
## Anthony Allen '18

*from* Redford, MI

**Major:** Chemistry & Philosophy

**Other Interests:**
Football

### Enantioselective Domino Nazarov/{4+3} Cycloaddition

*advisor* Albert Matlin

Development of an enantioselective domino Nazarov/{4+3} cycloaddition reaction through the trapping of the Nazarov oxyallyl cation intermediate with a diene. Chirality is introduced with the use of a chiral Lewis acid.

## Alyssa Altheimer '19

*from* Greensboro, NC

**Major:** Biochemistry

**Other Interests:**
Trombone

### Molecular Characterization of Colorimetric Metal Sensors

*advisor* Jason Belitsky

Recent events in Flint, Michigan and throughout the US have highlighted the potential for lead exposure through tap water. The ability to test lead concentrations at the point of use with a simple colorimetric assay could be of great value in preventing lead exposure. While working on synthesizing mimics of melanins, the biological pigments, the Belitsky lab found that coatings derived from the oxidative polymerization of catechols change color in response to binding metal ions, such as lead and copper. Currently, these catechol-based coatings are not selective or responsive enough to be practical sensors for lead, but we are working toward that goal by trying to understand these coatings at the molecular level, using tools such as IR spectroscopy. This semester, we are working on an assay for phenol content for the coatings, as well as the synthesis and characterization of new coatings and their optimization as colorimetric metal sensors.

## Alyssa Chow '20

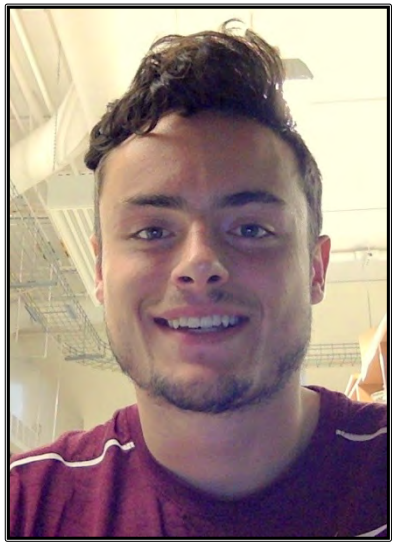
*from* Lorain, OH

**Major:** Biochemistry

### Synthesis and Structural Analysis of Pyridinium Metal Halides

*advisor* Catherine Oertel

Perovskite solar cells convert light energy into electricity by harnessing the properties of perovskite-structured hybrid inorganic-organic materials, generally involving an organic cation incorporated into an inorganic framework comprising metal cations and halide anions. In recent years, these devices have demonstrated promising growth in efficiency, thereby sparking interest in the exploration of hybrid metal halides. Our focus lies in the aromatic organic cation, pyridinium, and we work towards understanding the role that the pyridinium ion plays in the overall crystal structure, and ultimately the properties, of pyridinium metal halides. We have synthesized pyridinium lead bromide in solution and determined its crystal structure using single crystal X-ray diffraction. We have also synthesized pyridinium tin iodide using solution and solid state methods, and we are determining its crystal structure using powder X-ray diffraction. Preliminary work suggests that it is isostructural to pyridinium tin bromide.



## Connor English '18

*from* Billings, MT

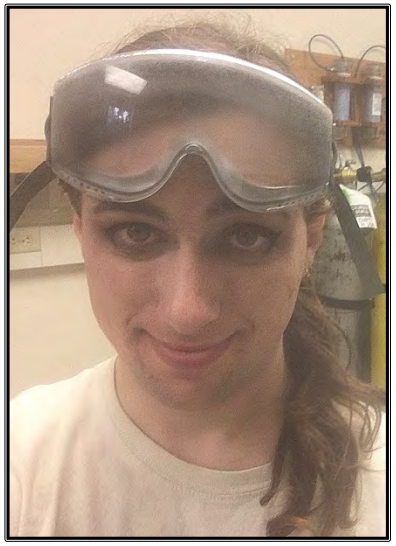
**Major:** Chemistry & Biochemistry

**Other Interests:**
Oberlin College Men's Soccer, Backpacking, Stand-Up Comedy, Organic Synthesis

### Development of an Enantioselective Tandem Nazarov Cyclization/Intramolecular Cycloaddition

*advisor* Albert Matlin

Nazarov Cyclization allows the synthesis of cyclopentenones from divinyl ketones. The utility of this reaction to produce cyclic and multi-cyclic molecules has generated a boom in research over the past 10 years. Many of the research groups studying this reaction are focused on the enantio-selective version of the reaction. In 2013, the Rawl group developed a chiral chromium "Salen" catalyst that produced <90% of one enantiomer for a variety of dienone substrates. Then, the West group expanded upon this reaction with a "Tandem Nazarov/Cycloaddition reaction." In this reaction, a diene was added to the reaction mixture which lead to the production of complex cyclic structures. Multi-cyclic systems containing an eight membered ring are challenging to synthesize. West's approach is important because it provides a simple and general approach to this problem. The goal of this project is to use Rawal's chiral Salen catalyst to develop an enantio-selective version of the West "Domino Nazarov/Cycloaddition" reaction.



## Arden Hammer '18

*from* Thousand Oaks, CA

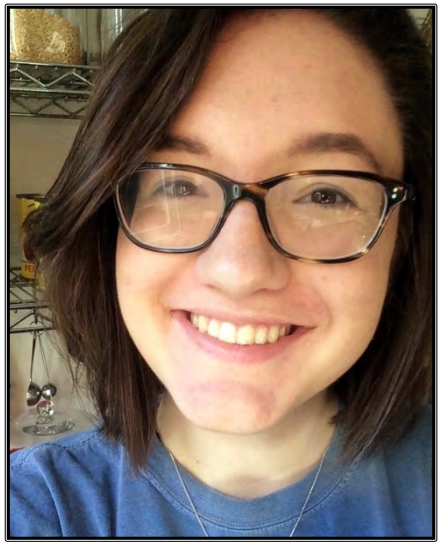
**Major:** Chemistry & Biochemistry

**Other Interests:**
petting dogs, bats, hiking, the sun, talking to nice people, science puns, classical music

## Synthesis and Structural Chemistry of Lead Oxide Carboxylates with Aromatic Ligands

*advisor* Catherine Oertel

Compared with organic molecules, hybrid inorganic-organic materials exhibit greater structural diversity, and strategies for predicting the structures they will form are less well developed. Lead oxide carboxylates are a family of hybrid inorganic-organic compounds in which edge-sharing $Pb_4O$ tetrahedra form extended inorganic substructures that are further coordinated by carboxylate ligands. Some members of this family have noncentrosymmetric crystal structures, resulting in unusual properties such as second-harmonic generation. Extended inorganic substructures may afford these compounds unique properties unlike those of other hybrid materials, such as high thermal stability and mechanical anisotropy. We have synthesized two novel lead oxide carboxylates with isomeric naphthoate ligands in order to probe the role of ligand shape in directing the condensation, topology, and symmetry of extended inorganic motifs. The structural patterns found may be applicable to other hybrid systems.



## Mikaila Hoffman '18

*from* Pittsburgh, PA

**Major:** Chemistry
**Minor:** Cognitive Science

**Other Interests:**
I've been a contributing artist for the Synapse for three years, and I enjoy reading in my spare time.

## Mechanistic Exploration of Co-Crystal Formation Reactions

*advisor* Manish Mehta

The goal of this project is to better understand the mechanism through which different co-crystal systems react. I will use a variety of techniques, including solid-state NMR and single crystal diffraction, to search for evidence for an intermediate or orientation requirement in the formation reaction of co-crystals. This is key information that is missing from the co-crystal literature, which has recently captured interest for the potential application of co-crystals to pharmaceuticals.

## Daniel Katz '19

*from* Washington, D.C.

**Major:** Chemistry

**Other Interests:**
Swing dancing, fishing

### Analysis of Nutraceuticals Marketed to Treat BPH

*advisor* Robert Thompson

Benign prostatic hyperplasia (BPH) or enlarged prostate is a disease affecting many older men. Treatment may involve pharmaceuticals or nutraceuticals that act to reduce the size and effects of the enlarged prostate. Three compounds – atraric acid, N-butylbenzene sulfonamide, and beta-sitosterol – have been identified as efficacious biochemicals in nutraceuticals. Of course, nutraceuticals marketed in the U.S. are unregulated and may contain more or less or none of these biochemicals. Our research aims at developing a method for quantifying the three compounds by liquid chromatography – mass spectrometry in commercial products sold for prostate health. Some of these products are marketed as Pygeum (from bark of an African tree), Saw Palmetto (from fruit of palm tree), and Usnea (from lichens). Once the analytical method has been fully developed, a dozen or so products will be analyzed in order to gain a sense of the contents of the products and how well they might work to ease the effects of BPH.

## Jorden Mandel '18

*from* Plantation, FL

**Major:** Biochemistry

**Other Interests:**
Football and Lacrosse

### Computational Structural Biology

*advisor* Zoey Hua

Spleen Tyrosine Kinase (SYK) is an enzyme that plays a central role in initiating signaling in B-cells of the adaptive immune system. SYK has a tandem dual SRC Homology 2 (tandem SH2) domain that can bind to the doubly-phosphorylated Immunoreceptor Tyrosine-based Activation Motifs (dpITAMs) found on the B-cell transmembrane receptor. Following SYK-receptor association, Tyrosine 130 (Y130) in the tandem SH2 protein is phosphorylated. Phosphorylation of Y130 is thought to cause a conformational change in the SYK tandem SH2 protein, which eventually lowers the binding affinity of the tandem SH2 domains to the dpITAM of the receptor.

The overall goal of this research is to understand the effect that a change in conformation of the tandem SH2 protein due to Y130 phosphorylation has on the binding affinity of SYK to dpITAM. Specifically, we are using docking programs such as Rosetta FlexPepDock to evaluate the binding interfaces formed between dpITAM and phosphorylated tandem SH2 protein. The results of FlexPepDock can then be loaded into VMD, a molecular modeling and visualization computer program, to view and determine the best docking poses and most plausible structures for the tandem SH2-dpITAM complex.

## Daniel Markus '19

*from* Rockville, MD

**Major:** Biochemistry & TIMARA [Double Degree]

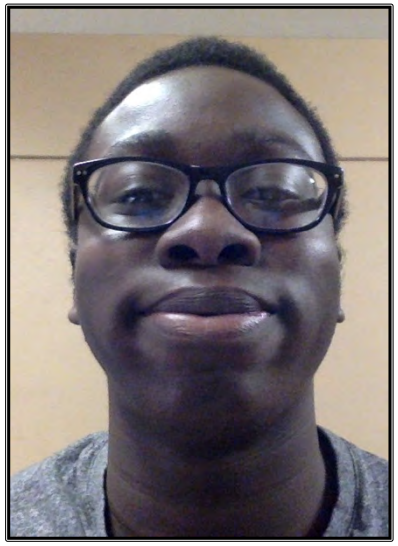
**Other Interests:**
memes, reminiscing about Kepler, saying "hey, that's a cool sound" because I am a TIMARA major, thinking about how I used to wear headphones all the time

### Influence of Experimental Conditions on Equilibrium Constant Determination for the Thrombin-Binding DNA Aptamers: Benchmarking the Model System

*advisor* Rebecca Whelan

Aptamers are single-stranded oligonucleotides, typically DNA or RNA, that have been selected to bind to a target with high affinity. DNA aptamers possess numerous advantages over antibodies including relative ease of synthesis and replication; predictable behavior in electrophoresis experiments; chemical simplicity; and facile labeling with fluorophores and immobilization handles. They are also more stable than unmodified RNA aptamers, which are subject to degradation by ubiquitous RNA-degrading enzymes. Of the DNA aptamers targeting proteins, the best characterized are the 15mer and 29mer for thrombin, a serine protease involved in the coagulation cascade. These aptamers are widely used as a model system to demonstrate proof-of-concept of novel analytical methods. Despite this widespread use of the thrombin and its aptamers, a wide range of apparent affinity has been reported for these interactions, with dissociation constant (Kd) values ranging from 0.5 nM to 255 nM for the 29mer and 37 nM to 455 nM for the 15mer.

My previous work explored the effect of various experimental conditions on determined Kd values for the two aptamers using Flourescence Anisotropy, and found that both aptamers display cooperative binding. My current work is further exploring this system using Affinity Probe Capillary Electrophoresis (APCE).



## Dom Ogunjimi '19

*from* Dolton, IL

**Major:** Biochemistry

**Other Interests:**
Reading, Drawing, Music, Guitar, Self-care

### Analysis of the Effects of Fluorescent Labels on Thrombin-Aptamer Binding Using Surface Plasmon Resonance

*advisor* Rebecca Whelan

Aptamers can bind to various biomolecules with high specificity. The aptamers 15mer and 29mer are well known aptamers that have been selected for binding to the plasma protein thrombin. The binding of these aptamers to thrombin has been characterized by the Whelan lab using two assays: affinity probe capillary electrophoresis (APCE) and fluorescence anisotropy (FA). The thrombin-aptamer system serves as a well-studied model system for the development of new analytical techniques. FA and APCE are both assays that require fluorescent labels to be attached to the aptamers. It is unknown whether these fluorescent labels impact the binding affinity of these aptamers for thrombin. Surface plasmon resonance (SPR) is a label-less assay that can also be employed to study target-aptamer binding. Currently, SPR is being explored as a method to determine the effects of fluorescent labels on thrombin-aptamer binding by comparing binding affinity measurements between labeled and unlabeled thrombin-aptamer interactions, further expanding our understanding of these thrombin-aptamer model system.


## Brendan Sheehan '18

*from* Middleton, WI

**Major:** Biochemistry & English

**Other Interests:**
Reading

### Analysis of BPH Nutraceuticals

*advisor* Robert Thompson

Benign prostatic hyperplasia (BPH) or enlarged prostate is a disease affecting many older men. Treatment may involve pharmaceuticals or nutraceuticals that act to reduce the size and effects of the enlarged prostate. Three compounds – atraric acid, N-butylbenzene sulfonamide, and beta-sitosterol – have been identified as efficacious biochemicals in nutraceuticals. Of course, nutraceuticals marketed in the U.S. are unregulated and may contain more or less or none of these biochemicals. Our research aims at developing a method for quantifying the three compounds by liquid chromatography – mass spectrometry in commercial products sold for prostate health. Some of these products are marketed as Pygeum (from bark of an African tree), Saw Palmetto (from fruit of palm tree), and Usnea (from lichens). Once the analytical method has been fully developed, a dozen or so products will be analyzed in order to gain a sense of the contents of the products and how well they might work to ease the effects of BPH.

## Benjamin Steger '19

*from* St. Louis, MO

**Major:** Biochemistry &
Trumpet Performance
[Double Degree]

### Synthesis of Eumelanin Analogues

*advisor* Jason Belitsky

Biological pigments known as melanins are ubiquitous but poorly understood biomaterials. Melanins have a range of fascinating properties that impact their biological roles and are beginning to be exploited for non-biological applications such as water purification. Eumelanin, the black to brown human pigment, is composed of oligomers of dihydroxyindoles that self-assemble into nanoparticles. Understanding this self-assembly process is a key challenge that we are addressing through the synthesis of well-defined dihydroxyindole oligomers. The Belitsky group has developed methods for the functionalization and coupling of dimethoxyindoles, utilizing reactions mediated by palladium, iridium, and bromine. This semester we will continue to optimize these reactions and expand their scope to construct dimethoxyindole oligomers with diverse shapes and sizes.

## Santino Stropoli '18

*from* Manhattan, NY

**Major:** Chemistry &
Violin Performance
[Double Degree]

**Other Interests:**
Classic rock style guitar and flamenco ukulele.

### Oligomerization Reactions of Isoprene-Derived Epoxides on Secondary Organic Aerosol Particles

*advisor* Matthew Elrod

A significant portion of the atmosphere's particulate matter consists of secondary organic aerosol (SOA), which has been implicated in human respiratory and cardiovascular disease, visibility loss, and climate modification. Extensive studies of SOA formation have identified epoxide intermediates as key species in the formation of isoprene-derived SOA. Recent work has suggested that isoprene-derived dimers constitute a significant fraction of SOA in the southeastern United States. We use nuclear magnetic resonance techniques to study acid catalyzed oligomerization of the isoprene-derived epoxide IEPOX-4.

## Andrew Sugarman '19

*from* Phoenix, MD

**Major:** Biochemistry

**Other Interests:**
Baseball, snowboarding, listening to music, weight training, being terrible at video games

### Computational Structural Biology

*advisor* Zoey Hua

Spleen Tyrosine Kinase (SYK) is a non-receptor tyrosine kinase residing in the cytoplasm of hematopoetic cells. SYK is prevalent in human B-cells and important for several signaling pathways governing a wide range of cellular activities, including differentiation, proliferation, and immune response.

Signaling in B-cell is initiated when two SH2 domains (tSH2) of SYK interacts with the doubly phosphorylated immunoreceptor tyrosine activation motifs (dpITAMs) of the B-cell immunoreceptor. It was observed in previous biophysical experiments that when Tyrosine 130 (Y130) of the tSH2 is phosphorylated, tSH2-dpITAM binding affinity is decreased.

The overall goal of the project is to understand the effect that this phosphorylation of Y130 has on the conformation of the SYK tSH2 so that a change in the binding affinity of SYK to the dpITAM is observed.

Multiple molecular dynamics (MD) simulations will be carried out in NAMD to explore the conformational space available to the phosphorylated tSH2. Analyses will be carried out in CHARMM and visualization of protein conformations will be in VMD.

## Cecilia Wallace '19

*from* Hancock, MI

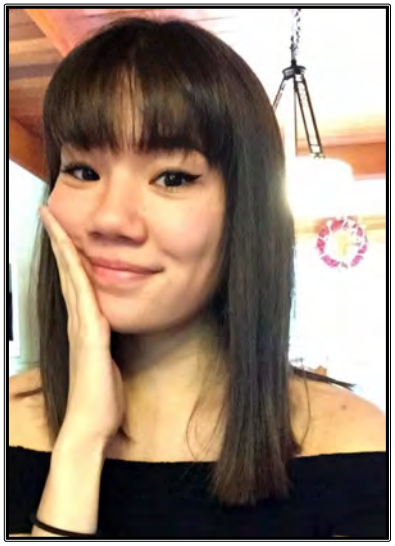
**Major:** 3-2 Engineering

**Other Interests:**
biochemistry, politics, CS, Student Senate, trying to learn Spanish, running

### Molecular Characterization of Colorimetric Metal Sensors

*advisor* Jason Belitsky

Recent events in Flint, Michigan and throughout the US have highlighted the potential for lead exposure through tap water. The ability to test lead concentrations at the point of use with a simple colorimetric assay could be of great value in preventing lead exposure. While working on synthesizing mimics of melanins, the biological pigments, the Belitsky lab found that coatings derived from the oxidative polymerization of catechols change color in response to binding metal ions, such as lead and copper. Currently, these catechol-based coatings are not selective or responsive enough to be practical sensors for lead, but we are working toward that goal by trying to understand these coatings at the molecular level, using tools such as IR spectroscopy. This we are working on an assay for phenol content for the coatings, as well as the synthesis and characterization of new coatings and their optimization as colorimetric metal sensors.



## Gabby Walsh '18

*from* New York, NY

**Major:** Biochemistry & Biology

**Other Interests:**
Cooking, food, travel, music, co-founder of Oberlin Multi-

### Analysis of HE4 Ovarian Cancer Biomarker Aptamer Candidates Generated by Magnetic Fluidic SELEX

*advisor* Rebecca Whelan

The Whelan lab uses systematic evolution of ligands by exponential enrichment (SELEX) to select aptamers, three-dimensional single-stranded DNA able to recognize a protein of interest, for ovarian cancer biomarkers. Using Galaxy and other bioinformatics platforms, I am analyzing five rounds of magnetic fluidic SELEX high-throughput sequencing data from this summer. The goal is to determine what DNA sequences best bind HE4 and then to analyze the binding strength of specific candidates using analytical techniques such as affinity probe capillary electrophoresis and fluorescence anisotropy.