Galen Brennan ’17
from Seattle, WA

Major: Biochemistry & Chemistry

Other Interests:
played on the Oberlin soccer team

Solution Phase Hydrolysis Reaction Kinetics of Atmospherically Relevant Isoprene-Derived Hydroxynitrates

advisor Matthew Elrod

I am working with Professor Elrod to synthesis and study the hydrolysis kinetics of various organonitrates that are found in the atmosphere. These organonitrates are of interest due to their derivation from isoprene, which is the second most abundant air pollutant found in the troposphere. The main goal of our study is to determine whether these organonitrates serve to directly impact the steady state concentration of tropospheric ozone, which is dictated by their rate of hydrolysis.

Alyssa Chow ’20
from Lorain, OH

Major: Biochemistry

Synthesis of Pyridinium Metal Halides

advisor Catherine Oertel

In the last few years, solar cells, used to convert light energy into electricity, are more commonly found in the form of perovskite solar cells, which function using material with a perovskite structure. They have become increasingly popular in the research field due to their promising growth in efficiency. The perovskite-structure materials used in these solar cells are hybrid organic-inorganic compounds typically involving an organic cation incorporated with an inorganic metal halide. This summer, we are working to synthesize, characterize, and determine the crystal structure of various pyridinium metal halides. We have synthesized pyridinium lead bromide in solution and determined its crystal structure using single X-ray diffraction. We have also synthesized pyridinium tin iodide through solid state reactions, and we will determine its crystal structure using its powder X-ray diffraction pattern.
Investigation of Atmospheric Mechanisms in Lactone Molecules

advisor Matthew Elrod

Recent literature has shown that hydroxymethyl-methyl-α-lactone (HMML) could act as an intermediate between the atmospheric Biogenic Volatile Organic Compound (BVOC), Isoprene, and Secondary Organic Aerosol (SOA) products. Because SOAs have been linked to health and climate issues, it is important to understand the viability of this intermediate oxidizing into the aerosol phase. This summer I am working on proxy lactone compounds (due to the instability of HMML) to try and determine their rate constants in the gas and aerosol phase using Flow Tube Chemical Ionization Mass Spectroscopy. The structural similarities of the compounds means that these rate constants should serve to model the likely behavior of HMML and reveal whether its reactions into the aerosol phase are significant.

Synthesis of pyridinium and ethylenediammonium lead iodides

advisor Catherine Oertel

Hybrid lead halide perovskites have exhibited remarkable photophysical properties and are prime candidates for application as solar cell absorbers. The properties of hybrid perovskites of the form ABX3 have generally been associated with the inorganic framework of linked BX6 octahedra. However, recent research suggests that the organic A-site cation may significantly influence the dimensionality and band structure of hybrid lead halide materials. To study the role of an aromatic A-site cation in hybrid lead iodides, we have synthesized pyridinium lead iodide and a solvate, pyridinium lead iodide • 1.5 DMF. Previously, we have characterized the optoelectronic properties of pyridinium lead iodide using diffuse reflectance measurements and density-of-states calculations. This summer, we will employ differential scanning calorimetry to investigate the possibility of structural changes due to ordering of the pyridinium ring at low temperatures. Additionally, we explore the synthesis of ethylenediammonium lead iodide in order to study the effects of the alkyl chain length in a diammonium A-site cation. We have determined new structures of two salts, ethylenediammonium dihydroiodide and ethylenediammonium monohydroiodide, which were reacted with lead iodide in the solid state. PXRD patterns provide evidence for the formation of new products in these solid-state reactions, encouraging the pursuit of the synthesis of ethylenediammonium lead iodide.
Arden Hammer ’18  
*from* Thousand Oaks, CA

**Major:** Biochemistry & Chemistry

**Other Interests:** dogs, bats, the sun, nice people, science puns, classical music

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**Synthesis and Structural Chemistry of Lead Oxide Carboxylate Hybrid Materials with Chiral Organic Ligands**  
*advisor* Catherine Oertel

Lead oxide carboxylates are hybrid inorganic-organic compounds in which distorted edge-sharing Pb$_4$O tetrahedra form extended inorganic substructures that are further coordinated by carboxylate ligands. Some lead oxide carboxylates have non-centrosymmetric structures that can give rise to novel optical properties, and synergy between their organic and inorganic substructures gives them the potential to display a unique set of properties, unlike those of either purely organic or purely inorganic compounds. However, not much is known about how ligand properties influence the structures and properties of these hybrid materials. Prior work has shown that noncoordinating to coordinating ratio of the ligand, as an approximation of ligand shape, is inversely correlated with dimensionality of the material. Our current work involves synthesis and characterization of new lead oxide carboxylate phases with chiral organic ligands in order to further elucidate how ligand shape governs the condensation and topology of extended inorganic motifs.

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Daniel Hill ’21  
*from* Oberlin, OH

**Major:** undeclared

**Other Interests:** chemistry, mathematics, ice hockey, reading, gardening

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**Oligomerization of $\beta$-propiolactone as a Model for the Formation of 2-MG Based Oligomers**  
*advisor* Matthew Elrod

Plants naturally emit biogenic volatile organic compounds (BVOCs) into the atmosphere. These BVOCs react with human introduced pollutants to form secondary organic aerosol (SOA) with the ability to effect air quality, cloud formation, and the Earth’s climate. Hydroxymethyl-methyl-$\alpha$-lactone (HMML) has been proposed as a species that could lead to the formation of methylglyceric acid based oligomers in SOA. However, HMML has no known synthesis procedure, and therefore, to determine if HMML could play a role in such reactions, we study a lactone that is very similar in structure, $\beta$-propiolactone (BPL). By studying the oligomerization reactions of BPL and the structural connectivity of the oligomers observed at varying possible atmospheric conditions, we aim to determine whether HMML could, in fact, lead to the formation of methylglyceric acid based oligomers in SOA.
Organochlorine pesticides (OCPs), including the well-known DDT, were used frequently in the 1960s, but are now banned in many countries. Despite being banned, it is possible OCPs may persist in the environment. This research will use EPA Method 8081B to analyze soil samples for OCPs with a focus on Dieldrin. The method uses a Soxhlet extraction followed by solid phase extraction (SPE) and evaporation to prepare samples for analysis by a gas chromatograph with an electron capture detector. The goal is to develop a laboratory experiment for an analytical chemistry course.
Dom Ogunjimi ’19  
from Dolton, IL  

Major: Biochemistry  

Other Interests: art, guitar, cooking, track & field  

Characterization of Thrombin-Aptamer Binding Using Fluorescence Anisotropy  

adviser Rebecca Whelan  

Without a general screening test for ovarian cancer, patients are most often diagnosed at advanced stages of the disease, where survival is the bleakest. Aptamers are potential alternatives to antibodies, which are currently used to probe for ovarian cancer, and may provide the basis for this general screening test. Development of these tests require a well characterized model system. Thrombin, a blood clotting enzyme, has two well-studied aptamers that often act as this model system. Literature values for their dissociation constants (KD—the measure of binding affinity) vary widely, making the thrombin-aptamer systems difficult to use accurately as models. Because of the literature KD’s wide variability, the Whelan lab characterized the thrombin-aptamer systems’ binding affinity in different buffer/ion environments using a fluorescence anisotropy assay. In FA, polarized light is shined onto fluorescently-labeled molecules, which then rotate and emit polarized light in various directions. Larger molecules, like protein-aptamer complexes, rotate more slowly and emit light in fewer directions resulting in higher anisotropy values. Aptamer concentration was held constant while thrombin concentration varied. Anisotropy values were gathered at each thrombin concentration and put into a Hill plot, from which the KD was derived. With these assays, the Whelan lab is measuring the strength of thrombin-aptamer binding while observing the effects of ions. By establishing criteria for “normal” thrombin-aptamer binding and ionic effects on this binding, the thrombin-aptamer system can be better utilized as a model system. As a model system, the thrombin-aptamer system can be used to test new target-aptamer assays and potential diagnostic tests for ovarian cancer and much more.

Rhodamine 110 Degradation Assay  

adviser Rebecca Whelan  

Rhodamine 110 is a fluorophore meaning that when excited by light emits light. Rhodamine 110 is used in Affinity Probe Capillary Electrophoresis as an internal standard to account for the variability in injected sample volume. The machine shines a laser at a sample and reads the amount of light the sample fluoresces. However, Rhodamine 110 has been found to be unstable and fluoresces less over time. My project is to determine the best condition for the Rhodamine 110 solutions to be kept at, and, if possible, to determine the rate of the degradation of the Rhodamine 110 solutions. I prepared fifteen solutions of Rhodamine 110 by using five different buffer solutions and making three solutions per buffer. One of each buffer solution was kept in a freezer at about -20°C, one of each in a refrigerator at about 4°C, and one of each at room temperature. The samples were kept in 2mL eppendorf tubes covered in aluminum foil to minimize light exposure, as it is known that Rhodamine 110 is sensitive to light. Every day I would prepare a dilution of each solution sample as a test sample. I put the test samples in a 96 well plate and inserted the plate in a spectrophotometer. The spectrophotometer would shine a light at each test sample and read how much light each sample emitted. Using this information, I observed the overall trend of the degradation of each sample to determine the optimal environment for a Rhodamine 110 solution.
Cancers are known to produce unique biomolecules or biomarkers that can be detected using diagnostic tests. CA-125 and HE4 are two biomarkers used in clinical tests to detect ovarian cancer, which responds favorably to treatment when diagnosed at its earliest stage. These tests, however, often produce both false positives—identifying cancer when it is not present and false negatives—failing to detect biomarkers that are present. The Whelan lab aims to create a new diagnostic tool by using aptamers as a way to detect these biomarkers.

Systematic evolution of ligands by exponential enrichment (SELEX) is one method used to select aptamers. Aptamers are short oligonucleotides, (usually RNA or single stranded DNA) that bind to a target with high affinity and specificity. The selection process requires amplifying DNA. Conventionally, polymerase chain reaction (PCR) is used to create double stranded DNA (dsDNA). This dsDNA needs to be converted to single stranded DNA (ssDNA). Alternatively, asymmetric PCR can be used to preferentially amplify one strand of DNA by using a greater amount of forward primer to create excess single stranded DNA. This is the strand of interest and can be used in subsequent SELEX processes. ssDNA can be separated from the primers using an agarose gel and then purified using a commercially available kit.

We are exploring a novel fluids based SELEX approach, which allows for continuous washing of the magnetic beads. This washing removes loosely bound DNA allowing aptamers with the highest affinity to remain bound to HE4. This summer we will select aptamers for HE4 by completing 5 rounds of SELEX using this approach that combines magnetic bead separation, fluids and asymmetric PCR.

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

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 in the southeastern United States 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 part 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.
Gabby Walsh ’18
from New York, NY

Major: Biochemistry & Biology

Other Interests:
cooking, eating, sleeping, and cats.

Optimization of 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. This summer I have worked on various projects optimizing SELEX. In addition to characterizing a new protocol involving a fluidics washing platform to separate weakly binding aptamer candidates, I helped to develop gel extraction of single-stranded DNA. I have also created several methods to reliably quantify DNA before and after each round of SELEX so that the proportion of DNA to protein of interest may be controlled for during selection. Using three methods - Nanodrop absorbance spectroscopy, gel electrophoresis, and capillary electrophoresis - I have made several calibration curves and visual comparisons for accurately measuring DNA. Moving forward, I hope to use capillary electrophoresis to characterize the binding of novel aptamers to our protein of interest.