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Audrey Seligman and Marcos Ortega (Advisor)
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Macalester College, St. Paul, MN

The French paradox is a phenomenon in which the French have a lower incidence of cardiac problems than expected considering their high fat diet. This has sparked interest in the cardioprotective and cancer preventative properties of a molecule that is in many foods that are a part of the typical French cuisine, resveratrol (RSV). The goal of this study was to investigate the relationship between RSV and Copper II (Cu(II)), and their ability to exacerbate DNA damage. DNA damage will ultimately up regulate or restore wild type p53, leading to downstream effects that will cause apoptosis, killing the cancerous cell. In addition, this study investigated the protective effects of RSV from Iron III (Fe(III)) mediated DNA damage. It has been hypothesized that RSV in the presence of Cu(II) would act as a pro-oxidant and would intensify DNA damage through the formation of reactive oxygen species (ROS). When RSV was at a low concentration, and in the presence of DNA, it would act as an antioxidant and through a direct interaction with DNA, protect DNA from Fe(III) mediated DNA damage.
This study used DNA gel electrophoresis assays and bacterial transformations. The results of this study showed that increased incubation time led to a higher percentage of DNA that was converted from supercoiled to relaxed DNA. When Ethylene Diamine Triacetic Acid (EDTA) was added to the reaction there was no conversion from supercoiled to relaxed DNA. Fe(III) causes DNA damage in a dose-and-time-dependent manner; Fe(III) treatment leads supercoiled DNA to become catenated. RSV prevents Fe(III)-mediated DNA catenation. With a pre-incubation of either Fe(III) or DNA, this phenomenon is exaggerated. This study concluded that Cu(II) and RSV-mediated DNA damage is time-dependent and absolutely dependent on the presences of Cu(II). For the first time the mechanism of DNA protection by RSV from Fe(III)-mediated damage was investigated; RSV has a protective effect against Fe(III)-mediated damage, and lower concentrations of RSV had greater protective effects, suggesting antioxidant effects.

CELLULAR AND MOLECULAR BIOLOGY

ALTERNATIVE SPLICING IN ARRHYTHMOGENIC RIGHT VENTRICULAR CARDIOMYOPATHY

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Arrhythmogenic right ventricular cardiomyopathy (ARVC) is a disease which arises from mutations in desmosome proteins. Mutated desmosomes compromise cell adhesion and result in myocardial atrophy and fibrofatty replacement of necrotic or apoptotic tissue, ultimately interfering with electrical signaling and leading to arrhythmias. This research investigates a point mutation in exon 13 of the gene JUP which codes for the protein plakoglobin. The point mutation is removed post-transcriptionally in the first heart field, resulting in a gain of function. To determine a mechanism for this differential splicing, RNA-binding protein (RBP) genes of interest which are differentially regulated between first and second heart fields have been identified by RNAseq. Altered patterns of expression of these genes between WT and mutant cell lines have been quantified over an 11-day growth period using qPCR. Altered expression patterns of RNA-binding proteins over the growth period may indicate their binding at exon 13. Some target RNBs show significant differences in expression between WT and mutant tissue and therefore may be implicated in the alternative splicing of ARVC.

BISPHENOL-A ALTERS NEUTROPHIL RECRUITMENT IN A ZEBRAFISH MODEL

Jackson Raynor, Sandy Carson, Apoorva Handigol, and Debby Walser-Kuntz (Advisor)
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The prevalent use of bisphenol-A (BPA) in food containers, thermal receipts, and other products provides an environmental challenge to the immune system. BPA disrupts the action of physiologic estrogens by binding to estrogen receptors and has previously been shown to impact immune responses. We are exploring the impacts of *in vivo* BPA exposure on the development and function of the zebrafish innate immune system. Our earlier work in mice showed that BPA exposure decreases the expression of KC, a chemokine whose function is to recruit neutrophils to a site of inflammation. Quantitative PCR experiments in the zebrafish model indicate that CXCL8, the homolog of

mouse KC, shows a BPA-dependent reduction in expression at days 3, 4, and 5 of development. To determine if the reduction in chemokine secretion has a functional outcome, neutrophil recruitment to an injury site was measured in transgenic zebrafish expressing GFP under a neutrophil-specific myeloperoxidase promoter (MPO). Day 4 MPO embryos that have developed in the presence of 0, 10, 100, or 500 ng/mL BPA are given a tail cut and neutrophil movement is tracked over time using fluorescence microscopy and ImageJ. Zebrafish embryos developing in BPA show reduced neutrophil recruitment to the site of tail injury compared with controls, correlating with the reduction in CXCL8 expression. Together these data demonstrate that BPA exposure during early zebrafish development alters baseline innate immune signaling as well as injury responses.

DIFFERENTIAL PROTEIN EXPRESSION COMPARISON BETWEEN FIBROLAMELLAR HEPATOCELLULAR CARCINOMA PATIENT VERSUS NORMAL SUBJECT

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Fibrolamellar hepatocellular carcinoma, FL-HCC, is a rare hepatic malignancy that is a variant of hepatocellular carcinoma (HCC). It is not associated with chronic liver disease and has a young age of onset. FL-HCC is characterized by laminated fibrous layers interspersed between the tumor cells. The relative survival of patients with FL-HCC in the U.S. is 73% at 1 year and 32% at 5 years with no effective therapy for unresectabel/metastatic FL-HCC. What is known about the cause of FL-HCC is very limited. The usual suspects in typical HCC-like mutation in tumor protein 53 (TP53) and Catenin Beta 1 (CTNNB1) are not seen in FL-HCC. Most recent discovery through next gen sequencing revealed a heterozygous deletion of approximately 400kb on chromosome 19 in all samples that underwent transcriptome and whole-genome sequencing. This deletion endpoint fell within two coding regions: the first exon of DNAJB1 (a heat shock protein) and the trailing nine exons of PRKACA (catalytic subunit of protein kinase A). Various work has been published on the genomic screening and transcriptomic screening of comparing FL-HCC tumor sample with normal sample; however, none has been on the proteomic scale of work. Our collaborator at the Mayo Clinic has recently conducted proteomic screening on FL-HCC tumor sample and has identified differential expression in several candidates. This project aims to verify the expression of these proteins utilizing western blot analysis.

ESTABLISHING A NOVEL MURINE MODEL OF CONTACT ALLERGY-PROVOKED GENITAL PAIN USING THE HAPTEN DINITROFLUOROBENZENE

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Vulvodynia is an understudied chronic vulvar pain condition with an unknown etiology that affects up to 8-16% of 15-60-year-old women. Epidemiological studies have found that history of allergies increases the risk of developing vulvodynia. We have developed a murine model of vulvodynia utilizing the hapten irritant dinitrofluorobenzene (DNFB). Ten daily topical applications of DNFB in previously sensitized ND4 Swiss mice induced increased innervation of cutaneous $CGRP^+$ nerves, mast cell infiltration, and sensitivity to pressure on the labiar skin in ND4 Swiss mice—all of which are consistent with the clinical diagnosis of vulvodynia. DNFB-induced contact hypersensitivity on the labia also provokes a local and consistent upregulation in Interferon-gamma (IFN- γ) expression. Our model is a new tool to study the enigmatic neuroimmune pathologies of chronic pain conditions, specifically the relationship between allergies and chronic pain. Because DNFB is known work via mast cell-driven pathways, this model can be used to explore novel mast cell-targeted therapeutic strategies that may provide new ways to treat and manage vulvodynia and other chronic pain disorders.

GLOBAL PROTEOME QUANTIFICATION DURING CELL CYCLE TRANSITIONS

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The cell cycle is a ubiquitous process that involves growth and replication of cells. Abnormal cell cycle signaling causes many diseases, and manipulating the cell cycle pathway with inhibitors has emerged as a promising area of drug research. We propose to identify the composition of cytoplasmic proteins during cell cycle transitions. We utilized Stable Isotope Labeling in Cell Culture (SILAC) as a highly versatile metabolic labeling strategy that relies on the incorporation of stable isotope-coded amino acids.We employed SILAC methodology, together with mass spectrometry, to quantitatively assess the perturbation of protein expression during cell cycle transitions.
Method: The leukemic cancer cell line (Jurkat) was grown in three different conditions: light (R0,K0), medium (R6,K4), or heavy (R10,K8) amino acid-labeled media, for a sufficient period of time (over five cell divisions) to ensure 95% labeling. Serum-free

RPMI medium was added to synchronize cell cultures overnight. The cell cycle was arrested at the G1/S stage for the R6,K4 group through the use of hydroxyurea, and at the G2/M stage in the R10,K8 group through the use of nocodazole. The R0,K0 cells were used as a control group (no treatment). Equal amounts of protein lysates from each group were then combined and submitted for LC-MS/MS analysis.
Results: We identified different proteins expressed in the cytoplasm when Jurkat cells were arrested at different cell cycle stages. In addition to SILAC, immunoprecipitation enabled the identification of direct interactions between proteins of interest and indirect interactions with protein complexes that are formed during cell cycle transitions. Once cellular compositions and interacting partners have been identified, we will test novel drugs that stop cancer cell growth and proliferation.

INTERACTIONS BETWEEN MALARIA AND SYSTEMIC CYTOMEGALOVIRUS INFECTION: A COMPARISON OF UL144 GENOTYPES IN MINNESOTA INFANTS WITH CONGENITAL CMV AND AFRICAN CMV STRAINS IN CHILDREN WITH MALARIA

Andrew Kemal Kirchmeier[1], Claudia Fernández-Alarcón[1], Nelmary Hernandez-Alvarado[1], Mark Schleiss[1] (Advisor), Chandy John[2] and Dibyadyuti Datta[2]
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Human cytomegalovirus (HCMV) is the most common congenital viral infection in the USA. Sequelae include sensorineural hearing loss and mental disability. The UL144 open reading frame (ORF), a highly variable region, encodes a tumor necrosis factor receptor homologue. Sequence variation is useful in understanding the epidemiology of the infection. Therefore, we analyzed variations of the UL144 gene in HCMV-positive clinical isolates obtained from Uganda and Minnesota. 33 samples from Uganda in children with active malaria were examined. There was, interestingly, a trend toward improved survival in children with malaria who had concomitant CMV DNAemia: 7 of 20 surviving children had CMV viremia (35%) while only 3/14 fatal cases (21%) had DNAemia. 3 samples were successfully RT-PCR amplified. 25 qPCR verified HCMV positive samples were sequenced: 7 clinical isolates (CIs) and 5 cell-culture adapted derivatives (CCAD) from the USA, 3 CIs and 10 clone colonies from Uganda. We were able to amplify a 737 base pair (bp) DNA product from the UL144 gene of HCMV from these samples by conventional PCR using previously published primer pairs. Sanger sequencing was performed on the resulting positive PCR amplification. Sequence variation was analyzed using bioinformatics. Phylogenetic analyses indicated that the nucleotide and amino acid (aa) sequences of the samples diverged into three major groups: subgroup 1A, 7/25; subgroup 1C, 4/25, and group 3, 14/25. Results suggest that strain variability is conserved between the two countries. Further characterization and analysis of strain variation of UL144 with an increased sample size could provide better understanding of the molecular epidemiology between strains of HCMV in Minnesota, with the samples from Uganda providing insight about intercontinental variability. Trends toward improved survival in the setting of CMV reactivation require further examination, but may reflect salutary modulation of the anti-malaria cytokine response following CMV reactivation.

INVESTIGATION OF A POTENTIAL *C. elegans* PERILIPIN GENE: LIPID DROPLET VISUALIZATION IN PLIN-1 RNAI KNOCKDOWNS

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Perilipins are proteins located in the membranes of lipid droplets. In many organisms, perilipins are responsible for regulating fat storage and metabolism. Abnormalities in fat storage have been linked to obesity, type II diabetes, heart disease, and cancer. In mammals, a lack of perilipin leads to lower body weight and decreased adipocyte size, while overexpression of perilipin results in obesity and increased adipocyte size. The somatic cells of the nematode C*aenorhabditis elegans* store and metabolize fat in a manner similar to mammalian adipocytes, but until recently perilipins were not thought to regulate the process. However, a *C. elegans* gene with sequences homologous to perilipins was recently identified. Subsequent studies have attempted to demonstrate that this gene, named *plin-1,* regulates lipid turnover in *C. elegans,* but the results have been inconclusive. This study aims to provide further evidence for the role of *plin-1* as a perilipin in *C. elegans.* Knockdown strains of *C. elegans* were created by RNAi inhibition of *plin-1* using a plasmid containing a segment of *plin-1* to produce dsRNA. The successful creation of the plasmid was verified with PCR using *plin-1*-specific primers, restriction enzyme digests, and DNA sequencing. Additionally, the plasmid was recreated using Phusion polymerase, a high-fidelity polymerase, rather than Taq polymerase, and this plasmid will be used in a second RNAi inhibition trial. Preliminary visualization of the lipid droplets

of *plin-1* knockdowns indicates that decreased *plin-1* expression results in smaller lipid droplets, opening up the exciting possibility of using *C. elegans* as an *in vivo* model to examine the mechanism of fat storage.

ISOLATION AND IDENTIFICATION OF ANTIBIOTIC-PRODUCING BACTERIA FROM SOIL

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Antibiotic resistance is a rising threat. It is limiting the ability to treat bacterial infections and can lead to premature death. Some of the most common infections that exhibit antibiotic resistance are caused by a group of six bacteria, known as the ESKAPE pathogens. To address the problem of resistance, we have partnered with the Small World Initiative (SWI), an organization that trains undergraduate students in a worldwide effort to discover new antibiotics. Our goal is to identify antibiotic-producing bacteria from soil samples, as soil is a well-known source of antibiotic-producing bacteria. We collected soil samples from two locations in Minnesota and isolated over 100 individual bacteria. We tested these bacteria for inhibition of the growth of safe relatives of the ESKAPE pathogens. We found four bacteria that inhibited the growth of at least one of these safe relatives. We used microscopic, genetic, and biochemical analyses to determine the genus of the isolates. Sequence analysis of the 16S rRNA genes showed that one of the isolates had 99% identity to *Streptomyces,* two had 99% identity to *Pseudomonas,* and one had 91% identity to *Bacillus.* Results of Gram staining and biochemical tests were consistent with these findings.

POLYGENIC AND DIRECTIONAL EVOLUTION ACROSS PATHWAYS IN *Cryptococcus neoformans*

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Cryptococcus neoformans is a pathogenic fungus that causes meningoencephalitis. The global burden of *Cryptococcus neoformans* is large: it is responsible for 620,000 deaths each year and disproportionately affects those who are immunocrompromised. There are two subspecies of *Cryptococcus neoformans:* D is predominant in Europe, while A is more prevalent in the rest of the world. The AD hybrid is heterotic: more virulent and stress resistant than each of the individual parent subspecies. The first part of this analysis examines the differential expression between the parents and the hybrid to elucidate possible pathways and mechanisms for increased virulence of the pathogen. The second part of this analysis investigates the evolutionary divergence between subspecies A and D by comparing allele-specific differential expression within the hybrid. We use a novel statistical approach to look for cis-regulatory changes indicative of directional evolution.

REPEATED EXPOSURE TO A COMMON COSMETIC PRESERVATIVE METHYLISOTHIAZOLINONE (MI) PROVOKES ALLERGY-DRIVEN CONTACT HYPERSENSITIVITY IN A MOUSE OF VULVODYNIA

Erica Arriaga-Gomez and Devavani Chatterjea (Advisor)
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Methylisothiazolinone (MI) is a biocide preservative commonly used in cosmetics and household paints. Studies in the US and in several European countries have shown that MI can cause allergic sensitization in human subjects. We have developed an MI-driven model of allergy-driven mechanical sensitivity in outbred ND4 Swiss mice. Repeated exposure to MI on the labiar skin produced increases in tactile sensitivity, eosinophil activity, mast cell density, and local levels of IL-6 and IFN-gamma was found in MI-sensitized mice. Therefore, we have established a new household chemical-driven contact hypersensitivity model that can be used to evaluate allergy-driven changes in mechanical sensitivity to touch and pressure. Given the epidemiological associations of a history of allergies and development of chronic unexplained vulvar pain, our studies have the potential to illuminate the roles of ubiquitous allergenic cosmetic preservatives in the etiology of this and other pain conditions.

SOURCING THE DOORS TO BACTERIAL SUGAR HIGHS: INVESTIGATING TONB-DEPENDENT RECEPTORS CC_0446, CC_0539, AND CC_1136 IN *CAULOBACTER CRESCENTUS*

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TonB-dependent receptors (TBDRs) are active transporters that facilitate the sequestering of nutrients in Gram-negative bacteria. Until recently, TBDR

substrates were thought to be limited to iron and vitamin B12, but now carbohydrates are also included. *Caulobacter crescentus* has 65 different TBDRs, an outstanding number compared to other bacteria like *Escherichia coli,* which has 7. The plethora of TBDRs present in *Caulobacter* is coherent with the oligotrophic, aquatic environments it inhabits. In this study, we seek to identify the substrates of three putative TBDRs: CC_0446, CC_0539, and CC_1136. Based on the genomic neighborhoods of these genes, we hypothesize that TBDR CC_0446 and CC_0539 transport the sugar GlcNAc, and CC_1136 transports sucrose. TBDRs are most highly expressed when they are needed by the bacteria; thus, we analyzed the gene expression of TBDRs CC_0446, CC_0539, and CC_1136 in glucose compared with either GlcNAc or sucrose. We found that GlcNAc increases the expression of CC_0446 195-fold but does not affect the expression of CC_0539, while sucrose increases the expression of CC_1136 57-fold.

CHEMISTRY

3D PRINTING AND OPEN-SPACE SPECTROSCOPY

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With the advent of the computer-age in the mid to late 20th century has come the development of sophisticated scientific equipment for myriad chemical analyses. Indeed, the field of spectroscopy alone has seen significant advancements in data collection, processing, and analysis due principally to the incorporation of microprocessors. While it is clear computers have revolutionized the field of instrumental chemical analysis, their impact is pervasive through every segment of our modern lives. From word processing, data management, and Computer Aided Design in our work environments to social media, crowd funding, and digital news at home, technology is utilized everywhere. This work seeks to explore the potential incorporation of the relatively new field of 3D printing into the design and "at-home" manufacture of optomechanical equipment for open-space spectroscopy. The primary goals of this work were the design of an optical cage system, with associated accessories, that is printable on any entry-level commercially available 3D printer along with the testing of said cage in comparison with other similar available optomechanical components. All equipment was designed on freely downloadable software and other than the 3D printed parts, which required the use of a 3D printer, only included components available at typical hardware stores. Design struggles and considerations will be discussed. Through cost analysis and measurements of beam deflection we have shown that, while not equal to available equipment, these components are much cheaper and likely suitable for basic to intermediate spectroscopy applications.

THE ASSEMBLY OF CARBON MACROCYCLES THROUGH ALKENE METATHESIS

Joseph Romo and Dennis Cao (Advisor)
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The assembly of supramolecular macrocycles has recently become an area of intensified research interest. Their unique and symmetric structures have the ability to encapsulate other molecules within their structural cavity and can be designed to bind with charged or neutral substrates. We are attempting to synthesize pentameric macrocycles by exploiting the 109° angle of sp3 carbons to direct the assembly of their pentagonal shapes—the interior angle of a pentagon is 108°. Di-topic alkene monomers will be exposed to alkene metathesis conditions with the hypothesis that these macrocycles will be the thermodynamically favored products of the metathesis equilibrium.

COMPUTATIONAL ANALYSIS OF ORGANIC PHOTOVOLTAIC ELECTRON DONOR CANDIDATES

Mitchell Lahm and Rollin King (Advisor)
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The most common current theoretical model used to calculate the power conversion efficiency of an organic photovoltaic cell, the Scharber Model, is a gross approximation. Two new external quantum efficiency models are proposed to better model absorption of spectral light. These models use Gaussian and Lorentzian functions centered on the oscillator strengths with heights corresponding to their respective first five excitation energies for each electron donor molecule. The power conversion efficiency according to each model was determined for 21 previously identified candidates. The ranking in power conversion efficiency according to each model is reported.

COMPUTATIONAL STUDY OF PHASE-TRANSFER CATALYSIS

Tony Schaefer and Joshua Layfield (Advisor)
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Liquid-liquid phase-transfer catalysis is a means of greatly increasing the rate of reactions that occur across

a water-organic solvent interface. Detailed information about the catalysis mechanism remains unknown. To this end, classical molecular dynamics simulations are employed to model catalyzed ion transfer across a water-cyclohexane or water-chloroform interface. A variety of quaternary ammonium phase-transfer catalysts (PTC's) are tested computationally to investigate their effect on the free energy barrier to the ion's transport, the solvation of the ion, and the relative orientation of the catalyst-ion pair. Different PTC's are used so that structural characteristics of more effective PTC's can be identified.

COMPUTATIONALLY INEXPENSIVE METHODS FOR PREDICTING OXYGEN-SENSITIVITY OF PRIMARY PHOSPHINES

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A variety of primary, secondary, and tertiary phosphines, with known air-stabilities have been modeled using semi-empirical and *ab initio* methods. Comparisons are made to a published benchmark indicating SOMO energies of the related radical cation for each respective phosphine can give a clear indication of expected phosphine sensitivity toward ambient oxygen. We have established the same trend for sensitivity using the significantly less "costly" semi-empirical PM6 and RM1 methods as well as by a simple Hartree-Fock method utilizing the small 3-21G basis set.

DETECTION OF HYDROGEN SULFIDE WITH A FLUORESCENT PROBE

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Hydrogen sulfide (H_2S) has most recently been identified as a gasotransmitter that, when produced in excess, is linked to neurological disease such as Alzheimer's, and Down syndrome. The exact concentration of H_2S *in vivo* is highly disputed. Currently, no non-destructive detection methods that are both sensitive and selective, and have fast reaction kinetics, are available. The goal of this project is to develop a fluorescent probe that enables the detection of H_2S *in vivo*. First, the H_2S probe, coumarin-DNP (1-floro-2,4-dinitrobenzene), will be synthesized and characterized by 1H NMR (nuclear magnetic resonance spectroscopy). Coumarin and coumarin-DNP will be characterized by collecting fluorescence excitation and emission profiles. Then, the response of coumarin-DNP to H_2S will be investigated. The hypothesis is that H_2S will selectively remove the DNP group and regenerate the coumarin fluorophore. The sensitivity of the probe will be evaluated by measuring the magnitude of coumarin fluorescence in the presence of increasing concentrations of H_2S.

DEVELOPMENT OF SMALL-SCALE FLOW TEST METHOD FOR QUANTIFICATION OF UREA ADSORPTION ONTO ACTIVATED CARBON

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The effects of chemical modifications on assorted activated carbon samples were evaluated for their ability to adsorb urea from solution by using a flow system and ultraviolet-visible spectroscopy (UV-Vis). Activated carbons of various pore sizes were subjected to soak treatments in different concentrations of iron nitrate or copper nitrate solutions with and without oxidation in nitric acid or hydrochloric acid and/or pre-treatment in sodium diethyldithiocarbamate (SDDC) or nitrilotriacetic acid (NTA). Carbon samples were subjected to a urea solution flow treatment in a novel syringe flow apparatus. A p-dimethylaminobenzaldehyde (PDAB) colorimetric assay was used to determine the urea concentration in filtrates for multiple fractions. Breakthrough curves for different carbon samples show the highest urea uptake observed for the samples treated with iron.

DIHYDROXYLATION OF LIMONENE

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Currently, Rochester Community and Technical College students in Organic Chemistry 2128 perform a dihydroxylation lab on cyclohexene. To make this lab more interesting, cyclohexene was replaced with limonene, a natural compound found in lemons. Using limonene creates a more interesting lab because its source is found in everyday life and the compound has more double bonds, making it an improved starting material. The goal of this project is to compare the products synthesized using the three methods of dihydroxylation (Woodward, potassium permanganate, and oxone) and the thin-layer chromatography (TLC) process. The reaction process was completed using the cyclohexene, which produced one or two products for each method. Then the lemon peels were steam distilled, in order to obtain the limonene. The limonene was then used in place of the cyclohexene, in order to establish the efficacy. After collecting the limonene, the student ran the dihydroxylation reactions (and TLC process)

using the same three methods–the Woodward, oxone, and potassium permanganate. Additionally, the results also showed that the oxone method provided the most products of all three methods, which was contrary to the hypothesis and past students' results. Progress toward purification and structural determination will be presented.

DISCOVERY OF A NOVEL MECHANISM FOR OPENING A CYCLOPROPYL RING

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In the process of carrying out a simple substitution reaction, an unexpected imidazolidinone byproduct was formed. During the exploration of the formation of this byproduct, we discovered a novel mechanism for a cyclopropane ring opening. The alkyl group on the 4-position of the imidazolidinone comes from the cyclopropyl ring of cyclopropylamine. A protonation of the cyclopropane ring is proposed and supported by several experiments and other examples. Characterization of the products formed from an intermediate iminium ion as well as the proposed mechanism is discussed.

ELECTROCHEMISTRY WITH HOUSEHOLD ITEMS

Ker Thao and Heather Sklenicka (Advisor)
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As chemistry advances and reaches the vast community in the higher education world, we as students struggle with grasping its step-child: Electrochemistry. What really happens when chemical and metals are grouped together? This study is about introducing college students to the basics of electrochemistry and relating it to everyday household items, in hopes to conduct enough electricity to possibly power a LED bulb for a couple of minutes. In order to understand this study, voltage testing of basic chemistry lab solution, varies metals, the model 152 Mult-Echem Half Cell Module and the configuration of standard cell potential for each solution was taken. Multi half-cells were tested and used to create enough voltage to power a LED bulb. After determining the research data, household to solutions will be tested to see if it is able to produce enough voltage to conduct electricity.

EXAMINATION OF THE RELATIVE IMPACT OF TRIS(DIISOPROPYLPHOSPHINOMETHYL)PHENYLBORATE AND TRIS(DIPHENYLPHOSPHINOMETHYL)PHENYLBORATE IN SALTS OF [M(CO)3(PHBP3)]- (M = CR, MO, W)

Shuruthi Senthil and Paul Fischer (Advisor)
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The development of tris(phosphino)phenylborates ($PhBP_3$), commonly referred to as strongly donating scorpionates, has facilitated the synthesis of transition metal complexes with novel electronic structures. The modular nature of these borates permits alternate substituents at phosphorous as the most direct way to modulate ligand donation. To date, tris(diisopropylphosphinomethyl)phenylborate and tris(diphenylphosphinomethyl)phenylborate are the most utilized ligands of this class. While the former is undoubtedly more electron-rich than the latter, the vast majority of complexes prepared to date with tris(phosphino)borates are charge-neutral and zwitterionic, where the borate negative charge balances a positive formal charge of the metal fragment. The Fischer group is exploring the chemistry of tris(phosphino)borates towards zerovalent group VI metals. This poster will provide a detailed comparison of the relative impact of tris(diisopropylphosphinomethyl)phenylborate and tris(diphenylphosphine methyl)phenylborate at the metal centers in salts of $[M(CO)_3(PhBP_3)]$- (M = Cr, Mo, W) in light of the strongly donating scorpionate classification of these ligands.

EXPLORING THE CARBON CHEMISTRY OF THE GALACTIC INTERSTELLAR MEDIUM: PHOTOCHEMICAL STABILITY STUDIES OF POLYCYCLIC AROMATIC HYDROCARBONS BY ARGON MATRIX ISOLATION SPECTROSCOPY

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Infrared emission bands ubiquitous in the interstellar medium of the Milky Way and other galaxies have revealed that a significant portion of all carbon in the universe is in the form of polycyclic aromatic hydrocarbons (PAHs). PAHs are tremendously stable organic molecules composed of aromatic carbon rings, observable in outer space by distinct IR fluorescence

signals emitted when pumped by UV radiation from nearby stars. PAH-rich gas clouds in interstellar space play a central role in the flow of matter in the galaxy and hold implications for the origins of organic and potentially pre-biotic chemistry. Infrared observational spectra can be deciphered with additional data from theoretical computation, *in situ* nanosatellite missions, and laboratory spectroscopy experiments. The PAH isoviolanthrene ($C_{34}H_{18}$) was among the chemical species tested in low earth orbit conditions aboard the NASA Space Environment Viability of Organics (SEVO) nanosatellite mission. The infrared spectrum and photochemical stability of isoviolanthrene can be further studied via argon matrix-isolation FTIR spectroscopy methods, a means to simulate interstellar medium conditions in a controlled laboratory environment.

EXPRESSION AND PURIFICATION OF RECOMBINANT PERILIPIN 2 FROM MOUSE HEPATOCYTE LIPID DROPLETS

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Lipid droplets are energy storage organelles that are essential to most eukaryotic cells, including hepatocytes. The mechanism of lipid droplet formation in normal and diseased states is not well characterized. Perilipin 2 (Plin2) is a lipid-binding protein that is found at the surface of the lipid droplet. Mutations in the gene coding for Plin2 cause alterations in lipoprotein profiles and levels of plasma lipids in humans. Functional domains within the protein have been identified, but the 3D structure remains unknown. High-resolution structural studies of Plin2 will improve the understanding of its role in the influx and efflux of lipids in the lipid droplets. In order to obtain a significant quantity of purified Plin2 for structural studies, the expression and purification of Plin2 must be optimized. Results of expression and purification of recombinant Plin2 will be discussed.

GREEN CHEMISTRY IN THE ADVANCED INORGANIC LABORATORY: MECHANOCHEMICAL SYNTHESIS AND CHARACTERIZATION OF HOMOLEPTIC BIS-CHELATE COPPER(I) COMPLEXES

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Green Chemistry plays an important role in chemical synthesis as it works to implement chemical reactions and procedures that not only minimize the use of toxic solvents and hazardous chemicals, but also reduce waste and energy consumption. Mechanochemistry is a promising area of chemical synthesis that utilizes mechanical energy input, typically grinding, and requires little to no solvent. In an effort to incorporate Green Chemistry labs into the undergraduate curriculum at St. Catherine University, we designed a viable, mechanochemical synthesis of homoleptic bis-chelate Copper(I) complexes to be implemented in advanced inorganic laboratory courses. Specifically, the procedure involves a solventless grinding reaction of diimine ligands (N^N = 2,9-dimethyl-1,10-phenanthroline (dmp), 2,2-biquinoline (biq), or 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (Ph_2dmp)) with $[Cu(NCCH_3)_4](BF_4)$ in a 2:1 molar ratio, respectively, to form $[Cu(N^N)_2](BF_4)$. Three reaction methods were utilized to synthesize $[Cu(N^N)_2](BF_4)$ following either a two-step or a one-step process. A generic thermal synthesis and a solvent-free mechanochemical synthesis were executed using the two-step process. A one-step, solvent-assisted mechanochemical reaction was also performed. Comparisons were made between the three reaction methods in light of green chemistry parameters such as yield, solvent use, energy input and waste, as well as time and cost. All resulting homoleptic Copper(I) complexes were characterized using a variety of methods including ^{1}H NMR, ATR-IR, ESI-MS, UV-vis, solid-state photoluminescence, and X-ray crystallography. The focus of this lab is to expand student comprehension of mechanochemistry and green chemistry principles, as well as practice a variety of characterization techniques and compare similar reactions using practical and green chemistry parameters.

HYDROGEL EXTRACTION OF CONTROLLED SUBSTANCES: CHARACTERIZATION AND OPTIMIZATION OF DRUG DETECTION USING DIFFERENT INSTRUMENTAL METHODS

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Leona et al. extracted and detected organic dyes from art objects using hydrogels and Surface Enhanced Raman Spectroscopy (SERS).[1] Other applications of these gels have not been published. This study aims to (a) characterize the small-molecule extraction process and (b) identify other applications for extraction via hydrogels. Extraction efficiency was studied controlling for pH, ionic strength, and extraction times. An unidentified chemical species that leached from the hydrogels could present problems if applied to forensic or cultural heritage objects and act as an interference species with some detection methods. Both SERS and High Performance Liquid Chromatography (HPLC)

have exhibited selectivity and sensitivity issues, which were overcome using Liquid Chromatography-Mass Spectrometry (LC-MS). Two drug classes were studied by LC-MS as model systems: caine drugs using benzoylecgonine (BZ) and amphetamines using 3,4-Methylenedioxymethamphetamine (MDMA). The limit of detection was 12.7 ng/mL and 0.5 ng/mL for BZ and MDMA, respectively. Extractions of crystallized, pure drugs off of banknotes showed average equivalent extraction amounts of 60 ng/mL each. Extraction of a 1:1 mixture of drugs detects a 6:1 ratio of BZ to MDMA, illustrating a difference in affinity for the polar hydrogel/solvent system. Reproducibility in both extraction and detection methods needs improvement. For example, the relative standard deviation of the MDMA extraction is 33% and detection is 53%. Current work is focused on improving the extraction's sensitivity, selectivity, and reproducibility by changing extraction and chromatographic mobile phases.

(1) Leona, M.; Decuzzi, P.; Kubic, T.; Gates, G.; Lombardi, J. Nondestructive Identification of Natural and Synthetic Colorants in Works of Art by Surface Enhanced Raman Scattering. *Anal. Chem.* **2011,** 83, 3990-3993.

HYDROTHERMAL SYNTHESIS AND CHARACTERIZATION OF TWO-DIMENSIONAL TIN SULFIDE NANOSHEETS

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Layered metal chalcogenides are emerging as two-dimensional (2D) materials with a wide range of electronic, optical, chemical, mechanical, and catalytic properties. Like graphene, these materials may be separated to form single- or few-layer nanosheets. Here we report on our efforts to synthesize nanosheets of tin monosulfide via a green hydrothermal synthesis. Specifically we discuss strategies to controllably produce single- or few-layer nanosheets with large lateral dimensions (> 1 micron). The resulting nanosheets are characterized UV-visible and Raman spectroscopy, atomic force and transmission electron microscopy, and X-ray diffraction.

INVESTIGATING THE REACTIVITY OF CUMINALDEHYDE AND ISOVALERALDEHYDE TOWARD DNA

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Aldehydes are among the compounds that are commonly used in the production of food and cosmetics and, therefore, come in contact with human bodies more often than expected, which makes it important to have a deep understanding of their properties and biological activity. Aldehydes have been known to be involved in the process of chromosomal aberrations and have a potential to react with DNA bases to form adducts. Little is known about the nature and biological potential of these adducts. The goal of this research is to obtain more information with regards to the composition of the two adducts formed in the reactions of isovaleraldehyde and cuminaldehyde, with 2'-deoxyguanosine. This information is necessary for studying their genotoxicity as well as for understanding the reactivity of aldehydes toward DNA. This research focuses on purification and further structural determination of the adducts that were previously found to form in the reactions of isovaleraldehyde and cuminaldehyde, with 2'-deoxyguanosine. In these reactions, L-arginine was used to facilitate the reaction while each of the aldehydes was independently reacted with 2'-deoxyguanosine in methanol in a sealed flask with constant stirring. The reactions were further analyzed using ^{1}H NMR, HPLC, and TLC.

ISOLATION OF ACTIVE COMPOUNDS IN ANTIBIOTIC-PRODUCING BACTERIA

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Antibiotic resistance is a global phenomenon that continues to worsen with every passing day. Tuberculosis, a disease caused by *Mycobacterium* tuberculosis, was responsible for about 1.8 million deaths in 2015, and even with available treatments, the disease persists and continues to gain resistance. The research focused on uncovering the diverse flora of antibiotic-producing bacteria that is required to fight against this growing problem of antibiotic resistance. This study is focused on bacteria collected from soil samples collected at Bethel University. Initial screening observed several colonies that create zones of inhibition when grown on nutrient media with other bacterial species. To further assess potential antibiotic-producing properties, three isolates of bacteria (I1, I2, and I4) were grown in nutrient broth solution, centrifuged (16,000 X g), and the supernatants tested through well-diffusion on nutrient agar against *Bacillus subtilis* (*B. subtilis*) and *Escherichia coli* (*E. coli*) lawns, for zones of inhibition. Bacterial cultures were allowed to grow for 24-h, 48-h, 1-week, and 2-week time intervals to determine if resource depletion served as a trigger for antibiotic production. A portion of each supernatant was then concentrated under vacuum. Preliminary results with both the original and concentrated samples showed no zones of inhibition with either *E. coli* or *B. subtilis.*

Isolate supernatants of I1, I2, and I3 will be tested again for zones of inhibition using disc diffusion, and new isolates will be used for a wider population to assay. Other growth strategies will also be investigated to induce antibiotic production. Supernatants of isolates that test positive as antibiotic producers will be analyzed through separation and spectroscopy techniques to identify the antibiotic compound.

OPTIMIZATION OF POLYCAPROLACTONE MICROSPHERE SIZE THROUGH SYNTHESIS MANIPULATION

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This experiment manipulates the quality of microspheres by changing experimental parameters in the synthesis process. First, chloroquine will be synthesized from chloroquine phosphate with a separation using a basic aqueous phase and an organic phase. Then the chloroquine will be encapsulated in spheres of polycaprolactone. This process will be optimized to form larger microspheres. These microspheres, when injected into the blood stream, will dissolve and release chloroquine at a controlled rate. In this experiment, chloroquine will be dissolved into an organic layer (dichloromethane) with polycaprolactone then mixed with an aqueous layer (polyvinyl alcohol) under a large shear force. Once the dichloromethane is evaporated, polycaprolactone precipitates with the chloroquine forming microspheres with a diameter in the range of 50-200 μm. Variables such as time, amount of organic solvent, amount of aqueous solvent, and amount of drug will be varied to maximize the size of these microspheres, which will be observed under a microscope for size determination and allowed to soak in aqueous solutions to determine how well the chloroquine is released from the microspheres.

OPTIMIZATION OF WARFARIN SYNTHESIS IN THE UNDERGRADUATE TEACHING LABORATORY

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The synthesis of warfarin has been used in the second-semester organic chemistry class at Rochester Community and Technical College. Originally used as a rat poison in 1948, warfarin is now commonly used as an anticoagulant. It is an example of an asymmetric synthesis, which will allow students to analyze their samples by optical rotation. Students have had difficulty with obtaining enough product for characterization. To address this issue, three reactions of varying quantities were prepared and different methods of purification tested. The melting point, IR spectrum, and optical rotation of the product was obtained when possible. Results will be presented.

OPTIMIZING C-TERMINAL PEPTIDES FOR INHIBITION OF HIV-1

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Infection by enveloped viruses requires fusion of a viral and target cell membrane. In HIV-1 this process is mediated by gp41, a surface glycoprotein that upon recognition of receptor sites extends its N-terminus into T-cell membranes. Short α-helical peptides derived from gp41's C-terminus bind this extended structure, inhibiting a conformational rearrangement required for fusion. To overcome common instability challenges for peptide therapeutics, we grafted a C-terminal peptide sequence onto a PH domain, a stably folded protein with a solvent-exposed helix, and optimized protein-protein surface contact by mutating residues that most directly contact the N-terminus of gp41.

PSI4: THE DETERMINATION OF FORCE CONSTANTS IN GEOMETRY OPTIMIZATION

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Psi4 is an open-source quantum chemistry program that uses ab initio calculations to perform efficient and high accuracy simulations for various chemical systems. OptKing is a presently functioning program used by Psi4 to optimize geometries of input molecules and fragments. The purpose of this project is to translate portions of the OptKing function from C++ to Python, eliminate Psi4-dependent code, and integrate alternative methods for the determination of force constants for stretching, bending, and torsions within the input molecule or fragment to be used in Hessian matrices. The three methods implemented were outlined in published papers by H. B. Schlegel, T. H. Fischer, and R. Lindh; these methods calculate force constants using equations derived from covalent radii, period-depended constants, empirically determined constants, and bond length. These methods were then tested using Psi4's set of molecular test cases and compared to the results of the default set of force constants in Psi4's geometry optimizer. The implementation of the alternative methods for determining force constants allows for more efficient and accurate calculations for specialized

cases in which one method is superior to another. Furthermore, the translation of the optimizer from C++ to Python allows for wider platform usage and less dependence on Psi4, allowing OptKing to be utilized by multiple quantum chemistry programs given a standardized input.

SOLID-STATE CHEMISTRY OF DIMERS OF A STERICALLY HINDERED BENZONITRILE OXIDE

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Nitrile oxides yield heterocyclic compounds by means of 1,3-dipolar cycloaddition reactions; for example, reaction of a nitrile oxide with a nitrile in solution yields a 1,2,4-oxadiazole. We are examining the possibility that nitrile oxides might be co-crystallized with nitriles and that subsequent solid-state cycloaddition might yield a heterocyclic product different from that obtained upon reaction in solution (1,2,5-oxadiazole vs. 1,2,4-oxadiazole). Success of this approach requires (1) a nitrile oxide sufficiently reactive to undergo cycloaddition with a nitrile but not so reactive that it reacts with either the nitrile or with itself (by dimerization) before the incorporation of both components into the crystal, and (2) an overall similarity in molecular space-filling requirements between the components to allow formation of mixed crystals (solid solutions). Our observation that several nitrogen-containing heterocycles assume crystal structures isomorphous with their corresponding *N*-oxides suggests that nitriles may be capable of co-crystallization with their corresponding nitrile oxides. Having determined the crystal structure of the sterically hindered 2,6-dichlorobenzonitrile oxide in previous work, we have begun co-crystallization studies using 2,6-dichlorobenzonitrile oxide and 2,6-dichlorobenzonitrile. We have also determined the crystal structure of one of the three dimers potentially obtained upon dimerization of 2,6-dichlorobenzonitrile oxide, the *bis*(2,6-dichlorophenyl)oxadiazole-*N*-oxide. The crystal structure is disordered, with molecules located upon crystallographic twofold axes even though the molecules lack twofold symmetry. Future work includes final refinement of this disordered structure and determining the crystal structure of the *bis*(2,6-dichlorophenyl)dioxadiazine, the one dimer in the 2,6-dichlorophenyl series yet to be examined crystallographically.

SOLID-STATE NITRILE OXIDE DIMERIZATION: CRYSTAL STRUCTURES OF 2,3-DICHLOROBENZONITRILE OXIDE AND ITS SOLUTION DIMER

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Nitrile oxides dimerize in solution to form three possible products: a furoxan, a dioxadiazine, or a 1,2,4-oxadiazole-*N*-oxide. We are using single-crystal X-ray diffraction to determine whether the molecular packing arrangement of the parent nitrile oxide determines which product is formed upon solid-state dimerization. We report here the crystal structure of 2,3-dichlorobenzonitrile oxide, formed by dehydrohalogenation of the corresponding hydroxamic acid chloride, and the crystal structure of *bis*(2,3-dichlorophenyl)furoxan, formed by dimerization of the nitrile oxide in solution. The nitrile oxide crystallizes in the monoclinic space group $P2_1/c$ with four molecules occupying general positions in the unit cell. Unlike our previously determined 4-chlorobenzonitrile oxide crystal structure, which includes close oxygen···chlorine contacts but no close chlorine···chlorine contacts, the crystal structure of 2,3-dichlorobenzonitrile oxide includes no close oxygen···chlorine contacts but does include close chlorine···chlorine contacts. The crystal structure of the furoxan includes both oxygen···oxygen and chlorine···chlorine contacts. A close centrosymmetric approach between neighboring fulminate groups in the nitrile oxide crystal structure suggests that the "head-to-tail" dioxadiazine or oxadiazole *N*-oxide dimers might be favored in a solid-state dimerization, but the large molecular motions possible even in the solid state render this conclusion speculative. Future work will involve the identification of the *solid-state* dimerization product as well as preparation of polymorphic forms of the nitrile oxide to determine any dependence of the product obtained on the crystal structure of the parent nitrile oxide.

SOLID-STATE STUDIES OF BENZONITRILE OXIDES AND THEIR DIMERS: CRYSTAL STRUCTURE OF A 1,2,4-OXADIAZOLE

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Nitrile oxides, compounds containing the fulminate group (CN^+-O^-), have long been known to be useful in solution reactions, particularly in 1,3-dipolar cycloadditions, but their solid-state properties and reactivity have been understudied. We are interested in crystallographically examining the parent nitrile oxides and their three possible solution-phase dimers — the

furoxan, the dioxadiazine, and the 1,2,4-oxadiazole-*N*-oxide — to determine whether different polymorphs of a given nitrile oxide could yield different products upon solid-state dimerization. We have been examining a series of selected benzonitrile oxides, including 4-nitrobenzonitrile oxide and 2-chlorobenzonitrile oxide, and have obtained infrared spectra that indicate that we have successfully synthesized these parent benzonitrile oxides and can monitor their solid-state dimerization. We have also examined selected dimers, and in that process we have now obtained the crystal structure of a compound that we obtained in an attempt to prepare and crystallize one of the two "head-to-tail" dimers of 4-nitrobenzonitrile oxide, the *bis*(4-nitrophenyl)-1,2,4-oxadiazole-*N*-oxide, by solution-phase dimerization of the benzonitrile oxide in the presence of a catalytic amount of triethylamine. The compound actually obtained has proved to be the *bis*(4-nitrophenyl)-1,2,4-oxadiazole, not the *N*-oxide. Previous workers have determined that this deoxygenated product can form upon reaction of the initially formed oxadiazole *N*-oxide with the reactant benzonitrile oxide. Our ongoing work will include obtaining a complete set of solid-state molecular packing arrangements (crystal structures) for the parent benzonitrile oxides and their dimers in the 2-nitrobenzonitrile oxide, 3-nitrobenzonitrile oxide, 4-nitrobenzonitrile oxide, and 2-chlorobenzonitrile oxide series.

SYNTHESIS, CHARACTERIZATION, AND ELECTROCHEMISTRY OF MELLITIC TRIIMIDES

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Aromatic diimides have been extensively studied for their electron-accepting properties. These aromatic diimides can exist in the neutral, anionic, and radical states. As a result, they are very good at spreading out electrons over the entire molecule, which gives rise to useful properties of the molecule, such as good electron-conducting abilities. This work, however, examines the more electron-deficient aromatic triimides. Aromatic triimides can exist in 4 different states: the neutral state, the singly charged radical, double-charged radical, and triple-charged radical states. This suggests that triimdes provide a better environment for delocalization. Individual mellitic triimides are C3 – symmetric, three electron accepting molecules. This ability to accept three electrons, each at a distinct and well-separated potential, is an unusual ability, especially for a simple organic system. The planar nature enhances their stacking ability. They can, therefore, stack and assemble to form stable supramolecular structures, which can be of very great importance in the field of sustainable engineering. Studies of naphthalene diimides (NDIs) have shown its uses to include the making of nanotubes, molecular sensors, thin films, and field- effect transistors (FETs). Theoretically, triimides should be able to serve better in these capacities.

SYNTHESIS OF A PFTASE SUBSTRATE CONTAINING A TERMINAL OLEFIN CAPABLE OF TETRAZINE LIGATION

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Enzyme substrate promiscuity can be used to label proteins with non-natural functionality. The enzyme used in this work, Protein Farnesyltransferase (PFTase), normally catalyzes the addition of a farnesyl group to a cysteine near the C-terminus of proteins with a "CAAX" motif. In this motif, "A" represents an aliphatic amino acid and X is a variable amino acid. PFTase has also been shown to transfer a wide variety of non-natural isoprenoids to "CAAX" proteins, including several with bioorthogonal functionality. Ras proteins are an important class of "CAAX" proteins that are mutated in up to 30% of human cancers. PFTase has been successful in transferring non-natural substrates with bioorthogonal functionality to Ras proteins using copper-catalyzed click chemistry. Unfortunately, due to copper's cytotoxicity, clickable isoprenoids cannot be targeted *in vivo* using this process. Presented here is the synthesis of a bioorthogonal PFTase substrate that does not require a copper catalyst for subsequent bioconjugation reactions on enzymatically modified Ras proteins. This synthesized isoprenoid chain contains a terminal alkene which can undergo an inverse electron demand Diels-Alder cycloaddition with a fluorescent BODIPY-tetrazine probe. The terminal alkene reacts with the tetrazine and imparts fluorescent properties onto the Ras protein. This bioconjugation strategy can be used to locate and quantify the amount of Ras proteins in living cells.

SYNTHESIS OF NOVEL OXAZOLIDINONE ANTIBACTERIALS

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The selective force from the ubiquitous use of antibacterial drugs over the past century has pressured bacteria to evolve resistance to their mechanisms of inhibition. This has created a need for the rapid development of new antibacterial drugs which employ new mechanisms of bacterial inhibition; one such innovation has been the development of Oxazolidinone

antibacterials. These drugs target the ribosomes of the bacteria and inhibit protein synthesis, effectively causing cell death. A novel Oxazolidinone structure incorporating a fused cyclic ring system has displayed incredible potency against *Mycobacterium tuberculosis* and other drug-resistant strains of bacteria. This research is aimed at synthesizing a new series of compounds based on this fused cyclic ring system that incorporate other functional groups into their structure with the hopes of increasing their effectivity as antibacterial agents. A carboxylic acid functional group was added to facilitate entry of the drug into the bloodstream and to make the molecule more water soluble, potentially causing it to bind more strongly to the ribosome. These molecules were synthesized using an eight-step synthesis. More recently, a four-step synthesis has been devised to synthesize the Oxazolidinone derivatives whose functional groups contain acidic protons.

TOWARD CORE-FUNCTIONALIZED NAPHTHALENE DIIMIDE

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Core-functionalized naphthalene diimides (cNDIs) are promising candidates as organic redox materials that could be used in applications including organic light-emitting diodes (OLEDs), photovoltaics, and other organic electronic devices. A diverse variety of cNDIs exhibiting varying degrees of electron deficiency and intramolecular charge transfer features have been reported in the literature. However, functionalization of the NDI core with imide groups has not been explored to date. We hypothesize that the crowding of imide groups on the naphthalene core to form naphthalene tetraimides may lead to new chemical and physical properties. Thus, we set out to synthesize the two different possible regioisomers of naphthalene tetraimide. The routes, challenges, and optimizations associated with these synthetic efforts will be discussed.

ECOLOGY AND ENVIRONMENTAL SCIENCE

BEACH SAFETY: MONITORING LEVELS OF *E. coli* IN RECREATIONAL WATER AREAS

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High levels of *Escherichia coli* in recreational swimming beaches are linked to high levels of fecal-borne pathogens. Because of this link, state and county officials across the United States routinely monitor swimming beaches for high *E. coli* levels and close them if the amount of *E. coli* exceeds a predetermined safe level. Over a period of three months during the summer of 2016, we measured *E. coli* levels weekly at three sites centralized around a single lake in Ramsey County, Minnesota. In order to determine the amount of *E. coli* at each site, we used membrane filtration and growth on modified mTEC agar. We found that *E. coli* levels at two sites, one of which was a swimming beach, routinely exceeded recommended standards. Actions taken included retesting, posting signs at the beach and electronic notices recommending that the public refrain from swimming.

COMMUNITY COMPOSITION AND FLORISTIC DIVERSITY IN DIFFERENT SUCCESSIONAL STAGES OF A TROPICAL DRY FOREST, COSTA RICA

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Tropical dry forests are threatened by habitat loss, yet conservation and restoration efforts in the past century have increased the amount of secondary forest area worldwide. Study of the successional patterns that secondary forests exhibit as they establish and grow can be used to inform more successful restoration efforts in deforested areas. The goal of this project was to investigate how community composition and floristic diversity compare in secondary dry tropical forest areas of different successional age. I resampled permanent plots of five different ages (17, 22, 29, 33, and 41 years) established by Reyes-Cordero in 2012 in northwestern Costa Rica. The most abundant families were Malvaceae, Fabaceae, Rubiaceae, Boraginaceae, and Sapindaceae. The most ecologically important species were *Chomelia spinosa, Cordia alliodora, Cordia panamensis, Guazuma ulmifolia*, and *Luehea speciosa.* Species composition was distinct among sites, although I found no correlations between richness, diversity, mortality and recruitment, basal area, or distribution across diametric classes and successional age. It is possible that successional age does not account for these dynamics past a certain age, and that the sites in this study have already surpassed this point.

DEGRADATION OF FOOD WASTE IN SIMULATED SEPTIC TANK

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Septic systems, used by over 20% of US households, treat sewage (wastewater) sequentially through septic tanks followed by leach field treatment. Current Minnesota Rules require septic tank capacity to increase by 50% with the installation of food waste (FW) disposal (Minnesota Rules, Part 7080.1930, Subpar 2), because it may induce sludge accumulation and deteriorate tank effluent. A lab-scale experiment was conducted to assess the effect of additional FW in sewage on the performance of septic tanks. Simulated septic tanks at 1 liter were operated at 15°C for 209 days with an average hydraulic retention time of 7.7 days. The addition of food waste disposal (FWD) to sewage increased the total chemical oxygen demand (tCOD), soluble chemical oxygen demand (sCOD), total phosphorus (TP) and total nitrogen (TN) by 34.8%, 35.0%, 7.9% and 5.0% in influents, respectively. Consequently, FW addition increased 17.7%, 9.9%, 3.8%, and 4.7% for tCOD, sCOD, TP, and TN in effluent compared with the effluent from the tank fed solely with sewage. Therefore, septic tank has stronger treatment capacity with FW addition, increasing removal performance in effluents. Total solids due to FW addition in influent increased by 80 mg/L from sewage but increased by 40 mg/L in effluent. Total suspended solids (TSS) due to FW addition in influent increased from 202 to 278 mg/L by 37.6% while the effluents yielded total suspended solids of 7 mg/L and 22 mg/L, respectively, both lower than 60 mg/L as restricted by Minnesota Rules, Part 7080.2150, Subpar. 3, Item K. The sludge volume showed an increase of 4.9% with additional FW, considerably lower than the expected value of 37.6% estimated from influent TSS data, indicating that the effect of FW on sludge accumulation was not substantial. In conclusion, septic tank results indicate marginal reduction in water quality with FW addition, but do not show negative impact on septic tank performance. Although sludge accumulation from FW was evident, values do not suggest significant difference between septic tank with sewage and that with additional FW. The finding from this study gives public understanding in water quality and septic tank performance with the usage of food disposal units and may lay a path for possible improvement in regulations on septic tanks.

DISTURBANCE IN PRAIRIE ECOSYSTEMS: THE EFFECTS OF FIRE ON RESTORED PRAIRIES IN SOUTHEASTERN MINNESOTA

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Much of the tall-grass prairie ecosystem has been converted to agriculture. Since 1989 St. Olaf College has restored approximately 61 ha of agricultural land to prairie to conserve biodiversity and provide educational and recreational benefits for the community. The main disturbance in prairies, fire, reduces non-prairie species and provides openings to maintain the diversity of prairie species. Each section of St. Olaf prairie is burned every 2-5 years and since prairie sections were planted with a similar mix and burned at different times, comparisons can be made among sections. This study shows that more recently burned prairies had higher species diversity and higher levels of soil moisture, organic matter, and nitrates. Changes in levels of phosphates, ammonia, and bulk density of the soil were not significantly different between the burned and unburned treatments. Over the course of the growing season nitrate and ammonia levels increased across the study area while phosphate levels showed no statistical difference over time. Additionally, the species composition of prairie sections burned in the current year was different from those burned in previous years. While the burned areas contained more grasses and slightly more legumes, the unburned sections were dominated by forbs. The burns allowed more light and moisture to reach the seed bank as the fire removed the large duff layer. This, in addition to the increase in organic matter created by burning dead plant material and soil type variation across sections, can lead to biological and chemical diversification of the prairie ecosystem.

EFFECTS OF LAND MANAGEMENT AND AGRICULTURE ON RICE AND HEATH CREEK IN SOUTHEASTERN MINNESOTA

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Anthropogenic effects, especially agriculture, on stream ecosystems have led to large changes in water quality. This study analyzed the effects of riparian buffers on variation in water quality and macroinvertebrate diversity in two streams in southeastern Minnesota: Rice Creek (a spring-fed stream) and Heath Creek (a lake-fed stream). It was hypothesized that macroinvertebrate populations and diversity in Rice Creek could be lowered by chemical changes in the water caused by agriculture, including excess nitrates

and ammonia, while Heath Creek would be less affected due to lack of proximity to agricultural fields and the use of riparian buffers by farmers. Abiotic characteristics including nitrates, ammonia, conductivity, pH, dissolved oxygen, and temperature were also measured. Results showed no significant differences in abiotic characteristics with different land use patterns along Heath and Rice creeks. Previous studies have shown higher nitrates in Rice Creek. However, the data in this study did not show a difference in macroinvertebrate diversity and population size, despite the disparity in nitrate concentrations in each creek. The Shannon-Simpson diversity index from the different sites showed no significant difference in diversity among the four sites. Mean species tolerance levels were not significantly different among sites and count data showed that both Rice and Heath creeks had small populations of macroinvertebrates. With the small numbers of macroinvertebrates and lack of diversity, this monitoring project can be used to spur land management changes in each creek system.

EFFECTS OF MOISTURE DIFFERENCES ON SOIL MICROARTHROPOD ABUNDANCE, AND DIVERSITY IN GREEN ROOF SYSTEMS

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An increase in urbanization has caused a massive loss of green space worldwide. A newly popular way to mitigate this loss is the building of green roof systems. Green roofs provide a variety of benefits, some of which are: betterment of the surrounding air quality, providing a habitat for wildlife, and lowering energy cost for buildings. One of the key components of a healthy green roof is the soil microarthropods. These organisms help with leaf litter decomposition and they also affect the nutrient cycling of the soil. Soil moisture content has been identified as a main limiting factor for ground level microarthropods, but little is known about how soil moisture affects these populations in green roof systems. In this study, we created two watering treatments, natural rain water only and natural rain water with supplemental watering, to determine if the soil moisture plays a role in the abundance and diversity of the microarthropods. The results of the study showed that green roof beds that received no supplemental watering had higher abundances of microarthropods as well as more species diversity. These data provide implications on how to better maintain green roof systems in order to maximize environmental benefits in the future.

THE EFFECTS OF RECREATIONAL TRAILS IN THE RESTORED TALLGRASS PRAIRIE OF THE ST. OLAF COLLEGE NATURAL LANDS

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The once prominent tallgrass prairie of North America is now a fragmented and highly disturbed ecosystem. Although many factors, such as fire, grazing, and agriculture act as disturbance forces in the tallgrass prairie, there are other disturbances that may also contribute to its deterioration. One such disturbance is edge effects, which may be established by recreational trails. This study investigated the presence of mowed trails in three tallgrass prairie sites in the St. Olaf College Natural Lands. Plant growth, quantified as biomass, was measured at three distances (0, 25, and 50 m) from the trail in each site. Additionally, the study examined other factors related to plant growth in the tallgrass prairie, which included the presence of fire, and the percent moisture and organic matter of the soil. The results demonstrated that mean biomass was not significantly different among the distances from the trail, but was significantly different among the prairie sites, which had been burned at different times. The most recently burned sites had the greatest mean biomass. Lastly, mean percentages of soil moisture and organic matter were significantly different with distance from the trail, suggesting differences due to edge effects. The percentages of organic matter and soil moisture were highest at 25 m from the trail and lowest at 0 m. Overall, this study suggested that trails do not affect plant growth in the tallgrass prairie, but may influence soil characteristics, which may have implications for the future management of the St. Olaf College Natural Lands.

THE HISTORIC RANGE OF THE *Siro* MITE HARVESTMEN IN THE PACIFIC NORTHWEST, ACCORDING TO PALEOCLIMATE DISTRIBUTION MODELING

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Species distribution modeling is a relatively new tool in the field of biogeography. The general idea is that one can predict the full range of a species or group of taxa by analyzing the abiotic factors at locations where the group has already been located, and running a computer model to identify other nearby areas with similar conditions. Most such studies are run using present-day climate data, although they can also predict a group's range at a specific point in the past or future, if the

distribution model is projected onto ecological data layers that represent the relevant timepoint.
I ran three paleoclimate distribution models on the *Siro* genus of mite harvestmen (*Arachnida, Opiliones,* Cyphophthalmi), endemic to the American Pacific Northwest, in order to compare their probable range at the Last Glacial Maximum (LGM), mid-holocene (MH), and their current distribution. LGM, MH, and present-day spatial data for nineteen climatic variables were downloaded, and eventually thirteen were included in the final models after pairwise correlation analyses to screen for redundant variables.
My results show a distinct lack of LGM suitability for *Siro* in southern Idaho, where present-day specimens of a particular species, *S. kamiakensis,* have been collected. However, the MH model shows that by that time period, the genus probably migrated to the area. Out of the thirteen climate variables used in the final models, total annual precipitation was found, by a wide margin, to be the most predictive of an area's habitat suitability for *Siro* mite harvestmen. I suggest further investigation to verify these preliminary results, including hypotheses to explain the isolation of *S. kamiakensis* from the rest of the genus.

IMPACTS OF *Rhamnus cathartica* ON ARTHROPOD DIVERSITY AND RICHNESS

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Common buckthorn (*Rhamnus cathartica*) is an invasive shrub in North America. Its ability to alter soil chemistry and grow quickly in dense thickets makes this species a serious competitor to native flora. Areas with high levels of buckthorn have low diversity of native plants. Because low plant diversity is linked to low arthropod diversity, areas with high levels of buckthorn may also yield low arthropod diversity. In this study, we examined woodlands within 16 parks in the Twin Cities metropolitan area. An equal number of study sites for each of four categories of buckthorn (cleared, 0-1m tall, 1-2m tall, and over 2m tall). At each location, we surveyed vegetation, arthropods, and songbirds to assess whether buckthorn height or relative density impacted the diversity and richness of birds, arthropods, and native plants. We found that arthropod diversity and richness increased with the presence of buckthorn in the shrub layer. In contrast, a concurrent study showed higher concentrations of buckthorn were associated with reduced bird diversity.

MONITORING POCKET GOPHER PRESENCE AND THEIR EFFECTS ON SOILS IN RESTORED AND REMNANT PRAIRIES

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The plains pocket gopher, *Geomys bursarius,* is considered a key ecosystem engineer in the tallgrass prairie because of its tunnel excavation and mound formation processes, which create a mosaic of soil conditions that have far-reaching impacts on the prairie community. Gopher colonization and presence in restored prairies is fundamental to the process of reestablishing tallgrass prairie ecosystems. Although there has been some colonization of pocket gophers at Carleton's Arboretum, St. Olaf's restored prairies have not been colonized. We documented the presence and density of pocket gopher mounds in areas of high gopher activity in both restored and remnant prairies and examined the effect of mound formation on soils by quantifying certain soil characteristics both on and off mounds. We found that gopher mound density was higher in remnant than in restored prairies and that mounds were highly clustered. We found no significant differences in soil density, moisture, or organic matter content either between remnant and restored prairies or between on and off mound locations. It may be that the pocket gopher's conspicuous absence from St. Olaf's restored prairies is due to the isolation of these prairies rather than soil conditions that might make them unsuitable for gopher colonization.

NATURAL AND ANTHROPOGENIC DRIVERS OF FRESHWATER MACROPHYTE COMMUNITY COMPOSITION IN VILAS COUNTY, WISCONSIN

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Aquatic macrophytes play a pivotal role in the chemical, biological, and physical processes of lake ecosystems. We surveyed macrophyte populations in 28 study lakes distributed across Vilas County, Wisconsin, to describe patterns of community composition and evaluate drivers of community assembly on a regional scale. We first used the Aquatic Macrophyte Community Index (AMCI) to characterize the biotic integrity of these populations. The majority of the study lakes received high AMCI scores, indicating the presence of robust and relatively undisturbed macrophyte communities. Species diversity and richness appeared to be distinguishing factors between lakes with high versus low AMCI scores. We next employed random forest modeling to identify influential environmental and

anthropogenic drivers of species diversity, richness, and AMCI values. The resultant models described 52 percent of the variation in species diversity, 39 percent of the variation in richness, and 22 percent of the variation in AMCI scores. Variable selection methods classified water alkalinity, basin hydrology, and the proportion of wetlands within the riparian zone as the most important drivers of diversity, richness, and AMCI values, respectively. Better understanding the interplay between environmental conditions and aquatic macrophyte communities will inform effective freshwater resource management.

PREDICTORS OF TREE GROWTH IN A TROPICAL DRY FOREST IN GUANACASTE, COSTA RICA

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Tropical dry forests are one of the most threatened tropical ecosystems in the world and are primarily composed of secondary forests regrown within the past 50 years. In the dry forests of the Guanacaste Conservation Area in northern Costa Rica, wildfires and cattle grazing are the main causes of deforestation. In the absence of fires and grazing, forests grow back naturally. Successful regeneration techniques depend on understanding forest dynamics and tree growth, yet there have been very few studies on how tree growth changes depending on stand structure. This study aimed to identify the best predictors of tree growth rates in a tropical dry forest of Guanacaste, Costa Rica, using diameter, species, stand age, number of lianas, and tree crown shape and position as possible predictors. Data were collected in 2012, 2013, and 2016 from permanent plots in five different naturally regenerating forest stands ranging from 17 to 44 years old. Diameter and height of nearly 3,000 trees were measured. For each stand, average growth rate, biomass, and carbon sequestration were calculated and species composition was characterized. Heliophylous (sun-preference) trees had a significantly higher growth rate than both fast- and slow-growing sciophylous (shade-preference) trees. There was no pattern relating stand age to growth, yet mean growth rates varied between stands; trees in the 29-year-old stand and the 41-year-old stand grew significantly faster than trees in the 17-, 22-, or 33-year-old stands, so differences in structure and species composition were more important factors affecting tree growth.

ECONOMICS AND BUSINESS

INCOME INEQUALITY AND THE SOLOW MODEL

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The Solow Growth Model is one of the cornerstones of the discipline of economic development. Despite decades of research, few, if any, studies have specifically addressed how the components of this model interact with the dynamic and influential variable of income inequality. Previous research has explored how this variable impacts either the broad and general concept of economic growth, or the specific and narrow factor of savings rates, which in turn may affect capital share measures endogenous to the model.
This study explored the relationships between the components of the Solow Model (capital, labor, capital share, and output) with the Gini index. The data included capital stock at constant national prices, number of persons engaged (in the work force), gross domestic product, and the Gini index of 20 different countries. This data was used to calculate capital share and Solow's Residuals for each country, and was provided by the Federal Reserve Economic Database of St. Louis and attributed to the World Bank. This research not only derived correlations between these variables, but also utilized impulse response functions to more firmly determine causality.
Significant positive correlations exist between all of the components of the Solow Model and the Gini index of income inequality. However, these relationships do not necessarily reflect the underlying causality mechanisms identified through impulse response functions. Additionally, the significance and strength of all correlations were not entirely consistent among all countries. Furthermore, the causalities distinguished through the impulse response functions were frequently significant, but again inconsistent between countries. This study interprets these relatively noisy connections as largely indicating that income inequality is influenced by the Solow Model components, rather than serving as a causal factor itself. This finding is contrary to the hypothesis, and is somewhat counterintuitive. More research will be necessary to further untangle these distinct but interwoven variables to further not only the field of economic development, but the humanitarian endeavors it inspires.

ENGINEERING

DEVELOPING AND EVALUATION GRID SEARCH METHODOLOGY TO DETERMINE THE DEAD TIMES IN MULTIPLE INPUTS DYNAMIC MODELING

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Continuous-time glucose monitoring (CGM) conclusively improves glucose control by providing frequently sampled information that allows users to associate changes in their glucose levels with changes in their behavior by using Block-oriented modeling (BOM), which is a multiple-input modeling approach for nonlinear dynamic processes. Current implementation of BOM into feed-forward control (FFC) results in linearization of the model and decomposition into separate components for each input. This work presents a multiple-input BOM FFC approach that does not linearize and decompose the BOM into separate components for each input. This implementation uses a new FFC law that uses the complete BOM in the time domain. The approach is demonstrated with a Wiener model for a simulated continuous stirred tank reactor (CSTR) with four (4) measured inputs. The Wiener model is nonlinear in the physically based dynamic parameters of the transfer functions and linear in the static parameters of the static gain function. The static gain function has a second-order linear regression form with interaction and quadratic terms. The Wiener model is built under open-loop conditions using a Box-Behnken statistical experimental design consisting of 27 sequential step tests. Under a sequence of multiple input changes, the addition of this feed-forward controller to the feedback controller reduced the standard deviation of the controlled variable from its set point by 70% in comparison to the response with only feedback control.

IMMUNOLOGY

ESTABLISHING A MODEL OF MC-DRIVEN ONGOING AIRWAY INFLAMMATION IN OUTBRED ND4 SWISS MICE

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Asthma is a widely prevalent disease characterized by ongoing airway inflammation and obstruction of the airways, which result in recurrent episodes of wheezing and shortness of breath. Various allergen-induced mouse models of asthma have been used to study the complex pathophysiology of the disease, but none to date use outbred mice. This study seeks to develop a model of MC-driven ongoing airway inflammation in outbred ND4 Swiss mice. Two well-established experimental models of asthma have been tested. One challenges mice intranasally with House Dust Mite (HDM) 5 days a week for 5 weeks, while the other sensitizes mice intraperitoneally with 0.05 mg ovalbumin (OVA) and challenges 9 times intranasally. In the HDM model, we observe mild increases in various immune cell populations in the lungs and cytokine levels in the bronchoalveolar lavage (BAL), and a statistically significant increase in lung IFN-γ levels. In the OVA model, we found increases in FCER1+ dendritic cell and inactivated eosinophil populations in the lungs but no changes in mast cells, which have been shown to drive OVA responses in C57BL/6 mice. Asthma is a disease of immense phenotypic variability – patients express diverse immune cell populations in the airways and have largely varying degrees of symptom severity. An outbred mouse model would better capture this heterogeneity, with the potential of providing novel insights into the intricate and variable pathophysiology of this disease. We are particularly interested in a model with MC-driven responses given the breadth of evidence from the literature implicating MCs in various features of asthma.

MATH AND COMPUTER SCIENCE

LINKING AMAZON ECHO AND TWITTER

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The purpose of my research project was to connect Amazon Echo and Twitter so that one could send tweets via voice command. I explored options including directly programming the two together as well as using third-party services to connect them indirectly. After conducting an extensive literature review, I determined there was a need to utilize a connection between voice-activated devices and social media to aid communication for older adults. My resulting hypothesis was that it is beneficial to provide an additional communication tool, specifically Amazon Echo, allowing those who are less-able to stay

connected with family. I addressed the following questions during my project:

1. Can Amazon Echo and Twitter be linked at all?
2. If a suitable third-party application exists, can the two be linked indirectly instead?

The answer to the first question seems to be yes, but the implementation is still in progress. The second answer, however, appears to be no. This led to expanded research in programming options to link the two directly. Using Alexa Skills Kit, Twitter API, and JSON, I am working to make an Alexa Skill to allow for a direct connection. Due to the complexity, the project will be handed off to future students.

STEM PERSISTENCE, TRAJECTORIES, AND OPEN QUESTIONS AT ST. OLAF COLLEGE

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Throughout their college career, students at St. Olaf College have the ability to switch from their planned major to another major due to the nature of a liberal arts college, which aims to provide students with a broad general knowledge and exposure to all areas in the arts and sciences. National data show that students especially switch out of majors in Science, Technology, Engineering, and Mathematics (STEM). Using St. Olaf transcript data we employed an algorithm that classifies students as STEM and Non-STEM. Our data consist of transcript data from 9,753 students and intention and declaration data from 2,784 students. We evaluated the success of our model by comparing our algorithm's classification with students' self-reported intention and transcripted declaration data at three points during their college career, and analyzed how a student's demographic information and previous AP classes affect the algorithm's ability to correctly identify these students. The sensitivity of our algorithm was 73% at first semester and 94% at sophomore year. The specificity of our algorithm was 82% at first semester and 76% at our sophomore year. Our results showed that most demographic groups had similar percentages of successful classification, which suggests that our algorithm is not affected by different demographics. Our research also explored the influence of GPA on a student's STEM persistence and finds that students are more likely to persist in STEM majors if their GPA in these classes is higher.

TACTILE LEARNING THROUGH RASPBERRY PI

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The practice of tactile learning has been historically used to increase student understanding as well as interest in a subject. In this study, tactile learning is applied to computer programming using electronic circuitry, LEDs, Raspberry Pi, and the Python programming language. Using a set of learning models, instructors require students to review the instructional material, answer a set of questions, and then apply what they have learned by building the circuitry and the code to interact with the LED lights. Each circuitry module explains how to build the circuitry and how the circuitry worked. The lessons and circuitry exercises gradually become more complex to show students more complicated examples of how the Python code can be used. By combining these aspects, students can learn the material and apply what they learned with hands-on examples providing instant visual confirmation of success. Through the learning modules, students are encouraged to modify the exercises to experiment with the circuitry code and LEDs configuration to create new results. The experimentation enhances student understanding of the subject and how to apply their knowledge to hands-on material. Raspberry Pi was selected as the hardware platform due to the portability and cost efficiency of the system. This hardware is open source and there is easy access to the GPIO pins, which is needed for the circuitry and code to work. The results of this study demonstrate that an inexpensive hardware kit can be integrated into programming instruction to provide a tactile learning experience for students.

NEUROSCIENCE

CHARACTERISTIC SPIKE-AND-WAVE DISCHARGES LINK DYSTONIC ATTACK PROGRESSION AND ABSENCE SEIZURES IN EA2 MOUSE MODEL TOTTERING

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Episodic Ataxia type II (EA2) has been attributed to global mutation in the CACNA1A gene, encoding the P/Q-type voltage-gated calcium channel. An orthologous mutation in mice has been used to model

EA2 in the tottering mouse (tg/tg), which exhibits a similar array of symptoms as patients, including absence seizures, dystonic attacks, and a wobbling gait. Though the physical characteristics of the dystonic attacks have been widely discussed, we aimed to characterize the neurophysiological basis of the condition. Previous findings in our lab using flavoprotein autoflourescence imaging found high-power low-frequency oscillations (LFOs) in the cerebellum and the cerebral cortex, with a change in their properties with the severity of the dystonic attack. While the flavoprotein imaging monitors a mesoscopic level of neuronal activity, we aimed to look at specific motor cortical neuronal populations using electrophysiological methods in awake, head-fixed tg/tg mice. Characteristic spike-and-wave discharges (SWDs) were consistently observed under baseline conditions and tended to build up during the onset of the attack, disappear during the peak severity of the attack, and re-emerging during recovery. It was also observed that SWDs were highly synchronous across the cortex and suppressed motor output, verifying a link between absence seizures and SWDs. The relation between the frequency of the SWDs and observed dystonic attack suggests a strong physiological link between the two. By studying the neurological characteristics of EA2, it may become possible to develop more effective interventional and chronic therapies to improve the quality of life in affected patients.

CIRCULATING MICRORNAS AS POTENTIAL BIOMARKERS FOR EPILEPSY

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Epilepsy is a neurological disorder characterized by high-frequency action potentials in the brain. Delayed and misdiagnosis can lead to developmental difficulties in children. Hence there is a critical need for early diagnostic biomarkers. MicroRNAs (miRNAs) are small noncoding RNA molecules that have a significant role in health and disease. Recently, circulating miRNAs have been identified in body fluids, allowing them to be used as biomarkers. However, the diurnal variation in miRNA expression is not known. We hypothesize that miRNA expression levels vary with sampling time. Our objective is to understand variation in blood miRNA expression following seizures. Whole blood samples were collected twice (AM and PM) in PAXgene blood RNA tubes (Qiagen, CA) from five canines with naturally occurring epilepsy, maintained at the University of Minnesota Veterinary Medical Center. MiRNAs were extracted using PAXgene blood miRNA kit (Qiagen, CA) and quantified by small RNA sequencing on an Illumina HiSeq 2000 platform. Statistical analyses were performed to determine the differences between groups. We identified ~180 unique canine miRNAs in whole blood. Four out of the five dogs displayed upregulation of miRNAs in the AM compared with PM samples. Our preliminary analyses revealed differential expression of miRNAs between the two time points of sample collection and that sampling time should be considered while interpreting miRNA expression analysis. We will perform further studies to investigate the temporal regulation of miRNA expression following seizures in these dogs to identify optimal sample collection time points in a clinical setting.

FUNCTIONAL NETWORK CONNECTIVITY IN SCHIZOPHRENIA: THALAMOCORTICAL CIRCUIT DYNAMICS DURING COGNITIVE CONTROL PERFORMANCE IN NON-HUMAN PRIMATES

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Deficits in cognitive control are a core feature of schizophrenia and represent some of the most debilitating and the most poorly treated symptoms of the disorder. Even though a dysfunctional dopaminergic system has been traditionally viewed as the underlying cause of schizophrenia, antipsychotics targeting dopamine neurotransmission fail to resolve these cognitive symptoms, sparking interest in the glutamatergic system's contribution to the schizotypal neuropathology. The prefrontal circuitry has been shown as a key component of the executive control network and its glutamate-mediated connectivity to other brain sites might provide insight on the etiology of schizophrenia. In light of imaging studies implicating hypofunction of the mediodorsal thalamic nucleus (MD) in schizophrenics, this study hypothesized that the neurons of the MD are involved in cognitive control in a way that is similar to the prefrontal cortex (PFC). With the use of the Dot Pattern Expectancy Task, context-processing performance was assessed in two Rhesus monkeys, while simultaneously recording from the neuronal populations of the PFC and the MD. Neurons were sorted off-line based on waveform and clustered with respect to what stimulus (cue, probe, or response) they tend to encode primarily. The findings indicate that the populations of the MD respond to task-specific stimuli in a similar distribution as the PFC and include

neurons that exhibit bias toward cue-types, highlighting the importance of the MD circuitry in context processing. Once this study makes use of glutamate antagonists, it has the potential to shed light on the specific mechanisms of dysconnectivity in schizophrenia.

THE GUT-BRAIN AXIS: ROLE OF GUT MICROBIOTA MODULATION ON ANXIETY

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The neuroscience of anxiety is increasingly complicated, with complex interactions between genetic and environmental factors. The gut microbiota can act as a modulator of mental health through host-microbiota interactions. Gut microbiota modulation, through antibiotic or probiotic use, may serve as an alternative treatment to traditional anti-anxiety medications, as both have shown decreased anxiety effects on the elevated plus maze (EPM). The effects of gut microbiota modulation on different baseline anxiety levels is not known. In this protocol, rats were pretested on the EPM to determine baseline anxiety, and then were treated with antibiotics or high-strength/short-course probiotics. Rats were evaluated at the end of treatment for differences in anxiety. Antibiotic tests showed high-anxiety rats with decreased anxiety and low-anxiety rats with increased anxiety, but no difference between antibiotic-treated animals and controls, or between different anxiety levels. Probiotic treatment also showed high-anxiety rats with decreased anxiety and low-anxiety rats with increased anxiety. There was no difference between probiotic-treated animals and controls, but there was a differential effect of treatment on different anxiety levels, largely due to effects from the high-anxiety group. Together, these results suggest that differences in anxiety seen across trials are likely due to repeated exposure to the EPM alone, creating decreased anxiety for high-anxiety rats and increased anxiety for low-anxiety rats. The probiotic treatment did suggest an effect of lowered anxiety on high-anxiety rats, but no significant effect for low-anxiety rats. Future studies could utilize high-anxiety rats alone to determine if high-anxiety animals show significant drug effecst, and to determine if probiotic treatment serves as an anxiolytic for high-anxiety rats alone. Further research will be necessary to explore potential anxiolytic properties of antibiotics and probiotics, and to explore the different responses of varying anxiety levels to repeated exposure on the elevated plus maze.

USING CONDITIONAL AUTOPHAGY INHIBITION IN MICE TO STUDY NEUROLOGICAL DISORDERS

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Autophagy is a cellular mechanism involved in the clearance of aggregated cytosolic proteins, and has been studied in relation to neurodegenerative disorders such as Parkinson's disease and depression. This project aims to create a mouse model of neurodegenerative disease and affective disorder through a conditional, targeted knockout of the autophagy associated *Atg 5* gene. Mice carrying a floxed *Atg 5* allele were cross-bred with transgenic mice carrying a Cre-recombinase enzyme driven off an inducible, neuronally expressed promoter. Resultant progeny were genetically selected to carry both the floxed *Atg 5* allele and the Cre recombinase, thus allowing induction of gene deletion to occur at a defined age. Conditional knockout mice were induced at 6 weeks of age and assessed via a battery of behavioral and physical tests, including open field, beam traversal, grip strength, RotaRod performance test, gait analysis, clasping analysis, black and white box, cookie preference, sweet solution preference test, amphetamine-induced open field, and replenishment of L-Dopa. In addition, expression of autophagy-related proteins was assessed using western blot techniques. Preliminary data suggest that deletion of the *Atg 5* gene results in the development of a manic phenotype revealed by increased activity observed in the open field test within 5 weeks of gene deletion. No evidence of motor impairments was noted at this time point post-induction. However, at 9 months post-induction a significant neurological phenotype emerged with knockout animals continuing to demonstrate increased open field activity, but now also demonstrating reduced ability to remain on the spinning RotaRod, reduced grip strength, abnormal gait, uncontrolled tremor, and abnormal clasping reflex. Treatment with L-DOPA did not block the tremors. Deletion of the *Atg 5* gene results in age-dependent development of behavioral and physical changes associated with the phenotype of "mania" and "neurodegeneration." This novel mouse model is amenable to screening studies for the discovery of novel small molecule drugs for the treatment of psychiatric and neurological disease.

ORGANISMAL AND PHYSIOLOGICAL SCIENCES

MERCURY DISTRIBUTION IN NEONATAL RAT PUP ORGANS AFTER MATERNAL MERCURY EXPOSURE

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Previous research has shown that when females are exposed to mercury during pregnancy, the metal crosses the placental barrier. This consequently affects the fetus and may lead to offspring with birth defects or developmental disorders (Davidson, 2004). Methylmercury can be found in highest concentrations in large predatory fish (2017 Minnesota DNR Fishing Guide). The indication is that the consumption of any amount of mercury-contaminated fish by a pregnant woman will be detrimental to the health of her developing child. This research gives us insight into some of the organs that accumulate the mercury from the placenta.
Pregnant rat dams were injected intraperitoneally with 0.1ml of a 0.9% saline solution with or without 20µg of methyl mercury chloride per day for 20 days of their 21-day gestation period, amounting to a total of 400µg of MeHgCl during pregnancy. Upon birth, the rat pups were eviscerated and eleven select organs were collected, pooled by organ type, weighed, and stored at -20C. Tissues were homogenized in 16N nitric acid and centrifuged at 40,000 rpm for 30 minutes. The volume of each supernatant was determined and then passed through a 0.45µm filter to clarify. All samples were stored at -20C until analysis with atomic absorption spectrometry at the University of Minnesota. The results of this analysis indicate that specific organs preferentially take up mercury during gestation. A quantitative comparison to untreated controls is provided for each organ.

PHYSICS

ANALYZING THE EFFECTS OF MASS SUBSTRUCTURE IN GRAVITATIONALLY-LENSED SYSTEMS

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The ΛCDM cosmological model predicts the existence of mass substructures, thousands of which purportedly populate the dark matter halo of the Milky Way and other galaxies. Only about 20 have been observed around the Milky Way; gravitational lensing is the only currently developed tool to address this issue. To account for the discrepancy in number of mass substructures seen in the dark matter halos of galaxies, gravitational lens-fitting simulations were performed to test whether the mass models used to describe these systems are unique. With no *a priori* knowledge, simulated quad-imaged lens systems were tested to see whether any effects due to any added dark matter substructure could be seen. The χ^2 goodness-of-fit statistic, as well as average image separation and RMS of image separation were found to be below resolution thresholds, and conclusively illustrated that it is technically possible in some cases to fit a smooth mass model to a gravitational lens system with added substructure. This study aids in the understanding of galactic structure and ultimately testing the ΛCDM cosmological model.

LOW-COST MICROBIAL FUEL CELL

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This paper outlines a procedure to construct a low-cost microbial fuel cell (MFC) using a strip of copper, aluminium, a potted plant, and some simple electronics. Power is generated using plant waste as nutrients for anaerobic bacterial respiration within the soil.

PSYCHOLOGY

THE EFFECT OF PARTICIPATION IN HIGH SCHOOL COLLISION SPORTS ON ATTENTION AND COGNITIVE FUNCTIONING

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This study builds on previous research exploring the effects of concussive and sub-concussive impacts resulting from participation in collision sports on cognitive functioning and reaction time. While concussive impacts have been shown to have detrimental cognitive and behavioral effects, it is unclear to what extent sub-concussive impacts, like those received in collision sports, have similar consequences. The cognitive functioning of male college students who played collision sports in high school (concussed and non-concussed) were compared with male college students who played non-collision

sports (concussed and non-concussed). All participants were under the age of 25 and had participated in one or more sports for at least sophomore through senior years of high school. Subjects were fitted with a 64-electrode electroencephalogram (EEG) net and performed a 3-tone auditory oddball task. The task consisted of participants' listening to three different tones played at random: a standard tone, occurring 80% of the time; a distractor tone, occurring 10% of the time; and a target tone occurring 10% of the time. Participants pressed a button when they heard the target tone. Data about the severity of concussions was collected as well. Preliminary results show that the concussed collision group had higher amplitudes in the p3b and n2 peaks on the event-related potentials (ERP) than the non-concussed collision group, suggesting that those people use more cognitive resources to effectively complete the task. It was also found that both collision and non-collision groups with concussions had increased latency for the p3b peak on the ERP. Groups did not differ in accuracy or reaction time to the target. There were also no differences found between the collision and non-collision groups.

SOCIAL SCIENCE

PSYCHOLOGICAL AND PSYCHOSOCIAL PREDICTORS OF ABSTINENCE VERSUS SUBSTANCE USE AMONG HIGH SCHOOL SENIORS: RESULTS FROM MONITORING THE FUTURE STUDENT SURVEY 2014

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Risky attitudes, social relationship factors, and health risk behaviors are associated with individual's choice to abstain or use (Musher-Eizenman et al. 2003) In the present study, we predicted that risky attitudes, friendships, and health risk behaviors would be associated with the choice of substance use. Sample: Data were from the 2014 Monitoring the Future and participants were 7,265 nationally representative high school seniors. Measures: Measures included thoughts about drugs, friends' involvement, and social and psychological attitudes. Three substance use groups were constructed (abstainer: 1,741 [23.96%]; user: 4,889 [67.29%]; non-common drugs: 635 [8.74%]). Results: Analyses suggested risky attitudes, social relationships, socializing in parties, and health risk behaviors were associated with substance use versus abstention (all p's <0.05). Abstainers tended to be more concerned if friends disapprove of drugs and found alcohol or marijuana use riskier than users did. Both found drugs such as cocaine quite risky (all p's <0.05). Abstainers believed that marijuana use should be illegal and those who use the drug are less sensible and hardworking (all p's <0.05).Conclusion: Risk attitudes, health behaviors, and friendships were predictive of use or non-use among high school seniors. Results suggest that prevention efforts may be aimed at changing attitudes regarding substance use risk, and encouraging relationships that are associated with abstention. Data from this study were accessed via ICPSR public access data sources. The Monitoring the Future study was funded by National Institute of Health, US Department of Health and Human Services, and the National Institute on Drug Abuse (ICPSR 36646).

THE RELATIONSHIPS BETWEEN STUDENTS' STUDY HABITS, SATISFACTION, AND EXAM SCORES IN CHEM100

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This study showed students spend their vast majority of time studying by reading the textbook, completing homework assignments, and studying specifically for exams. Also, as expected, the study showed student satisfaction increased directly with exam score. However, there were two small populations of students, one with low satisfaction and high exam scores and the other with high satisfaction and low exam scores, which differed from the main trend. This research was conducted in order to observe the study habits and student satisfaction in a general education level chemistry course. This study was conducted by asking the students enrolled in Chem100, Chemistry in Society, in the spring of 2017 at Minnesota State University, Mankato, to complete a post-test survey and record their student hours within an online calendar for each of their first two exams. The population of consented survey participation contained 74% of the class for both exam 1 and 2. As for the consent and participation on calendar completion, exam 1 consisted of 73% of students and the second exam, 65%.

THE ROLE OF INSTRUCTIONAL STYLE IN METACOGNITION

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Metacognition is the amount of awareness one has in monitoring their own thinking or learning. A way of testing metacognition is through knowledge surveys.

Knowledge surveys consist of 100 questions that include material similar to that of what the students would encounter on their assessment. Students answer if they believe they would be able to answer the question correctly and incorrectly if taking an exam with similar questions. Comparing matched questions from knowledge surveys with the actual assessment reveals the gap between what a student thinks they know and what they actually know. Studies have shown that higher-performing students will estimate their performance more accurately, having better metacognition, than lower-performing students. We used matched questions from the knowledge surveys and American Chemical Society General, Organic, and Biochemistry exam to compare four instructional approaches ranging from lecture to guided inquiry.

NOTES

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