# *Senior Thesis 2021*

ST. CLOUD STATE
UNIVERSITY
DEPARTMENT OF CHEMISTRY
& BIOCHEMISTRY

| Room 1 | Room 2 | Room 3 |
|---|---|---|
| Meeting ID: 991 8854 6119<br>https://minnstate.zoom.us/j/99188546119<br>Password: Chem491_1 | Meeting ID: 943 4968 7800<br>https://minnstate.zoom.us/j/94349687800<br>Password: Chem491_2 | Meeting ID: 98027264760<br>https://minnstate.zoom.us/j/98027264760<br>Password: Chem491_3 |

**Friday, April 23, 2021**
**4:00 p.m.**

4:00-4:20 p.m.

Room 3

Advisor:
Dr. Poole

## Yahya Abdulrahman

### Validation of a Novel Analytical Method for Hydroxyl Radical Reactions in Non-aqueous Solutions

**Abstract:** The reaction of hydroxyl radical was studied by conducting reactions in non-aqueous solutions. Hydroxyl radical derived product distributions in toluene indicate that addition of the radical to the *ortho* position is favored. The radical is almost four more time likely to attack at the *ortho* position than *meta*-. The data was obtained by analyzing the $^{1}$H NMR spectra of product distributions. To validate the analytical method the mass balance of hydroxyl derived products was calculated using the peak integrals. The product distribution was found and were based on the hydrogen abstraction and addition mechanisms. The mass balance of [*o,m,p*-cresol +benzyl] : [*tert*-butyl] was found to be between 73 %and 105%. This includes the uncertainty after correcting for the number of protons responsible for the resonance frequency of the *tert*-butyl adduct peak. The molar ratios and product distribution had little variation across a range of temperatures between 50°C and 75°C.

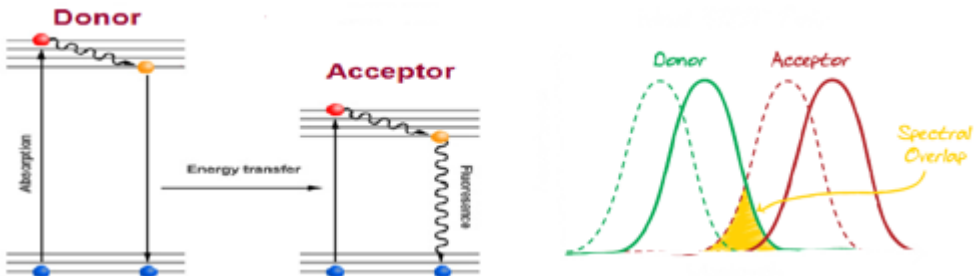
4:50-5:10 p.m.

Room 2

Advisor:
Dr. Bruender

## Jordan M. Bisping

### An Introduction to and Application of Fluorescence Resonance Energy Transfer (FRET)




**Abstract:** This work elaborates two/three different applications of FRET in biochemical investigations. In the first example, Dziedzicka-Wasylewska et. al used FRET to study the heterodimerization of human dopamine receptors. They determined that dopamine D1 and D2 receptors could form hetero-oligomers while remaining in the plasma membrane. In a 2009 study completed by Miyake-Stoner et. al FRET was used to study the structural changes of protein unfolding that occurred during the disruption of the protein's hydrophobic core. In the final example explored, Andersen et. al utilized FRET to study the interaction between amyloid precursor protein and its neuronal trafficking receptor to determine possible targets for the prevention of senile plaque formation.

4:50-5:10 p.m.

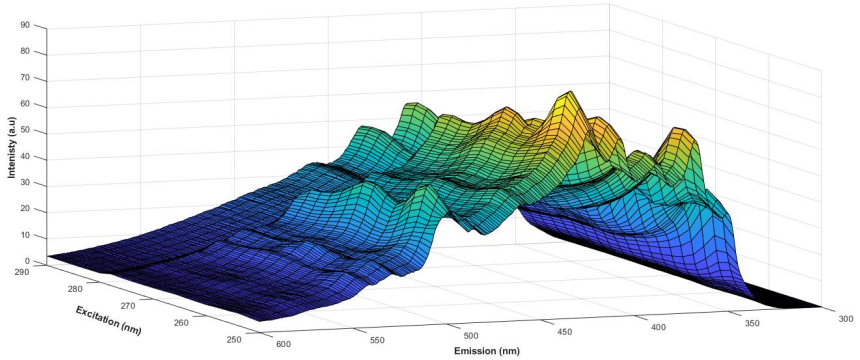
Room 3

Advisor:
Dr. Dvorak

## Ahmed Doudin

### Fluorescence Spectroscopy and PARAFAC Analysis to Time Resolve the Solid Phase Extraction of a Simple PAH Mixture on Whatman 1 PS Paper

**Abstract**: 2-dimensional datasets commonly referred to as Excitation Emission Matrices (EEMs) and the multi-way decomposition method Parallel Factor Analysis (PARAFAC) for the characterization of polynuclear aromatic hydrocarbons (PAH) (phenanthrene, naphthalene, and benzo(a)pyrene) extracted onto solid Whatman 1 PS filter paper is undertaken. The aim is to characterize these analytes in a single aqueous mixture solution via solid-phase microextraction (SPM) and PARAFAC analysis which can provide excitation signatures, emission signatures, and relative concentration of the three analyte species as a function of time over 60-minute period. Mass loadings of the PAH on the filter paper are at the sub-nanogram level. The work also explores the effects that the background signal has on the final analysis. PARAFAC was able to identify the emission, excitation, and extraction time profiles for the phenanthrene, benzo(a)pyrene, and background. It also distinguished the background spectrum of the filter paper with PAH loadings present. The approach did not observe the naphthalene signal as there was not enough of it in the aqueous mixture or the limit of detection (LOD) was too high. Spike recovery tests were applied to support the stated claim.




4:25-4:45 p.m.

Room 2

Advisor:
Dr. Jeannot

## Easter Emmanuel

### Wastewater-Based Epidemiology: Opioid Epidemic

**Abstract:** In a collaborative study by Arizona State University and the Center for Clean Water Technology, investigators sought the relation between opioid consumption and corresponding levels of the selected illicit drugs in wastewater in two unnamed mid-western cities. The wastewaters were analyzed for morphine, codeine, oxycodone, heroin, and fentanyl. Using liquid chromatography-tandem mass spectrometry (LC-MS), they analyzed samples of each city's raw water from wastewater treatment plants over the course of 2 years, during a heightened time of the opioid epidemic. The key findings from the study are discussed herein.

A second study by Biodesign Center for Environmental Health Engineering, the Biodesign Institute and Arizona State University tracked the narcotics consumption at an unnamed Southwestern U.S. university campus (Gushgari et al. (2)). Through wastewater-based epidemiology (WBE) twelve narcotics were sampled once a month from August 2017 to December 2017, for seven continuous 24-hours raw wastewater sampling periods from a campus generated wastewater plant. Under instrumental analysis using LC-MS/MS, the composite narcotics raw wastewater samples were analyzed for indictors of morphine, codeine, oxycodone, heroin, fentanyl, methadone, buprenorphine, amphetamine, methylphenidate, alprazolam, cocaine, and MDMA. These results are also discussed herein.

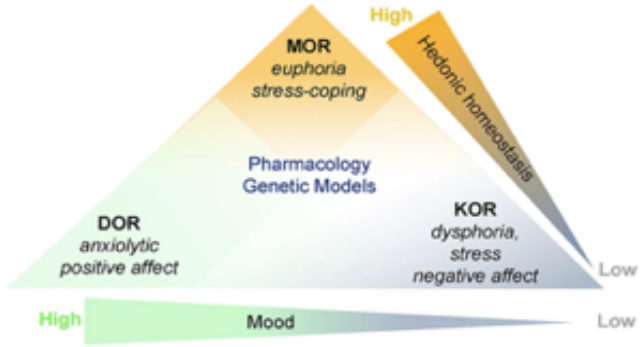
4:25-4:45 p.m.

Room 3

Advisor:
Dr. Jacobson

## Mackenzie M. Johnson

### Review of the Structural Basis of Opioid Treatment and Rehabilitation




**Abstract:** Opioids are pharmaceutical drugs to treat persistent or severe pain. Multiple research articles were analyzed, and it was found that gene cloning, brain mapping, the use of nanobodies, and rapid pace cloning with expression of the receptors are methods in studying endorphins and enkephalins. There are three major receptors that are responsible for signaling and controlling how the body reacts from the opioid drug. The three most common classifications of opioid receptors are preproenkephalin (κ (KOR)), pre-proopiomelanocortin (μ (MOR)), and pre-prodynorphin (δ (DOR). The MOR receptor is the main target for most opioid analgesics and is the most known receptor due to its interactions with the highly studied opioid, morphine. The MOR receptor is responsible for euphoria and stress-coping. The KOR receptor was found to be associated with dysphoria, stress, and negative effects, while the DOR receptor was found to be associated with anxiolytic and antidepressant activity. There are proposals that can be made on creating new pain reducing medication. One is discovering new amino acid interactions in the binding site of the receptors or altering amino acid sequences, so the receptors could exhibit different effects. Another way could be binding to a different receptor. Lastly, further studies could be conducted to determine a new receptor that has yet to be discovered to produce pain relieving effect, without producing mood altering effect.

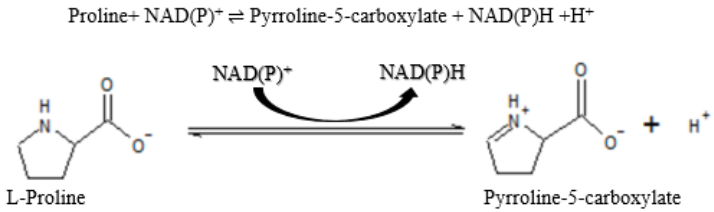
4:00-4:20 p.m.

Room 2

Advisor:
Dr. Bruender

## Xeroxa Joshi

### Expression, Purification and Characterization of Pyrroline-5-Carboxylate Reductase from *Sinorhizobium meliloti*




**Abstract:** The goal of the investigation was to characterize the function of the putative enzyme pyrroline-5-carboxylate reductase to confirm its proposed function in collaboration with New York Structural Genomics Research Consortium (NYSGRC). A plasmid containing the gene supplied by the NYSGRC, was expressed recombinantly in *Escherichia coli* and the protein was purified using Ni-NTA chromatography to obtain pure enzyme (<95%). The function of the purified enzyme was tested using a UV-spectrophotometer to detect the formation of NADH/NADPH (absorbs light at 340 nm) from the cofactor $NAD^+/NADP^+$ in the presence of either L-proline or L-4-thiazolidinecarboxylic acid (L-thiaproline). The enzyme catalyzes the oxidation of L-thiaproline, using $NAD^+$ or $NADP^+$, consistent with the function of the enzyme as a pyrroline-5-carboxylate reductase, which is the reverse of the reaction detected.

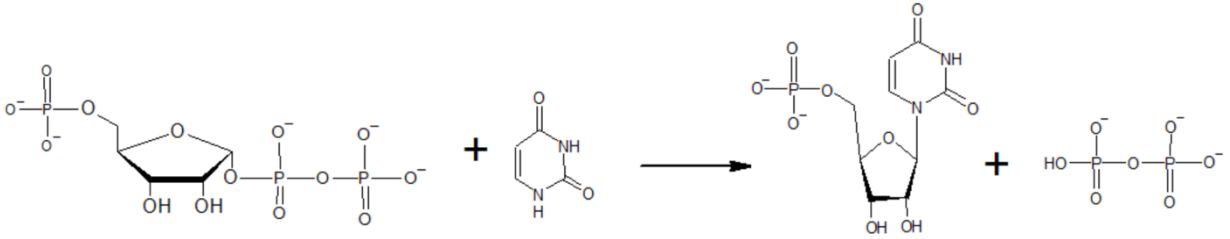
4:25-4:45 p.m.

Room 1

Advisor:
Dr. Bruender

## Brooke Schlangen

### The Study of the Phosphoribosyltransferase Activity



**Abstract:** Studies over the recent years have shown that the regulation of the phosphoribosyltransferase family is unpredictable, unkempt, and an intricate process. Control of these enzymes and the mechanisms that are included are important to understanding the basic rules of avoiding underlying syndromes. Phosphoribosyltransferase are transferases belonging to many different subclasses, including: uracil phosphoribosyltransferase, adenine phosphoribosyltransferase, and hypoxanthine-guanine phosphoribosyltransferase. In order to understand the role of the phosphoribosyltransferase in general they need to be functionally characterized. Therefore, a gene encoding for a hypothetical phosphoribosyltransferase from *Oceanicaulis sp*. HLUCCA04 was cloned and expressed, and the resulting protein was purified. The proposed enzyme was classified as a hypoxanthine-guanine phosphoribosyltransferase. In order to demonstrate this activity, the gene was cloned, expressed and the protein was purified. This work has shown that Guanine and Cytosine are not the substrates of phosphoribosyltransferase. At this time the function of KPP is still unknown but work is progressing in identifying the function of the enzyme.

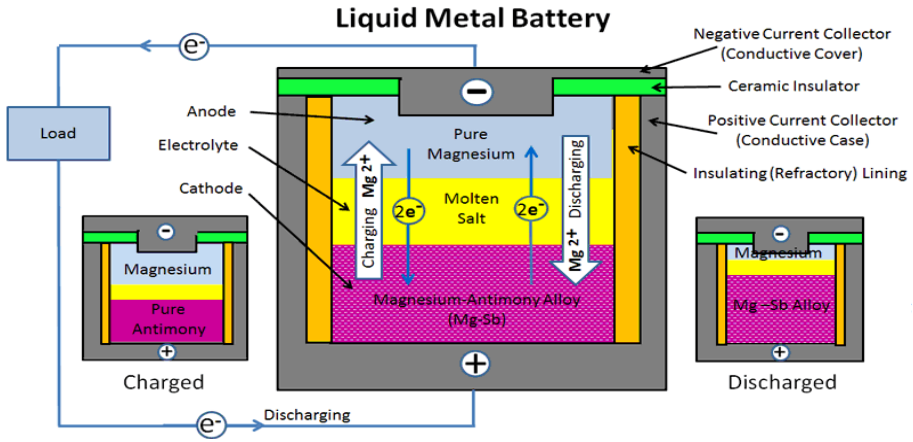
5:20-5:40 p.m.

Rooms 1, 2, 3

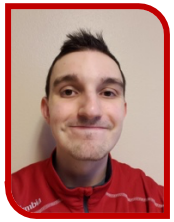
Advisor:
Dr. Dvorak

## Justin Schroepfer

### A Review of Design Principles, Electrode Material Types, and Current Research Directions of Liquid Metal Battery Technology




**Abstract:** The shift towards a carbon neutral society has advanced renewable energy technologies faster than ever before, creating the need to seamlessly interface renewable energy into the power grid. Quick, efficient, and reliable energy storage must be used to regulate the intermittency inherit with renewable sources as well as smooth power fluctuations in the grid. Liquid metal batteries (LMBs) make ideal candidates to fill the energy storage role given their cheap cost, high efficiency, long cycle life, and ease of scaling up. The high temperatures needed for LMBs to operate and associated issues such as high temperature hermetic seals and increased corrosion, motivates the study of not only elemental electrode pair materials, but also fusible alloy materials. The review presented will overview the design principles and material choices for liquid metal batteries, including the past and current advancements in LMB technology.



4:00-4:20 p.m.

Room 1

Advisor:
Dr. Mechelke

4:50-5:10 p.m.

Room 1

Advisor:
Dr. Bruender

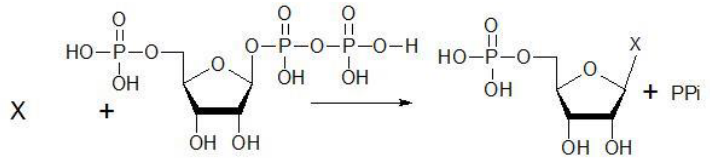
## Cody Smelik

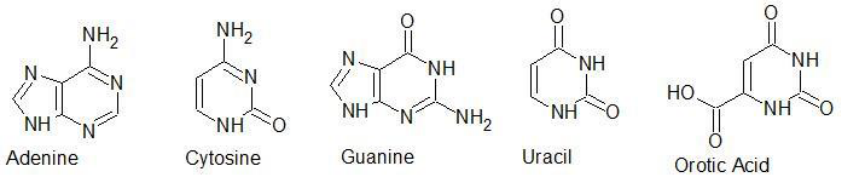
### The Evolution of Hydroboration Oxidation Reactions and the Future in Organic Chemistry

**Abstract:** Hydroboration oxidation reactions are two step reactions that allows addition of water to different alkenes in an Anti-Markovnikov fashion. Four reagents over time to improve regioselectivity and stereoselectivity in the final products. The 1st Generation of reagents discussed, the molecule $BH_3$ in tetrahydrofuran(THF) complex or dimer $B_2H_6$, combined with NaOH and $H_2O_2$ to provide good yield of desired Anti-Markovnikov products but resulted in a racemic mixture. The 2nd generation reagent of 9-borabicyclo[3.3.1]nonane(9-BBN) developed by Dr. Herbert Brown produced more regioselective favored products and was particularly successful in reactants that included multiple double bonds but lacked stereoselectivity. Dr. Brown also designed a 3rd generation hydroboration molecule, diisopinocampheylborane ($Ipc_2BH$), to achieve stereoselectivity while maintaining regioselectivity in certain alkenes. The 4th generation of reagent of trans-2,5-dimethylbororlane developed by Dr. Satoru Masamune aimed to achieve a high stereoselectivity across more types of alkenes compared to $IpC_2BH$. The following paper will discuss the origin of the hydroboration-oxidation reaction and follow the development of the key reagents, from the racemic mixtures to the highly regioselective and stereoselective reagents of today.

## Tylor Veldhuizen

### Characterization of the Uracil Phosphoribosyl Transferase Enzyme




**Abstract:** Enzymes hold the utmost importance in biological reactions, without enzymes life would not be sustained. Without enzymes activation energy of biological reactions would not be lowered and an organism's existence would not occur. Sequences of enzymes are entered into biochemical databases with proposed function. Characterization of enzymes in databases, like NCIB, is virtually non-existent. This study is focusing on phosphoribosyltransferase enzymes, particularly the uracil phosphoribosyltransferase enzyme. Phosphoribosyltransferase enzymes transfer D-ribose 5-phosphate from 5'-phospho-α-D-ribose-1'- pyrophosphate (PRPP) into a purine, or a pyrimidine by ribophosphorylation to make the respective nucleoside-5'-monophosphate. High-performance liquid chromatography (HPLC) was used to detect the absorbance of nucleobase. HPLC was used to display possible activity of the phosphoribosyltransferase enzyme with various nucleobases (adenine, cytosine, guanine, orotic acid, and uracil). The results from this experiment were mixed, however the enzyme displayed no activity when uracil was used as a substrate. The enzyme is proposed to be an uracil phosphoribosyltransferase enzyme, since uracil did not work, this proves the system is flawed and further characterization should be done before enzymes are entered into databases.