

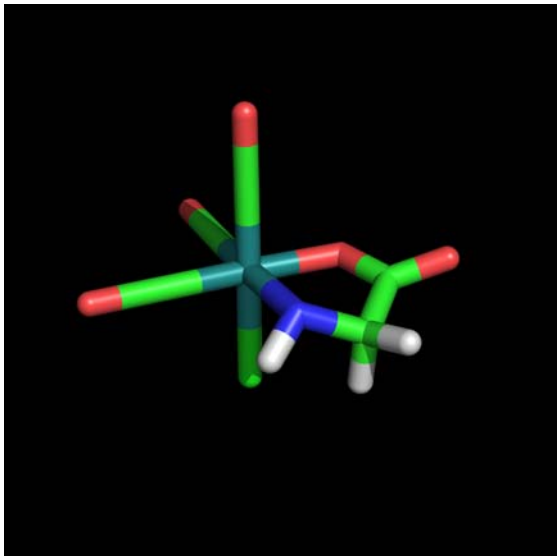
Within the department of electrical engineering at Notre Dame the Wistey group performs a wide variety of energy related activities. Using a variety of elements and a new combination of materials already in place within most solar labs, the researchers create lasers, photovoltaics, transistors, modulators, and detectors, the materials for new devices, and ultimately things like optical neural interfaces. Much of the current work revolves around the use of germanium as a material for transmitting light energy. The future of technology lies in the ability to use light energy rather than electrical energy to transmit signals. The physical properties of the current computer chip limits the speed at which information can be transmitted. Using light would significantly decrease the amount of time information would take to be transmitted and ultimately allow technology advances to once again seem endless.

Poster Presentation

The Structure and Dynamics of CORM-3 in Solution Studied Using FTIR and 2D-IR Spectroscopy

Joshua Ostrander
Advisor: Kevin Kubarych, Dept. of Chemistry, University of Michigan

Metal carbonyl complexes serve as excellent vibrational chromophores and absorb strongly in the infrared region of the electromagnetic spectrum. This has made Fourier Transform Infrared Spectroscopy (FTIR) and Two-Dimensional Infrared Spectroscopy (2D-IR) especially useful in the study of their structure and dynamics. In addition to this, metal carbonyl compounds have proved invaluable as vibrational probes because of their sensitivity to solvation environments. The "carbon monoxide releasing molecule" tricarbonylchloro(glycinato)runthenium (II) (CORM-3) has shown promise as a pharmaceutical in animal models of disease. Previous work on this molecule has suggested that in the presence of amino acid residues CORM-3 releases carbon monoxide and forms a metal-protein adduct. CORM-3's Reactivity to proteins has consequentially provided an excellent method to study hydrophobic hydration dynamics in a variety of model biological systems. Although CORM-3's reactivity and crystal structure have been well documented, its structure in solution is not well understood. In this study we present preliminary evidence of multiple isomers in solution dependent on the solvent composition, primarily using FTIR and preliminary 2D-IR measurements. The results indicate that the peak areas and frequency of transitions are dependent on the presence of water in solutions. In addition, evolution of the linear FTIR spectra over time indicates that CORM-3 may release small amounts of carbon monoxide in solution, despite the absence of any amino acids available for adduct formation.



Poster Presentation

Identifying the significance of the dual Peroxisomal Targeting Signals in *Arabidopsis thaliana* LACS7

Clarence Pascual
Ali Dorchak, Dept. of Molecular, Cellular, and Developmental Biology, University of Michigan
Advisor: Laura Olsen, Dept. of Molecular, Cellular, and Developmental Biology, University of Michigan

Peroxisomes are small organelles found in all eukaryotic cells, and are responsible for the catabolism of long-chain fatty acids and the breakdown of oxygen radicals (e.g. hydrogen peroxide) through the process of oxidation. Peroxisomal proteins are post-translationally localized to peroxisomes via a specialized peroxisomal targeting signal (PTS). Peroxisomal matrix proteins contain two possible signals: Peroxisomal Targeting Signal Type 1 (PTS1) or the Peroxisomal Targeting Signal Type 2 (PTS2). The protein under study in this project is *Arabidopsis thaliana* long-chain acyl-CoA synthetase 7 (LACS7). Acyl-CoA synthetase is responsible for the catabolism of long-chain fatty acids by directing them to the β-oxidation pathway. LACS7 is known to interact with the PEX5 receptor that is strictly associated with the PTS1 signal. While most peroxisomal proteins contain only a single PTS, LACS7 is characteristically unique because it carries a PTS2 as well as a PTS1 signal. We hypothesize that this phenomenon occurred as a way to increase the efficiency of import since acyl-CoA synthetase plays a very important role in a cell's energy production. With the use of site-directed mutagenesis, we were able to create five constructs of the LACS7 gene carrying PTS variations. An *in vitro* S-methionine. Localization of these proteins was performed using an *in vitro* import assay containing glyoxysomes isolated from pumpkin cotyledons. Our goal is to take advantage of the duality of signals in LACS7 protein and determine the efficiency of each import route.

Poster Presentation

Determining Heart Rate from Video

Aakash Patel
Advisors: Michael Villano and Charles Crowell, Dept. of Psychology, University of Notre Dame

There have been past successes both here at Notre Dame and elsewhere in developing methods to determine an estimate of an individual's heart rate from a video containing the subject's face (referred to below as a heart rate from video (HRFV) system). However, the integration of a ground-truth source to test the accuracy of these systems has been slower to occur. One purpose of the present research was to address this shortcoming by integrating a Contec CMS60C pulse oximeter as a ground-truth validation source for HRFV code previously developed here at Notre Dame. In addition, subsystems were implemented in the code to (1) allow users to select specific video sources if multiple inputs were present on the computer being used to execute the HRFV code, (2) analyze and export the original video after adding simultaneous overlays of estimated heart rate data from both HRFV system and the ground-truth source, and (3) output of the raw estimated heart rate data to a file for subsequent analysis. These enhancements were intended to facilitate the validation of the HRFV system as well as to make it a more versatile tool for use in future studies. In addition, since several parameters are available in the code that can affect the heart rate estimation process, the simultaneous output of both ground truth and HRFV estimates make it easier to select optimal parameter settings for any particular application. The above tasks were completed via the Boost libraries for serial communication and threading in addition to the OpenCV library for video capture and exporting. Exporting live video from a camera source via OpenCV proved to be problematic initially due to time sync issues between realtime and captured video. This challenge was addressed by determining and implementing proper time delays in code corresponding to a specified capture frame rate. A specific validation study has been designed and approved by the IRB to collect data from 10 subjects. If the HRFV system proves reliable, then the eMotion & eCognition lab will utilize this system in a variety of future projects.

Poster Presentation

The Geppetto Project

Nathaniel Pelz
Advisors: Michael Villano and Charles Crowell, Dept. of Psychology, University of Notre Dame

Previous studies in social cognitive neuroscience have documented the existence of an interference effect that occurs when two humans face one another while each performs a separate incompatible action. This effect predicts that observing an individual performing an action facilitates the observer's performance of that same action, while interfering with the performance of an opposite action. This interference effect has been reported to a lesser extent when a human is observing the motion of a humanoid robot, but is not present when a human is observing only the motion of a robotic arm. Other studies have indicated that a humanoid robot must have "realistic" (i.e. human-like) motion in order to properly induce the interference effect.

Our goal in the present research was to further explore this phenomenon by studying the extent to which the interference effect is present when interacting with the digital image of a Nao humanoid robot displayed on a video screen. However, in order to properly perform this study, it is necessary to program the Nao to move in a fluid, realistic way. Our approach to this goal was to record human arm movements using a Microsoft Kinect and transfer this data to the Nao robot arm, allowing it to move in the same way as the original human actor. To complete this task, we created a Microsoft Visual Studio program (written in C#) to read in a series of coordinates and move the Nao motors appropriately. We also altered an existing Kinect motion-recording program to send its captured human coordinates directly to the Nao control program in real-time.

Both programs are functional, and the Nao can effectively mimic human movements by reading in Kinect coordinates in real-time or from a saved file, but additional work is needed. The Nao imitation of a fluid human arm movement is still somewhat jerky, since the program is not yet able to convert Kinect coordinates to Nao coordinates via inverse kinematics with 100% accuracy. Our remaining effort on this project will be to address this issue.

Poster Presentation

Characterization of APC-induced microtubule branching

Jaqueline-Mae Picache
Advisor: Holly Goodson, Dept. of Chemistry and Biochemistry, University of Notre Dame

Every year, 57,000 people die of colorectal cancer in the United States. Many cases of colorectal cancer are initiated in the Wnt signaling pathway. This pathway is inhibited by the protein adenomatous polyposis coli (APC) which is coded for by the tumor suppressor gene APC. APC mutations are not the only cause of colorectal cancer but do cause cancer in many patients who have the mutation. In patients with colorectal cancer, the C-terminus of the APC protein is often disrupted due to missense and deletion of APC. This C-terminus is also known to bind microtubules. Literature indicates that cytoskeletal networks play roles in tumor initiation and progression. However, the mechanisms of involvement are not fully understood. Further investigation into the relationship between APC and microtubules should be done to clarify how cytoskeletal networks lead to tumorigenesis and progression. A potential project involves a recently observed phenomenon that APC causes branching of microtubules. The main objective of this project was to characterize the APC induced branching of microtubules phenomenon. In order to do so the following goals were achieved: 1) purification of the APC-C1 protein and 2) polymerization of APC-C1 bound microtubules by incubating unpolymerized tubulin with the protein. This combination was incubated with or without labeled tubulin seeds to determine if tubulin polymerization can occur on its own in the presence of APC without already polymerized tubulin. The polymerization was analyzed using a light scattering assay and florescent microscopy. Preliminary results suggest that branching of microtubules is possible but it remains unclear if APC is the cause.

Poster Presentation

Generation and characterization of *tnfa* and *nr2e3* transgenic zebrafish lines

Samantha Piekos
Manuela Lahne and Kristin Ackerman, Dept. of Biological Sciences, University of Notre Dame
Advisor: David Hyde, Dept. of Biological Sciences, University of Notre Dame

Following damage, zebrafish can regenerate all neuronal classes in the retina, making them an ideal model organism for studying the neuronal regeneration process. Specifically after light damage, photoreceptor cell death triggers Müller glia to re-enter the cell cycle and proliferate, creating neuronal progenitors that migrate to the outer nuclear layer (ONL) to replenish the lost photoreceptors. Tumor Necrosis Factor-alpha (TNFα) is an apoptotic factor, and our laboratory has shown that it is expressed in dying photoreceptors and in Müller glia. In development, Nuclear receptor subfamily 2, group 3, member 3 (Nr2e3) is a transcription factor involved in rod photoreceptor differentiation, and therefore it is hypothesized to be expressed in the progenitors and/or new photoreceptors in the ONL. Transgenic zebrafish allow for high fidelity labeling and cell tracking, making them effective tools for research on embryonic development and adult tissue regeneration. The development of *TNFα* and *nr2e3* transgenic zebrafish lines will enable further understanding of photoreceptor differentiation and regeneration. A BAC containing *TNFα*, a transposon iTol2-amp cassette, and a GFP-kan cassette inserted into the first intron of *TNFα* has been constructed. A BAC is currently being constructed for *nr2e3* following the same procedure. The *TNFα* BAC was sequenced, which confirmed the presence of these components, and was then microinjected into one-cell albino zebrafish embryos. Injected embryos were sorted for GFP expression. Potential GFP- positive zebrafish were crossed with albinos and the offspring were sorted for GFP expression. To confirm the transgenic GFP expression patterns, I performed *in situ* hybridization of albino zebrafish to characterize *TNFα* and *nr2e3* expression. These results will lay the foundation for using the *TNFα* and *nr2e3* transgenic lines to study retinal regeneration.

Poster Presentation

Thiolated gold and silver nanoclusters absorption of visible light

Julian Pilate-Hutcherson
Kevin Stamplecoskie, Dept. of Chemistry and Biochemistry, University of Notre Dame
Advisor: Prashant Kamat, Dept. of Chemistry and Biochemistry, University of Notre Dame

The absorption of thiolated gold and silver nanoclusters can be tuned in the visible (350 and 700 nm) region. Unlike their counterpart of larger nanoparticles, these few atom nanoclusters do not exhibit plasmon absorption, but exhibit molecular-like properties. Upon visible excitation, these nanoclusters are capable of injecting electrons into TiO2. There were several methods tested for the synthesis of these thiolated gold clusters, in every case Au3+ was reduced to Au0 in the presence of glutathione as a stabilizing agent. In one method Au3+ was reduced by refluxing with glutathione as the reducing agent. In other experiments Au3+ was reduced, at room temperature, by NaBH4 in the presence of glutathione. In yet another set of experiments silver nanoparticles were used in galvanic exchange to reduce Au3+, while they themselves become oxidized. Silver nanoclusters were also synthesized by reduction with the addition of NaBH4 again in the presence of glutathione as a stabilizing agent. All the synthesized gold and silver nanoclusters were able to absorb an appreciable amount of visible light up to 650 nm. These gold or silver clusters that absorb visible light may provide increased efficiency of TiO2 solar cells by absorbing more sunlight.

Oral Presentation

Double Folding Analysis of 6Li Elastic and Inelastic Scattering to low lying states on 208Pb

Benedict Pineyro
Advisor: Umesh Garg, Dept. of Physics, University of Notre Dame

Elastic scattering of 360 MeV 6Li ions from 2.9 degrees to 33 degrees from 208Pb. The data were fitted with a hybrid double folding model and a pure double folding derived from M3Y density dependent model. Distorted Wave Born Approximation (DWBA) calculations were performed with the fitted parameters to calculate cross-sections for inelastic scattering to low lying 3-states.

Poster Presentation

Dye Sensitized Solar Cells

Kenneth Poling
Ming Li, Dept. of Civil Engineering and Geological Sciences,
University of Notre Dame
Advisor: Chongzheng Na, Dept. of Civil Engineering and Geological Sciences,
University of Notre Dame

Solar Panels are designed to absorb light and convert light to energy that can be utilized by our society. TiO2 (titanium dioxide), a nanocrystalline film, allows electron conduction to take place. In order for the electrons to be charged by sunlight effectively, a charge transfer dye is needed. The dye absorbs light, and the light's energy excites electrons in the dye molecules. These excited electrons travel out of the dye molecules and into the TiO2 nanocrystals. In a solar cell, an electrolyte will also be needed to transport the electrical charge. In order to function, each solar cell will have an anode (positive charged electrode) and a cathode (negative charged electrode) charged plate. When these plates are attached a potential difference is the source for an electrical current. When the TiO2 forms nanocrystals a greater surface area to volume ration is created. This allows more TiO2 for a dye to soak, creating a more efficient surface area for sunlight absorption. Conceptually, the question of this lab experiment , is to investigate "Which dye, or dye product, will produce the highest level of electrical power?" Raspberries, blueberries, maple leaves, or carbon-nano-tubes? The intention of this experiment is not test the longevity or shelf life of the dye or product.

Poster Presentation

Crystalline InSb from Simple Electrodeposition of Sb onto the Reactive Interface of In Electrodes under Aqueous Benchtop Settings

Jessica Rafson
Eli Fahrenkrug, Dept. of Chemistry, University of Michigan
Advisor: Stephen Maldonado, Dept. of Chemistry, University of Michigan

In this presentation, I will discuss my recent efforts to directly reduce dissolved Sb_2O_3 at clean In(s) electrodes to produce crystalline InSb at room temperature. Conventional production of crystalline III-V semiconductors relies on sophisticated equipment, toxic precursors and energy intensive growth strategies which add cost at large scales. Recent work in our group has focused on developing a room temperature benchtop process that leverages the electrochemical reduction of Group V oxides in water on active group III metal electrodes to produce the respective crystalline III-V semiconductor. The developed setup required for the process is very simple: an In foil electrode is used in a standard three electrode cell containing a solution of dissolved Sb_2O_3 in NaOH. A potentiostatic bias is then applied at room temperature. Raman analysis of the resultant films confirms this method can reliably produce crystalline InSb. The necessity of an oxide-free metal electrode interface and methods to achieve this will be discussed. Results from time-dependent spectroelectrochemical measurements (<6h) will be shown that highlight a key balance between rates of electrodeposition and interfacial reaction. Additionally, incrementally changing the applied electrode potential from the thermodynamic reduction potential (-0.84 V vs. Ag/AgCl) to -1.85 V vs. Ag/AgCl increased the total quantity of deposited Sb. Decreasing the concentration of dissolved Sb_2O_3 M) by one order of magnitude subsequently decreases the amount of Sb deposited on the In electrode. Preliminary data for an electroless analog of the synthesis of crystalline InSb will also be introduced.

Poster Presentation

Characterization of fluticasone propionate microcrystalline drug product using quantitative polarization microscopy

Sashary Ramos
Gustavo Rosania, Dept. of Pharmaceutical Sciences, University of Michigan
Advisor: Gustavo Rosania, Dept. of Pharmaceutical Sciences, University of Michigan

Orally-inhaled fluticasone propionate, a potent corticosteroid anti-inflammatory agent, is one of the most prescribed inhaled drug products for the treatment of asthma. This drug product is formulated as a suspension of pure microcrystals in trichlorofluoromethane and dichlorodifluromethane with soya lecithin, and is administered to the lungs using a Metered-Dose Inhaler (MDI) device. Here, we developed a quantitative microscopic imaging method to characterize the aerosolized fluticasone propionate particles delivered directly from the MDI device. Taking advantage of the unique optical properties of fluticasone propionate microcrystals, we employed a quantitative polarization microscope to monitor the size, distribution, and birefringence properties of the particles at a specific angle and distance from the nozzle. The particles were captured on a glass surface, and using a quantitative retardance measurement algorithm, the birefringence properties of the fluticasone propionate microcrystals were used to quantify the properties of individual aerosolized particles produced by the MDI device. Experimentally, the area of the aerosolized particles ranged from .297 to 1265.624μm^2 at a distance of 15cm from the nozzle. The integrated retardance of the fluticasone propionate particles was linearly related to the area of the individual particles, consistent with an even distribution of fluticasone propionate microcrystals within each particle. Approximately 90% of the analyzed particles had an area from 0 to 100 μm^2, which is in the respirable range for inhaled particles; the remaining particles were too large to be considered in the respirable range. Based on the area distribution of the particles and the aerodynamic requirements necessary to achieve inhaled drug particle deposition in the airways, we estimated that a minimum of 50% and a maximum of 75% of the dose expelled from the device had the potential of reaching their intended site of action in the lungs. To conclude, our results demonstrate a polarization microscopy-based imaging strategy may be useful to optimize the characteristics of microcrystalline fluticasone propionate formulations and to study the performance of different MDI devices. Interestingly, this imaging strategy could also be useful to monitor the fate of individual fluticasone propionate particles as they dissolve *in vitro*, and potentially, *in vivo*.

Poster Presentation

Population genetic structure of Balinese long-tailed macaques (*Macaca fascicularis*)

Julia Resil
Amy Klegarth and Hope Hollocher, Dept. of Biological Sciences, University of Notre Dame
Advisors: Amy Klegarth and Hope Hollocher, Dept. of Biological Sciences,
University of Notre Dame

Increases in human population and subsequent urban development have a marked impact on the environment. Animal habitation in the vicinity of humans has a prospective possibility of having their dispersal patterns and species gene flow experiencing extreme distortion. This study examines genetic variation and population structuring of Balinese long-tailed macaques (*Macaca fascicularis*) in varying degrees of anthropogenic influence. Long-tailed macaques are not only known for their dispersal abilities but are also known extensively throughout Southeast Asia; conversely Balinese macaques are honored at Hindu temple sites and are offered varying degrees of food provisioning. This research is designed to examine the influence of varying levels of provisioning of macaque genetic variation. In spite of Balinese macaque's large population sizes, my hypothesis is that food provisioning will result in decreased dispersal, ultimately decreasing gene flow and more importantly decreasing genetic variation. This study is designed to determine the degree of genetic variation on Bali based on correlation of genetic distance and geographical distance. This method of study has been previously used to examine gene flow on Singapore via mitochondrial and nuclear datasets. A previous incomplete dataset from Bali generated a haplotype network with limited success on genetic variation relation to population structure. By using mitochondrial DNA to make haplotype networks it will be possible to visually analyze differences and similarities associated with Singapore and Bali respectively. Further tests on genetic variation will include more analysis with mitochondrial on the number of social groups per site and the number of matrilines per group. Furthermore we will be able to achieve sharper data on genetic variation that was previously discovered by a study that used nuclear DNA from Bali macaques. Future goals of this on going project would be to give preliminary data to be used for macaque management and study of anthropogenic environmental influences on other mammalians and eventually to other types of organisms.

Poster Presentation

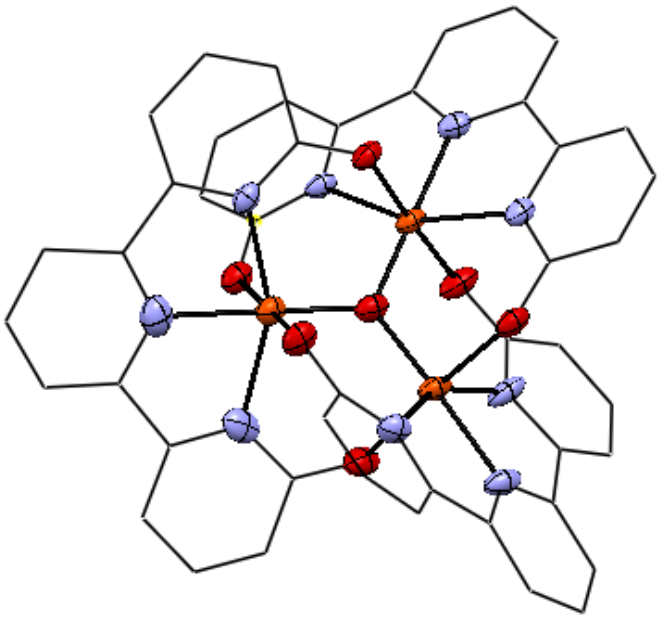
Structure and Catalytic Activity of Iron 6,6'-Dihydroxy Terpyridine Complexes

Grayson Ritch
Advisor: Nathaniel Szymczak, Dept. of Chemistry, University of Michigan

The ligand 6,6'-dihydroxy terpyrdine (dhtp) is a redox stable ligand with pendent hydroxy groups in the ortho positions of the furthermost pyridine rings. The ligand has been previously shown to switch between a neutral, anionic, and dianionic states at various pH ranges. It's proposed that dhtp would act as an intramolecular proton transfer agent within a metal complex promoting novel catalytic behavior.

To explore the use of this ligand in catalysis, several iron-dhtp complexes were synthesized and characterized with various auxillary ligands and counter ions. Several iron compounds with different anions were used as water oxidation catalysts using cerium ammonium nitrate as a chemical oxidant. An inherit issue with such complexes seem to be the formation of a catalytically inactive trimer in the presence of a base.

Iron compounds utilizing phosphine auxillary ligands were used to catalyze transfer hydrogenation reactions. A complex using trimethylphospine has been found to be monomeric in the solid state and shows promising potential as a transfer hydrogenation catalyst for electron rich acetophenones.



Poster Presentation

Functional characterization of the carbon dioxide receptor genes in *Culex quinquefasciatus* and *Culex stigmatosoma*

Olaf Rodríguez Gutiérrez
Advisor: Zainulabeuddin Syed, Dept. of Biological Sciences, University of Notre Dame

Carbon dioxide (CO_2) is an important chemosensory stimulus used by mosquitoes to locate their hosts, and is also implicated in sugar-feeding behavior. Detection of CO_2 in *Anopheles gambiae* was previously shown to be conferred by three receptors, *AgGR22*, *AgGR23*, and *AgGR24*, expressed together in an olfactory receptor neuron (ORN) in the maxillary palp (MP) sensilla. I studied whether the homologues of these *An. gambiae* CO_2 receptors are present in *Culex quinquefasciatus*, the West Nile virus (WNV) transmitting mosquito. *Culex* are the dominant mosquito vectors in North America. The recent WNV outbreak in southwestern U.S. and other regions have highlighted the importance of studying this genus. As a first step, I synthesized the cDNA from host seeking/CO_2 sensitive female and male mosquitoes. Using a set of degenerate primers, I amplified all the three receptors (*CqGr1*, *CqGr2*, and *CqGr3*) and cloned them into pCR-BLUNT-II vector. Full length amplified sequences revealed 78.0, 73.1 and 77.0 % homology with the *AgGR22*, *AgGR23*, and *AgGR24* receptors, respectively. In addition, I studied if the reported lack of CO_2 sensitivity in a closely related *Culex* species, *Cx. stigmatosoma*, is due to the absence of the CO_2 receptors in the genome. Since *Cx. stigmatosoma* genome has not been sequenced, I used *Cx. quinquefasciatus* primers to amplify these receptor genes from *Cx. stigmatosoma*. One gene, putatively named *CsGR2*, was successfully amplified from the cDNA. Preliminary single-unit electrophysiological experiments from the CO_2-senstive ORNs in *Cx. quinquefasciatus* and *Cx. stigmatosoma* revealed that both the species respond to increasing concentrations of CO_2 in a dose-dependent manner. I am in the process of studying whether microRNAs play a role in the differential CO_2 sensitivity in these two mosquito species.

Oral Presentation

Integration of Design and Energy Analysis Tools for Cooperative Energy Efficient Building Design

Clarissa Rogg
Advisors: David Go, Dept. of Aerospace and Mechanical Engineering, and Aimee Buccellato, School of Architecture, University of Notre Dame

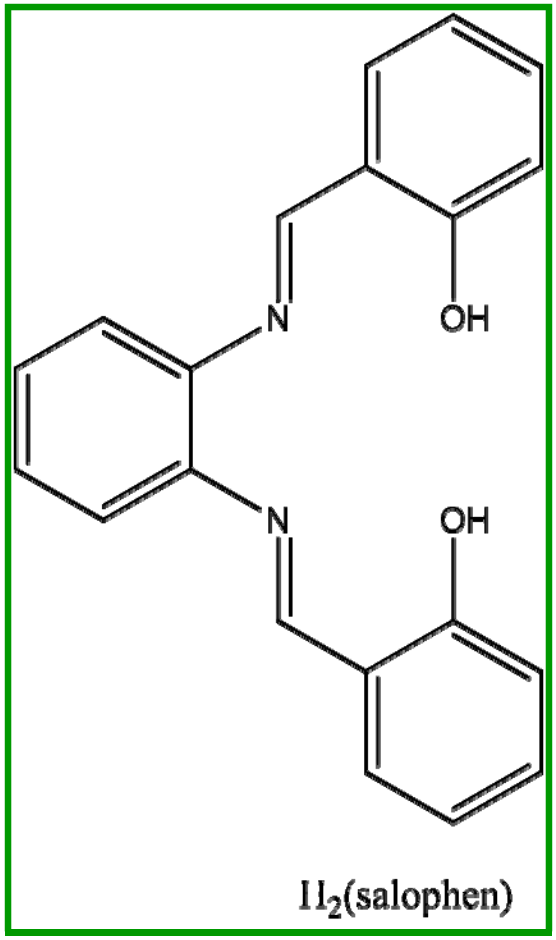
Buildings accounted for almost 40% of the total energy consumed by the United States in 2012. Reducing the energy consumption of buildings is a priority for the architecture industry. This creates a need for integrated CAD tools that assess energy performance throughout the building design process. Optimizing energy efficiency while maintaining comfort and safety standards as well as aesthetics and architectural form requires collaboration between architects and engineers, and they must have mastery of the integrated CAD and energy analysis tools. Students of architecture and engineering, therefore, need opportunities to develop design decision making skills informed by sound energy analysis and understanding of important archetypes that balance form and function. In this work, the tools for such a collaboration were explored and the basis for an undergraduate class on collaborative building design process was established. Architecture students will supply engineering students with building design plans so that the engineering students can run energy simulations and collaborate with architecture students about decisions to reduce energy consumption while maintaining comfort. For this work, buildings are modeled with SketchUp and simulated in the energy analysis program, EnergyPlus. Tutorials were designed to guide students through the energy analysis process and parametric studies of how design choices affect energy performance. Individual studies on the variation of orientation, materials, fenestration, HVAC systems, internal loads, scheduling, and location were conducted to elucidate the broad utility of EnergyPlus and to guide future design studies. Future work will be to include embodied energy analysis through the GreenScale tool to create a design and analysis framework that can be used by students to evaluate the total, lifetime energy performance of proposed building designs.

Poster Presentation

Development of s-block Organometallic Catalysts for co-polymerization of Polycarbonates

Ann Rutherford
William Buchanan and Kenneth Henderson, Dept. of Chemistry and Biochemistry,
University of Notre Dame
Advisor: Kenneth Henderson, Dept. of Chemistry and Biochemistry, University of Notre Dame

I worked with Dr. Henderson's group on a project to create catalysts that promote co-polymerization of carbon dioxide with epoxides to form polycarbonates from waste feedstocks utilizing ambient pressures and low temperatures. The intended polycarbonates are higher-value polymers with applications in many areas (i.e. lightweight, shatterproof lenses) and could potentially provide a cost offset to Carbon Capture and Sequestration efforts.



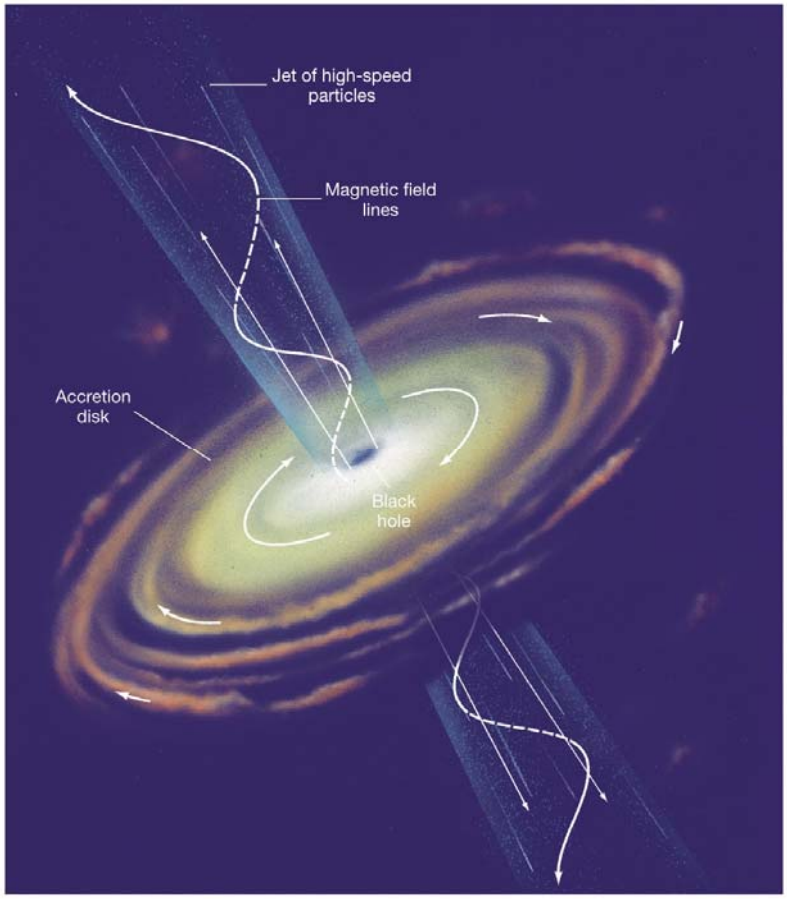
H_2(salophen)

Oral Presentation

Formation of relativistic jets along the axis of rotation of a black hole

Adrien Saremi, Aaron Sawyer, and Jared Johnson
Advisor: John Poirier, Dept. of Physics, University of Notre Dame

Black holes are well known to attract anything that passes their surroundings due to their large mass, but some also have the ability to eject matter in two powerful jets along their axis of rotation called **relativistic jets**. The main explanation to their formation is the magnetic field produced by the **accretion disk** located in the equatorial plane of the black hole, but can also be attributed to the twisting of space-time around the compact mass. Our project consists in studying the magnetic field produced by the accretion disk and how a particle can, under the influence of this B-field, move from its circular motion to an upward direction along the z-axis (axis of rotation). To do so, we designed a program that computes and draws the magnetic field lines of the accretion disk. Once this was done, we then designed another code to compute the trajectory of a particle, starting from different positions in the accretion disk. Our work also consisted of verifying our program's calculation, by establishing mathematical formulas to calculate the B-field in specific cases.



Oral Presentation

Beam Monitor Prototype Using Gas Discharge

Trevor Satterfield
Advisor: Manoel Couder, Dept. of Physics, University of Notre Dame

Nuclear astrophysicists study nuclear reactions to understand the energy production and nucleosynthesis in stars. Since Astrophysicists cannot directly measure the cross section of the atomic interaction in stars, experiments involving particle accelerators have to be used. Those reactions take place in stars at relatively low energy where the cross section is very small. In the laboratory, high intensity beam are required to measure those small cross sections. The high intensity beam may melt solid material in the interaction. In this work we focus on finding an alternative to the standard slits in order to evaluate the size and profile of the beam. As the beam travels through a vacuum, regardless of the quality of the vacuum, it interacts with the residual gas, mostly nitrogen. Research have been done by German physicists (F. Becker (2007) et al., Proc. DIPAC'07), at energies greater than 200 MeV/u with an intensity of approximately 10 nA. D. Seil (UU. 2005) has also done research but his beam energy and intensity was at 50 keV and 30 mA. However, no one has tested the energies and intensities between these ranges. Therefore, research at these energies is of great importance to Notre Dame due to the introduction of a new underground particle accelerator laboratory, DIANA, which will be able to reach even higher intensities. Results of a preliminary beam monitor prototype are presented.

Oral Presentation

Particle acceleration due to electromagnetic fields about an accretion disk

Aaron Sawyer
Advisor: John Poirier, Dept. of Physics, University of Notre Dame

It is known that accretion disks of in-falling matter tend to form about gravitating bodies. A model is presented for particle motion leaving a charged, rotating accretion disk. The motion of the particle was found to spiral out of the plane of the accretion disk, towards the z-axis of the gravitating body under certain circumstances. Frame dragging effects caused by a spinning black hole might explain how this vertical motion could then be funneled into a relativistic jet.

Poster Presentation

Role of cyclins in Müller glia and neuronal progenitor cell proliferation in the zebrafish retina

Sarah Semanek
Advisor: David Hyde, Dept. of Biological Sciences**,** University of Notre Dame

Age-related macular degeneration is the leading cause of vision loss worldwide. Currently, there are limited preventative therapies (Tsao et al., 2013) and lost human vision cannot be restored. Zebrafish are excellent vertebrate models for studying the visual system due to the similarity of its retinal structure and function to the human retina. In contrast to humans, zebrafish can regenerate lost retinal cell types after injury and restore vision. Photoreceptor cell death induces Müller glia to reenter the cell cycle and produce neuronal progenitors that further divide and migrate to the ONL, where they differentiate and replace lost photoreceptors (Vithelic et al., 2000). The mechanisms underlying this regeneration have not been fully characterized. To study how the Müller glia reenter the cell cycle, I am focusing on the cyclin gene family, which regulate progression through the cell cycle. In some cases, the mammalian retinal Müller glia upregulate early proliferation markers that are expressed during G1-phase, such as Cyclin D1, but do not undergo mitosis (Joly et al., 2011). To further understand the processes governing Müller glial cell cycle reentry and regeneration of the retina, I am generating transgenic lines of the cyclin family (*ccnb1*, *ccnd1*, and *ccne1*) using a transposon-mediated BAC transgenesis protocol (Suster et al., 2011). The transgenic constructs generated were microinjected into *albino* embryos at the one-cell stage. *In situ* hybridization was performed to confirm that the spatial and temporal expression patterns of the transgenic lines match that of endogenous mRNA. Gene specific DIG-labeled *in situ* hybridization probes were generated for *ccnb1* and *ccnd1* to localize the corresponding RNAs. The *ccnb1* transgenic line was designed to express GFP and the *ccnd1* line will express *mcherry*, which will allow us to differentiate between the different cell cycle stages. This would allow us to identify signaling pathways that are required for the progression from G1-phase to mitosis, potentially offering avenues for therapies.

Poster Presentation

Opportunistic Grid Computation for High Energy Physics

Dillon Skeehan
Advisor: Paul Brenner, Center for Research Computing, University of Notre Dame

In this poster, we present a general method for software and data access for opportunistic grid systems to aid in the analysis of high energy physics through the Compact Muon Solenoid (CMS) experiment at CERN. Traditional computational resource capabilities owned by CERN and associated institutions through the Worldwide LHC Computing Grid (WLCG) are the primary bottleneck for analysis, and in order to combat this growing concern, CERN has broadened its scope to employ opportunistic methods of computation for periods of high intensity data analysis. The computational method explored in this poster relate to CMS data analysis on opportunistic computational grids such as the Center for Research Computing High Performance Computing facility at Notre Dame. We show how CMS software and data may be accessed through the Parrot Virtual File System, a tool for accessing remote file systems, to allow for submission of jobs to grids with no previous connection to the CMS experiment. We then give an analysis of the eviction of these jobs and provide a comparison of performance between this new approach and traditional dedicated resources.

Poster Presentation

Hey! Can Someone Turn the Light On? SOS! (*Sustainably Off Sunlight)

Lynda Smith
Advisor: Prashant Kamat, Dept. of Chemistry and Biochemistry, University of Notre Dame

The search for more efficient and environmentally sound sustainable energy sources is one of the most important endeavors imaginable. Currently we are mostly at the mercy of a fossil fuel economy, not knowing what the prices will be, knowing the demand will only go up and the available supply diminish. The release of CO_2 continues to contribute to global warming as we continue to burn these fuels. Why is research on alternative energy sources not an important global imperative? The Kamat Lab at Notre Dame is working to increase the understanding and efficiency of the solar cell (as well as other things). The "first generation" solar cells must be manufactured in a clean room with pure silicon which makes these cells expensive. These solar cells also do not capture a wide range in the visible light spectrum-thus reducing their potential efficiency. Researchers at the Kamat Lab are investigating alternative ways to capture solar energy- using Quantum Dot Solar Cells (liquid junction and solid-state)-some to produce electric current, others to split water into hydrogen and oxygen, with hydrogen available as a fuel source. This is the kind of research that contributes to improved and more efficient and economical types of sustainable energy. My goal is to bring the sense of urgency of developing alternative, sustainable forms of energy to my students and to allow them to see how they can understand the energy issue and can see some of the work being done to address this problem. I want my students to understand the importance of science and doing research-and I'm also hoping that many will find this an interesting and exciting idea that they may wish to explore further.

Poster Presentation

Revolutions of 1848: History of Contingency?

Emmanuel Sosa
Advisor: John Deak, Dept. of History, University of Notre Dame

The year 1848 was one of great turmoil as Europe broke out in a series of revolutions. From Sicily to Milan, all over France, extending to great parts of Central Europe, from Berlin to Budapest. Everyone from students to workers lead revolts to challenge authority in different parts of Europe. These revolutions are generally viewed as key points of a national awakening, many historians today believe them to be national revolutions. This project intends to go beyond the national narratives, by studying the residual effects of the French Revolution of 1789 and the events leading up to the year 1848. Europe was essentially a boiling pot which no lid could suffice. With a more precise study of local problems that afflicted different parts of the continent, such as social, economic and political conditions, (failing harvests, censorship, the rise of liberal politics, and in some cases accidents) it is clear to estimate that this problems were different from place to place. Thus, revolutionary conditions were much more local, not national: no revolution of that year is identical to the next or stems from the exact the same roots. It is crucial to study the time frame after the French Revolution leading up to that year and keep both eyes open as to what was happening in a local sphere rather than a national one.

Oral Presentation

Delineation of the role for Notch signaling during zebrafish kidney regeneration

Kristin Springer
Kristen McCampbell, Dept. of Biological Sciences, University of Notre Dame
Advisor: Rebecca Wingert, Dept. of Biological Sciences, University of Notre Dame

Kidney disease affects millions of people each year and while procedures such as hemodialysis are available to help those afflicted with kidney disease, no known cure exists. Zebrafish have the incredible ability to regenerate their kidneys upon acute injury; however, the exact mechanism by which regeneration occurs is not well understood. This ability, coupled with findings demonstrating similar patterns of development between zebrafish and human kidneys, makes studies of kidney regeneration in zebrafish especially promising. The Notch pathway is essential during nephron development, and thus we hypothesize that Notch signaling may be likewise essential during renal regeneration. Notch is a transmembrane protein with both an extracellular and intracellular domain. During development, ligands bind to the extracellular portion of the protein, resulting in the cleavage of Notch and release of the intracellular domain into the cytosol. This intracellular domain then travels to the nucleus where it modifies gene expression. The aim of this project is to investigate the role of the Notch pathway in kidney regeneration upon acute injury by gentamicin injection. The expression of Notch signaling components or their targets in renal development has not been previously examined in the zebrafish adult kidney. To assess the expression of Notch components in adult kidneys, we generated antisense riboprobes to a panel of genes including Notch receptors and ligands and used whole-mount in situ hybridization to assess the spatial localization in kidneys before and after injury. It was found that Notch ligand jagged2 showed fewer transcripts in injured kidneys suggesting downregulation. Conversely, a second Notch ligand, deltaC, showed transcript expression in cellular casts of injured kidneys. Ongoing studies include the completion of our gene expression timecourse with the use of qRT-PCR and section in situ hybridization to study expression of Notch components in kidneys before and after injury. Future studies investigating the effects of blocking and over expressing Notch may shed further light on the mechanism by which regeneration occurs.

Poster Presentation

Improved Efficiency of Negative Ion Electron Capture Dissociation (niECD) Through Charge State Reduction and Laser Activation

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Advisor: Kristina Hakansson, Dept. of Chemistry, University of Michigan

Post translational modifications (PTMs) are crucial for the structure, function and interaction of many proteins in their biological environment. Many positive ion mode tandem mass spectrometry (MS/MS) techniques cannot retain these PTMs1 and thus important information about biological function can be lost. Also, several PTMs are acidic and therefore ionize poorly in positive ion mode. Recently developed negative ion electron capture dissociation (niECD) produces c'/z•-type product ions without loss of PTMs2. However, due to the Coulomb barrier between negatively charged precursor ions and electrons, electron capture can be difficult and lower charge states are thus preferred. The effect of precursor ion charge state upon niECD efficiency was explored. Additionally, activation of precursor ions using an IR laser prior to niECD (AI-niECD)3 was investigated as a tool for increasing sequence coverage.
Five μM ubiquitin was prepared in 50:25:25 water:methanol:isopropyl alcohol. In addition 0.1% formic acid was added by volume. All experiments were performed on a 7 T Fourier transform ion cyclotron resonance (FT-ICR) mass spectrometer (SolariX, Bruker Daltonics, Billerica, MA). Analytes were introduced into the gas phase through electrospray ionization (ESI). Mass isolation was performed using quadrupole mass analysis prior to electron capture dissociation in negative ion mode. The electron capture efficiency was improved from 3% to 8% when the charge state of the precursor ions shifted from -4 to -3. In addition, increased efficiency by over 500% was observed when precursor ions were activated using an IR laser, presumably due to destruction of non-covalent interactions.

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Poster Presentation

Data Git: Provenance Extraction Tool Using Version Control

India Stewart
Judy Long
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Data and software provenance metadata provides the context necessary to understand, trust, and reuse scientific data, a critically important component of curating the massive datasets generated by High Energy Physics (HEP) experiments where data is not reproducible. Data and Software Preservation for Open Science (DASPOS) explores solutions to meaningful documentation and preservation of data to provide a model for HEP and other disciplines. To further this goal, we have prototyped and are testing the viability of Data Git (DGit), a tool for extraction and machine readable documentation of provenance metadata, using W3C standard ontologies. DGit is a Python wrapper for Git distributed version control that utilizes Git's handling of repository contents to extract and document provenance metadata of a repository in machine readable format, for the purposes of later querying. DGit demonstrates a useful model for capturing the state, contents, and changes of a repository, making the metadata accessible and linkable at a later point in time.

Poster Presentation

Analysis of SIRT1 Activity by Capillary Electrophoresis

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Advisor: Erik Guetschow, Dept. of Chemistry, University of Michigan

Sirtuins are a family of NAD-dependent protein deacetylases and are currently of great interest due to evidence suggesting their effect on aging and aging related disorders, such as Alzheimer's disease and Huntington's disease. Several methods have been developed to study the activity of sirtuins with mass spectrometry and fluorescence-based assay being most common. However, the most common fluorescence assay utilizes the Fluor de Lys fluorogenic dye, which has been shown to susceptible to false positive results. Capillary electrophoresis (CE) is a promising alternative to these methods that is able to overcome some of these challenges. In CE, a small sample is injected into a capillary filled with buffer solution and separated in an electric field based on the size and charge of the analytes. We have developed a method that utilizes fluorescently labeled peptides containing an acetylated lysine as a substrate for SIRT1. When SIRT1 deacetylates the substrate, the mobility of the peptide through the capillary changes and distinct peaks are observed for the acetylated and deacetylated peptides. The ratio of the signal peaks can be used to determine enzyme activities in the presence of various inhibitors and activators of SIRT1. By employing CE, results can be obtained quickly with high sensitivity. Several known inhibitors of SIRT1 were tested using this method and IC50 values of 674.5 nM for Ex-527 and 142.5 nM for Surmamin were measured, while resveratrol, a suspected activator, showed no signs of activation.

Poster Presentation

Determining the Significance of the ZNF217-PKM2 Interaction in the Metabolic Regulation of Breast Cancer Progression

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Advisor: Laurie Littlepage, Dept. of Chemistry and Biochemistry, University of Notre Dame

In 20-30% of early-stage breast tumors, chromosome 20q13.2 is amplified and is associated with poor patient prognosis. ZNF217 is thought to be the oncogene responsible for this amplification, making it a novel biomarker and potential therapeutic target. In this study, we hope to determine the significance of ZNF217's interaction with the M2 isoform of pyruvate kinase (PKM2), which plays a vital role in metabolic regulation. Two different truncation mutants were made from the full-length ZNF217 protein: an N-terminal truncation removing the first five zinc-finger binding motifs and a C-terminal truncation removing the two putative nuclear localization sequences. These two truncations were then cloned into two different vectors, N-terminally-tagged and C-terminally tagged GFP vectors, to ensure that there was no tag interference in ZNF217 function during localization. In total, four different ZNF217 truncation constructs were made for analyzing PKM2 interaction and to be compared with the full-length construct, known to interact with PKM2. Each construct was transfected into 293T cells along with RFP-tagged PKM2. The localization patterns of ZNF217 and PKM2 were monitored via fluorescence microscopy to characterize a nuclear or cytoplasmic interaction domain. The interaction was also verified by co-immunoprecipitation and western analysis of ZNF217 and PKM2. Future experiments testing the presence of metabolic factors in cells overexpressing ZNF217 will provide more insight into how the ZNF217-PKM2 interaction may affect metabolic regulation. I hypothesize that ZNF217 interacts with PKM2 to regulate metabolic factors like glucose intake and lactate production to create hypoxic and low-nutrient environments that promote tumorigenesis.

Poster Presentation

Ultrafast 2DIR probe on an organic polymer for a model HFL system

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The efficient extraction of petroleum through the use of hydraulic fracturing is apparent through its rapid and widespread adaptation. Despite the large-scale adaptation of hydraulic fracturing, relatively little is understood about the fundamental chemical dynamics of actual hydraulic fracturing liquid (HFL) solutions used in the process. HFL is a heterogeneous mixture of water, organic-polymers, and suspended particles, essential to the success of hydraulic fracturing. We are actively investigating new types of vibrational probes based on transition metal carbonyl complexes as sensors of their environments. Here we report on the development and the characterization of macro-molecular probes using Steglich esterification in order to study HFL solutions by two dimensional infrared spectroscopy (2D-IR). Using the piano-stool metal carbonyl (Benzyl)Chromium-tricarbonyl as an infrared active probe of the local hydration environment, we hope to gain insight into the how solvent dynamics respond to changes in composition of the HFL. This characterization will aid in developing a working model for how each component in the HFL affects the overall properties of the solution.

Poster Presentation

Effects of pH on Pore Size of poly(isoprene-b-styrene-b-dimethylacrylimade) Membrane

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The WATER Lab specializes in fabricating and testing polymeric membranes that can be used for filtration. Graduate student Jake Weidman has fabricated a membrane from a self-assembling block terpolymer, poly(isoprene-b-styrene-b-dimethylacrylimade) (ISD), that is being tested because of its sensitivity to pH. The structure of the ISD membrane contains a high density of nearly monodisperese pores, which results in performance that surpasses that of commercial nanofiltration membranes. After exposure to a simple acid solution, the polydimethylacrylamide block is converted to a polyacrylic acid block, which is pH sensitive. Under acidic conditions (pH < 4) the polymer chains collapse opening the pores and under basic conditions (pH > 9) the polymer chains expand causing pore swelling. Running consecutively increasing pH filtrates (spanning from pH 1-12) followed by consecutively decreasing pH filtrates have revealed a hysteresis in membrane permeability. The particular interest of this study is defining the hysteresis. Future experiments will test if pore size can be fixed by pretreating with a specific pH and then running experiments with DI water (pH=5.7). One projected application for the ISD membrane is the separation of valuable pharmaceutical products from unwanted products of pharmaceutical synthesis.

Poster Presentation

Does Visible Light Photolyze Hydroxocobalamin?

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Advisor: Roseanne Sension, Dept. of Chemistry, University of Michigan

Previous experimental data in which DNA cleavage successfully occurred has been attributed to the photolysis of hydroxocobalamin induced through illumination with visible light (T. A. Shell, D. S. Lawrence, J. Am. Chem. Soc. 133 (2011) 2148.). Theoretical simulations later suggested that it should be possible to induce the photolysis of the OH radical from hydroxocobalamin through excitation at the correct wavelength. In the work reported here experimental conditions used by Shell and Lawrence were explored in order to observe cob(II)alamin formation through steady state photolysis of hydroxocobalamin. Samples were prepared utilizing hydroxocobalamin in a buffer solution at various pH values, with neutral salts to vary the ionic strength, and with a radical scavenger. The samples were exposed to visible light from a mercury lamp in ten minute intervals. UV-Vis spectra were then taken in order to observe photoproducts. From the spectra it was determined that there was no noticeable photoproduct formation. Ultrafast transient absorbance spectroscopy yields an excited state lifetime of 2.9 ps consistent with the negligible photolysis in steady state measurements. Finally, additional information was obtained by performing a Gaussian decomposition of UV-Vis spectra of hydroxocobalamin and a compound known to photolyze under similar conditions, namely methylcobalamin. Our measurements and analysis suggest that the DNA cleavage observed by Shell and Lawrence must have proceeded through an alternate mechanism where cob(II)alamin was not formed.

Oral Presentation

Exploring the Collective Properties of Gadolinium-160

Zachary Tully
Advisors: Shelly Lesher and Ani Aprahamian, Dept. of Physics, University of Notre Dame

We have examined 160-Gd using the (n,n'γ) scattering reaction with energies from 1.5-2.8 MeV to better understand nuclear vibration. Collective vibration along the semi-major axis of the ellipsoidal (deformed) nucleus (termed γ-vibration) is well known. However, vibration along the major axis of the nucleus is undetermined. Our goal is to categorize this lesser known vibration by analyzing the isotope's decay properties. My role in this research primarily involves developing the excitation function for all spectra.

Poster Presentation

Experimental Studies on Field Emission-Driven Microdischarges

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Advisor: David Go, Dept. of Aerospace and Mechanical Engineering, University of Notre Dame

Microdischarges, defined as the passage of current through gas with dimensions less than 1 mm, have numerous applications including excimer radiation sources, sensors, plasma display panels, ozone generators, and biomedical devices. Field emission is the discharge of electrons from the surface of a solid material subjected to a strong electric field. At small enough scales ($d < 10$ μm) the electric field becomes large, and field emission can become an important source of free electrons in a microdischarge. In this work, we experimentally demonstrate the relationship between pressure and current for field emission-driven microdischarges in atmospheric air. Microdischarge devices are made of metal (titanium - Ti or tungsten - W) on silicon with a photoresist polymer as a spacer, where the polymer height determines the electrode gap. During the experiment current and voltage were recorded, and Fowler-Nordheim plots were used to confirm the presence of field emission. Then, the relationship between the pressure and current was examined by measuring current versus pressure from ~0.01 to 700 torr at a fixed voltage. These measurements show that current grows exponentially with pressure due to electron impact ionization of neutral gas molecules. This confirms theory stating that current scales as $i = \exp(\alpha d) \times iFE$, where α is the ionization coefficient, d is the gap size, and iFE is the field emission current at ~0.01 torr.

Poster Presentation

MD Simulations Reveal the Impact of Crystal Packing on the Post-SET Loop of NSD1

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Advisor: Heather Carlson, Dept. of Medicinal Chemistry and Chemistry, University of Michigan

NSD1 is a histone lysine methyltransferase with an active SET domain that likely plays a role in many diseases. Hyperactivation of NSD1 is found in multiple cancers and has been associated with cell immortalization and poor prognosis. This makes NSD1 a potentially fruitful drug target, yet the mechanism by which NSD1 regulates lysine methylation is not well understood. Recent crystal structures of NSD1 and the related histone methyltransferase ASH1L show the post-SET loop in two distinct auto-inhibitory conformations. The crystal structure of NSD1, however, appears to be influenced by crystal packing. We hypothesized that when allowed to move freely in solution, the loop adopts a conformation that is similar to ASH1L and is more representative of its native state in the cell. To investigate this, we ran molecular dynamics (MD) simulations of the NSD1 catalytic domain starting from both loop positions. We then performed cluster analysis in order to generate typical conformations adopted by the protein. Indeed, we found that the loop spontaneously adopts a stable conformation similar to ASH1L when the crystal packing contacts are removed and it is allowed to relax in solution. Our simulations clearly show transitions between the two auto-inhibitory states, which lends insights into controlling NSD1 and its methylation of histone lysines. These structure-function relationships and the ensemble of protein conformations from the MD may be useful for drug design.

Oral Presentation

CMS Upgrade Simulations

Edward Varty
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Due to the planned upgrades to the luminosity and energy of the LHC, the CMS detector is also planned to be upgraded. To account for the increased number of particles that will be produced, the CMS detector must have a more efficient method of filtering out uninteresting particles. This is done by the Level 1 Trigger, but the current trigger is not effective enough so a new method of separating particles is needed. Simulated particle tracks were analyzed by a trigger algorithm passed on by previous workers on this project. The results of this algorithm were evaluated and the algorithm was altered in order to increase the efficiency while decreasing the number of false particle tracks found. The current implementation of the algorithm is closer to what is required for the future hardware. There are still problems in the track finding. Some are inherent in the detector design while a few are still problems with the algorithm itself, but are not insurmountable.

Poster Presentation

Analysis of *lunatic fringe* in Renal Progenitor Patterning During Zebrafish Kidney Development

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Advisor: Rebecca Wingert, Dept. of Biological Sciences, University of Notre Dame

The zebrafish pronephros is a simple kidney organ composed of two nephrons with a shared glomerulus and a pair of tubules connected to the cloaca. Each pronephric tubule is segmented into functionally distinct sections: a proximal convoluted tubule (PCT), proximal straight tubule (PST), distal early segment (DE), distal late segment (DL) and pronephric duct (PD). However, where and when this pattern is established during embryogenesis has remained poorly understood. In young embryos, the renal progenitor cell field that will generate the pronephros is not divided into segments; instead it is divided into a rostral and caudal domain. My previous study indicated that these renal progenitor domains emerge in the early embryo as early as 3 somites. To continue studying renal progenitor patterning, *lunatic fringe* (*lnfg*) was identified as a potential gene of interest. *lnfg* is a regulator of Notch signaling; it refines the spatial localization of Notch-receptor signaling to tissue boundaries. In zebrafish, *lnfg* expression has been reported in many regions including the anterior-posterior axis of the neural tube, presomitic mesoderm (PSM), somites, and renal progenitors. However, the precise timing and expression domain(s) of *lnfg* in renal progenitors has not been described. We hypothesized that *lnfg* is also involved in renal progenitor patterning and segmental boundary specification of the pronephros. To investigate this hypothesis, we examined the expression of *lnfg* and performed morpholino knockdown of *lnfg* followed by whole mount *in situ* hybridization. *lnfg* morphants exhibited a slightly expanded PST and a reduced DE. Current efforts are aimed at looking at additional gene probes to better characterize the renal progenitor domains, such as the transcription factor *etv5*. To determine the function of these factors in nephrogenesis, future studies will be conducted to define the relationship between *lnfg*, retinoic acid, and the transcription factor *mecom*, which we have previously shown to be significant in nephrogenesis.

Poster Presentation

Investigation of Small Molecule Binding to the Exon Splicing Silencer in Human Immunodeficiency Virus Type 1 Tat Exon 3

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Advisor: Hashim Al Hashimi, Depts. of Chemistry and Biophysics, University of Michigan

Regulation of mRNA splicing is essential for the HIV virus, because both spliced mRNA and non-spliced RNA are key to its survival and proliferation (Si et al., 1998). Specifically, spliced mRNAs are used to make proteins, while non-spliced RNAs are exported out of the nucleus, through the Rev pathway, and then packaged into new viruses (Si et al., 1998). Such regulation is affected through different mechanisms, such as exon splicing silencers (ESS) and exon splicing enhancers (ESE). One such silencer is ESS3, located near splice site A7, which is also the beginning of the third exon found in tat mRNA as well as in many other mRNAs (Tange et al., 2001; Zhu et al., 2001). Its silencing action is activated through hnRNP A1, a protein that binds to ESS3 and prevents splicing of the mRNA transcript, specifically by the UP1 subunit (Tange et al., 2001; Zhu et al., 2001, Levengood et al., 2012). Our goal was to find a molecule that would bind to the to exon splicing silencer 3 (ESS3) of the HIV-1 virus and inhibit binding of hnRNP A1, thus preventing splicing inhibition and the creation of longer mRNA transcripts, which are important in later stages of the HIV virus' lifecycle (Levengood et al., 2012). To this end, we have prepared RNA constructs containing the hnRNP A1 binding region of ESS3 (SLESS3) for structure and small molecule binding characterization using NMR spectroscopy. The spectra reveal well-resolved resonances and establish suitability of this system for NMR-based high throughput screening against small molecules.

Poster Presentation

Stasis of Saltwater Tolerance in *Anopheles farauti* FAR1 Mosquitoes

Alyse Volino
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Saltwater tolerance in anophelines is a trait with important implications in disease transmission and human health. The existence of saltwater tolerant anopheline species means that anophelines can be found in a wider geographic distribution, which translates to a broader range of disease transmission. Mosquitoes of the species *Anopheles farauti* are a major vector of malaria. *Anopheles farauti* has been found to survive in brackish water in the environment, but a colony of the FAR1 strain of *An. farauti* has been maintained in freshwater in the laboratory since 1967. Removing selection pressure for osmoregulation by raising the larvae in freshwater may have resulted in loss of salinity tolerance. Thus saltwater tolerance of FAR1 mosquitoes was tested by assessing survivorship to pupation of larvae that were reared in water of varying salinities. Water salinity was found to be related to the percentage of larvae that survived to pupation, as well as the amount of time it took larvae to develop to pupation. As water salinity increased, survivorship to pupation decreased. Treatment with water at salinities above 60% that of seawater proved to be detrimental to pupation: no more than 40% of larvae in any treatment higher than 60% of seawater survived to pupation. Also, time to pupation increased as salinity increased, from 7 days in larvae reared in freshwater up to 11 days in larvae reared in 90% of seawater. The ability of FAR1 mosquitoes to survive to pupation in water of low to moderate salinities shows that the saltwater tolerance of *Anopheles farauti* has not been lost, even though freshwater laboratory culture conditions have made tolerance unnecessary for over 40 years.

Poster Presentation

S-Nitroso-N-hexanylpenicillamine (SNHP)-Doped Polymers: Synthesis, Leaching Stability, and Characterization of Nitric Oxide Release

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Advisor: Mark Meyerhoff, Dept. of Chemistry, University of Michigan

Nitric oxide (NO) plays a key role in multiple physiological processes, such as vasodilation, immune defense, and antithrombotic activity. As a result, materials that release NO at rates similar to the vascular endothelial layer that lines the inner walls of all blood vessels have been explored extensively for their application to blood-contacting biomaterials. Significant progress in this direction has been achieved with polymers doped with S-nitrosothiols (RSNOs), such as *S-nitroso-N*-acetylpenicillamine (SNAP); however, such materials can suffer from significant leaching of SNAP out of the polymer phase, decreasing NO release lifetime of the polymer and posing a potential biohazard. The objective of this study was to increase the lipophilicity of an RSNO doped within a polymer coating to reduce leaching. In a simple, two step synthesis, the amine group on penicillamine was derivatized with hexanoyl chloride and the resulting thiol was nitrosated with acidified sodium nitrite to yield *S-nitroso-N*-hexanylpenicillamine (SNHP) in good yield. Two biomedical grade polymers, silicone rubber and Elast-eon™ E2As, were then doped with SNHP to investigate RSNO leaching rates and controlled release of NO by thermal decomposition. SNHP leaches out of the E2As polymer layer extremely slowly, releasing 5% of the total doped compound during the first day of incubation in solution at physiological temperature, and only 8% release after 5 days. The SNHP-doped E2As also displays physiologically relevant levels of NO release for up to 5 days. Based on these results, SNHP is also likely to exhibit excellent storage stability within polymer films/coatings. The use of the new SNHP/E2As polymer formulation may prove useful for enhancing the biocompatibility of various biomedical devices such as intravascular catheters and grafts; animal studies to assess these applications will be conducted in the near future.

Poster Presentation

Synthetic processes of gold nano-sphere (NS) & nano-rod (NR) particles for the enhancement of solar cells

Justin Waller
Advisor: Prashant Kamat, Dept. of Chemistry and Biochemistry, University of Notre Dame

Gold nano-spheres (NS) and rod shaped particles (NR) were synthesized for the application to solar cell devices in order to enhance light absorption abilities and improve solar cell efficiency in energy conversion of solar light to electricity. These materials were designed to be equipped to solar cellular devices that displayed absorption compatibility, absorbing light of similar wavelength/frequencies, which are absorbed by the cell. Solar cells absorb and convert more efficiently with respect to the characteristics and optical properties of the shape differentiated particles. Gold (NS) particles were synthesized via citrate reduction method and seed mediated growth methods, while gold (NRs) were synthesized via seed mediated growth methods only. Particles were layered with silica coatings of various shell thicknesses, allowing particles to serve as a more suitable enhancing component to solar cell systematic devices, through prevention of unsolicited electron transfers.

Poster Presentation

Structure probing of the transcriptionally acting $preQ_1$ riboswitch using single molecule FRET (smFRET)

Jiarui Wang
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Advisor: Nils Walter, Dept. of Chemistry, University of Michigan

Riboswitches are regulatory elements found in the 5' untranslated regions of many bacterial messenger RNAs (mRNAs) that modulate gene expression in response to the binding of small molecule ligands. Riboswitches comprise two functional components: a ligand binding aptamer domain and an expression platform. The $preQ_1$ (pre-Queuosine) riboswitch from *Bacillus subtilis (Bsu)* has the smallest known aptamer that controls the expression of genes involved in the biosynthesis of Queuosine, a hypermodified nucleotide found in the anticodon wobble position of certain tRNAs. The aptamer domain of the $preQ_1$ riboswitch folds into a pseudoknot structure when bound to the ligand but the nature of its ligand-free state was unclear until recently. Notwithstanding some previous studies on the ligand-free *Bsu* riboswitch that suggested an extended conformation for the aptamer, recent NMR and especially single molecule FRET (smFRET) studies on the riboswitch proposed a pre-folded conformation with the single stranded A-rich tail interacting with the hairpin loop P1-L1. To directly probe the transient interactions of the A-rich tail with the P1 stem, we have developed a single molecule kinetic 'structure probing' assay using a fluorophore-labeled DNA oligo that is complementary to the tail. Preliminary data using the aptamer domain show that the binding kinetics of oligo to the A-rich tail are affected by the presence of the ligand as expected. In the presence of preQ1, the k_{on} of oligo binding to the A-rich tail decreased as compared to the no ligand condition, while the k_{off} did not show distinct change. Once established, our single molecule 'structure probing' assay using small DNA oligos can be used to investigate the conformation of any RNA under different conditions. Using this technique, the pre-folded state of the riboswitch will be investigated further by comparing the kinetics of oligo binding to the A-rich tail in isolation (without the P1-L1 stem-loop) and as part of the aptamer domain, which will provide information about the accessibility and therefore interaction between the A-rich tail and P1 stem in the absence of ligand. In addition, the full-length $preQ_1$ riboswitch will be studied using the above technique and using in vitro transcription termination assays.

Poster Presentation

Hurricane and Storm Surge Modeling at Notre Dame

Nicholas Weidner
Advisor: Timothy Stitt, Center for Research Computing, University of Notre Dame

Accurately predicting storms and hurricanes is critical to saving lives and reducing economic loss. Therefore, it is necessary to use the most current software and hardware technology available in order to improve the performance and fidelity of our predictive mathematical models. The Computational Hydraulics Lab (CHL) at the University of Notre Dame has developed a high-resolution storm surge model (DG-ADCIRC) to predict storm surges in coastal areas. The objective of my REU project was to port the existing parallel storm-surge code to the state-of-the-art Intel Xeon Phi Co-Processor system (Stampede) at the Texas Advanced Computing Center (TACC) and ideally demonstrate speedup on a set of benchmark calculations. The porting would be accomplished by identifying and vectorizing compute-intensive loops to be offloaded to the 61-core Xeon Phi coprocessors whilst leveraging their 512-bit vector units. Offloading excessive amounts of code can reduce the effectiveness of using the Xeon Phi coprocessors so the code was initially profiled in order to identify the code sections where the host processors spent the majority of their time (and demonstrated good potential for data parallelism). This analysis allowed us to focus coprocessor offloading to those regions. After determining the code hotspots our objective was then to rewrite those hotspots using Xeon Phi programming directives to successfully offload the code instructions and data and ensure successful compilation and execution on a sampling of test cases. As the REU research period nears its end we have successfully obtained a Xeon-Phi port of the DG-ADCIRC code and we are currently in the process of testing and analyzing its performance in direct comparison to the original version.

Poster Presentation

Methods for Cocrystal Synthesis

Milena Westarb
Advisor: Adam Matzger, Dept. of Chemistry, University of Michigan

This investigation centers on the development of a microfluidic system to screen for the formation of cocrystals between one or more sets of cocrystal formers in solution. The method discussed employed the use of a CO2 laser system to cut a pattern of microfluidic channels through a 75×25×2 mm piece of polymethyl methacrylate (PMMA).
The PMMA channel layer was then solvent-welded using 2-butanone to two other layers of the same dimensions: a top layer with access holes through which a glass pipet can push liquids, and a flat bottom layer acting as the substrate. The bottom layer was a standard 75×25 mm glass microscope slide, while the top layer was PMMA. When the solvent inside the device evaporated, the glass bottom layer could easily be removed from the assembly, allowing any solid crystalline material formed on its surface to be examined via microscopy, X-ray diffraction, or Raman spectroscopy.
Two microfluidic channel designs were tested. The first was designed to mix two cocrystal formers in solution in varying ratios. The second was intended for the same purpose, but using three or more different former solutions that could each be mixed with one parent solution without interacting with each other.
Microfluidic devices offer a valuable opportunity to expand cocrystal research because they can limit reagent waste, as well as improve the efficiency of the cocrystal screening process. This investigation aims to develop a system through which multiple cocrystal formers can interact in isolated conditions with a single parent compound, all on one substrate. Future work on such a method will include testing of the system with known cocrystal systems using both 100% ethanol (trinitrotoluene:phenothiazine) and water (acetylsalicylic acid:L-theanine) as solvents.

Poster Presentation

Receptor Interacting Protein Mediated Cell Death in ECM-detached Breast Cancer Cells

Russell Williams III
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Advisor: Zachary Schafer, Dept. of Biological Sciences, University of Notre Dame

The survival of mammary epithelial cells is largely dependent on their attachment to the extracellular matrix (ECM). When anchorage-dependent cells like mammary epithelial cells detach from the ECM, they undergo detachment-induced apoptosis, known as anoikis (Frisch, Francis. 1994). In order for breast cancer cells to metastasize, they must evade anoikis (Buchheit et al. 2012) as well as other anoikis-independent and poorly defined cell death mechanisms. For example, it has been shown that when anoikis is inhibited, ATP deficiency occurs and cells still die (Schafer et al. 2009). However, the precise cell death mechanism has not been identified. Our preliminary data suggest that this non-apoptotic cell death may be necroptosis, a programmed type of necrosis. Although little is known about the molecular mechanisms associated with necroptosis, it has been demonstrated that necroptosis requires receptor interacting protein 1 kinase (RIP1) and receptor interacting protein 3 kinase (RIP3) (Zhou et al. 2012). Our objective is to determine if necroptosis contributes to ECM-detachment induced cell death. We have compared the expression of RIP1 and RIP3 levels in attached and detached conditions in cancer cell lines and non-tumorigenic, mammary epithelial cells (MCF-10A) with oncogenes overexpressed. We found that in MCF-10A cells with Bcl-2 overexpression, RIP1 is up-regulated in ECM-detached conditions. Additionally, our lab has found that in the absence of apoptosis in Bcl-2 overexpressing cells the viability of cells treated with the necroptosis inhibitor Nec-1, increases compared to Bcl-2 cells treated with DMSO. This result suggests that these cells undergo necroptosis in the absence of apoptosis when detached from the ECM. We hypothesize that cancer cells may prevent the increase of Rip1 levels blocking necroptosis from occurring in ECM-detached conditions. Understanding ECM-detachment induced cell death processes is paramount for finding targets for novel therapeutic treatment approaches that target metastatic cancer cells.

Poster Presentation

Kinetics of Reaction of (MeClamp)Ti with Hydrazobenzene

Mark Wilson
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Carbon dioxide, CO_2, continues to be a problematic product while our demands for energy continue to increase. In order to address the issue of CO_2 release, and its abundance in the atmosphere, methods of CO_2 processing are being studied. While sequestering [capturing] CO_2 remains a popular option, another alternative would be to reducing/functionalizing the CO_2 into chemical fuels. We have studied the reaction of hydrazobenzene, PhNHNHPh, with a metal complex containing oxidized ligands, (MeClamp)Ti. In this reaction, the two hydrogens from hydrazobenzene are delivered directly to the ligand; if this takes place by a concerted mechanism, similar compounds could then be used for selective reactions with CO_2. The kinetics of the reaction have been studied using ultraviolet-visible (UV-Vis) spectrophotometry, including investigation of kinetic deuterium isotope effects.

Poster Presentation

Synthesis and Characterization of Five- and Six-Coordinate Ferrous Heme-Nitrosyl Complexes

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At low (nanomolar) concentrations, nitric oxide (NO) is involved in various important biological processes. However, at high (micromolar) concentrations, NO is toxic, which can cause septic shock and organ degradation. Interestingly, denitrifying bacteria efficiently detoxify NO through nitric oxide reductase (NOR) enzymes. In bacterial NOR enzymes, ferrous heme-nitrosyl complexes have been proposed as intermediates for N-N bond formation. Based on this, the synthesis of five- and six-coordinate ferrous heme-nitrosyls was investigated. The corresponding five-coordinate complexes [Fe(TPP)(NO)] (TPP^{2-} = tetraphenylporphyrin) and [Fe(T_o_-F^2PP)(NO)] (T_o_-F_2PP_2- = *o*-difluorotetraphenylporphyrin) were synthesized and spectroscopically characterized. First, the porphyrin co-ligands were synthesized, and then metallated using $FeCl_2$, resulting in the corresponding ferric chloride complexes. Next, the NO complexes were formed anerobically via reductive nitrosylation of these precursors in a solvent mixture of toluene and methanol. Finally, the corresponding six-coordinate ferrous heme-nitrosyls were synthesized by reaction with a nitrogen-donor ligand, here 1-methylimidazole. These complexes were characterized by UV-vis, IR, and EPR spectroscopy.

Poster Presentation

Genetic Differentiation among Populations of *Echinolittorina radiata* across East Asia

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Echinolittorina radiata is a species of marine periwinkle snail that can be found on the intertidal shores of East Asia across a wide range of latitudes. Because they are routinely exposed to long periods of heat and desiccation, they live close to their thermal limits and are highly susceptible to slight changes in temperature. For this reason, *E. radiata* is an ideal system for studying the effects of climate change. An international collaboration between researchers at the Chinese University of Hong Kong, the University of Hong Kong, Academia Sinica (Taipei, Taiwan), Xiamen University (Xiamen, China), and the National Museum of Nature and Science (Tokyo, Japan) is currently investigating the genomic mechanisms and regulatory networks underlying thermal tolerance and adaptive plasticity within the genus *Echinolittorina*. Here a mitochondrial DNA marker, namely cytochrome c oxidase I (COI), is used to assess the genetic differentiation of *Echinolittorina radiata* populations in Hong Kong, Japan, Ningbo, Qingdao, Taiwan, and Xiamen. Standard genetic diversity indices were calculated and a neighbor-joining phylogenetic tree as well as a haplotype network map were constructed. High levels of gene flow and low genetic variation were detected across all sites. Within-location genetic diversity approximates between-location genetic diversity. The results correspond with expectations given gene flow among all locations after a recent demographic expansion due to glacial retreat in the post-Pleistocene period. This project was funded by a Research Grants Council (RGC) grant of the HKSAR government #HKU782011. The Center for Undergraduate Scholarly Engagement, the College of Science, and Multicultural Student Programs and Services of the University of Notre Dame sponsored the presentation of this poster at the national Evolution conference held in Snowbird, Utah from June 21-25, 2013.



Figure 1. Apertural (left) and abapertural (right) view of an *E. radiata* from Japan Site A. Scale is 5 mm.

Oral Presentation

Summary of CMS Minimum Bias Pythia 8 Tunes

Hanyi Yi
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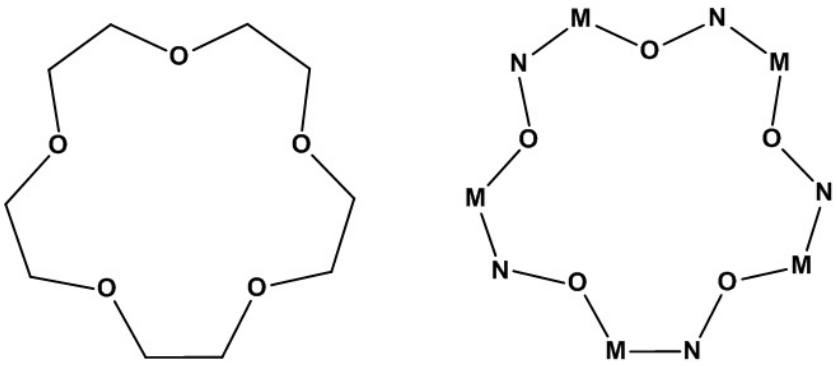
Pythia 8 is an event generator that generates high energy-collision events, such as proton collisions and electron collision. Upgraded from Pythia 6, however, the new version has not yet been enough tested and tuned for it to have reached the same level of reliability as the older one. Improving Pythia 8's performance in describing collider data involves two parts: first, adding new CMS analyses into Rivet, a toolkit for MC event generators and experimental data comparison, in order to expand the base of analyses to be compared to; second, running CMS analyses using Pythia 8 with different settings and compare the output data with real CMS data in order to get the most optimized minimum bias tune. We use Professor-1.3.1 as a tuning instrument, and we come to the conclusion that the new tune provides a more accurate and reliable prediction for CMS collisions.

Poster Presentation

Chiral Guest Recognition by Lanthanide Metallacrown Hosts with Threonine-based Ligands

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Supramolecular recognition has spurred interest among scientists due to potential implications in catalysis and separation. Metallacrowns (MCs), a unique class of macrocycles, are the inorganic analogues of crown ethers that contain metal-nitrogen-oxygen repeating unit. It has been shown that a hydrophobic cavity can be introduced over one face of the planar Ln(III)[15-$MC_{Cu(II)}$-5], where the central metal is a Ln(III) ion, the ring metal is Cu(II), and the ring consists of 15 atoms with 5 repeating units. The resulting cavity encapsulates aromatic carboxylates reversibly. Discussed herein, a new series of ligands are proposed in order to study the mechanism of chiral host-guest recognition in MCs. The ligand design is based on the four diastereomers of threonine and L-threonine hydroxamic acid (L-ThrHA) has been synthesized and characterized. Evidence of formation of Gd(III)[15-$MC_{Cu(II)}$ -5] with L-ThrHA has been observed by mass spectrometry and binding studies to chiral carboxylate guests are currently underway. Analogous MCs that employ Co(II) as the ring metal are also being studied for molecular recognition purposes.



Oral Presentation

Constructing and Testing a Beam line for 5U Accelerator and Germanium Gamma Ray Detector Tests

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The 5U accelerator at the Nuclear Science Laboratory will be used to produce charged beam of particles with high intensity, which is over 100uA, and with voltage up to 5MV. An evacuated beam line provides an obstruction free path through which the beam travels. Various devices along this beam line are needed to optimize transmission of the beam from the source to the target. And the latest commissioning tests will be presented. High Purity Germanium Detectors are used to detect gamma rays with high energy resolution. Data are collected from the detectors using a multi channel analyzer, and then analyzed with energy calibration and efficiency calculation. The newly constructed Georgina Array has been tested using a selection of known and unknown gamma sources.

Oral Presentation

Accelerator Mass Spectrometry (AMS) applied in the measurement of Zr

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Advisor: Philippe Collon, Dept. of Physics, University of Notre Dame

According to the momentum-over-charge ratio (P/Q), the technique of mass spectrometry (MS) can be used to obtain particle separation using magnetic analysis. However, there are many limitations to this technique when the concentration radioisotope of interest is very low compared to the isobaric background. Accelerator Mass Spectrometry can offer a better way to measure radioisotopes with very low concentrations by providing the possibility of using the standard detection method in nuclear physics. One of the experiments of the AMS group at the University of Notre Dame is to study the isotopes of Zirconium (Zr). Following the general principles of AMS, we designed, built and tested a Bragg peak detector in an attempt to provide better separation between ^{93}Zr and its isobar ^{93}Nb. We used it to trace different stable isotopes of Zirconium. We mapped ^{90}Zr through ^{94}Zr to predict the behavior of ^{93}Zr which is not stable and can only be found as a tracer in certain geological environments. The overall goal of the experiment is to allow the separation of ^{93}Zr from ^{93}Nb.

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