

**Anthony Allen '18**  
from Redford, MI

**Major:** Chemistry & Philosophy

**Other Interests:**

Football, weightlifting, guitar, listening to the Grateful Dead, losing at League of Legends, eating food (edible for the most part), breathing, sleeping, awaking at 5:45 am to do all the previously listed activities, walking, recounting embarrassing

life stories, going to Mass celebrated in languages that aren't English (Latin, Arabic, etc.) , watching the occasional Rom-Com, faking interest in making small talk, reading Plato's Dialogues or Shakespeare in my spare time

**Development of Enantioselective Tandem Cycloaddition/Nazarov Cyclization Reaction**

*advisor* Albert Matlin

This project in organic synthesis is an attempt to develop an enantioselective variant on F.G. West's tandem intermolecular [4+4] cycloaddition/Nazarov cyclization reaction towards keto-bridged cyclooctenes.



**Charlotte Andrews '19**  
from Laguna Beach, CA

**Major:** Biochemistry

**Minor:** Dance

**Other Interests:**

art museums, game nights, dancing, and being dramatic

**Screening of a library of serine protease inhibitors against PARL**

*advisor* William Parsons

PARL is a protease with an established role in mitochondrial maintenance and has been implicated in the pathology of neurodegenerative and metabolic diseases. I am spending Winter term optimizing a protocol to discover PARL inhibitors to further study the biology of this enzyme. I use SDS-PAGE-based assays with a PARL-reactive fluorescent probe to determine the effectiveness of candidate inhibitors in blocking PARL labeling.



**Riley Davies '19**  
*from Washington, DC*

**Major:** Chemistry

**Other Interests:**  
Several

### **Thermodynamics of Cocrystals**

*advisor* Manish Mehta

Cocrystals are substances composed of at least two distinct compounds engaged in non-covalent interactions and have properties not consistent with a standard mixture of these components. Scientists have recognized and studied cocrystals as distinct phases of matter for almost two centuries, but the popularity of this field has sharply increased in recent years, largely in the world of pharmaceuticals. The Mehta lab is currently pursuing two projects regarding the study of cocrystals.

The first project involves performing calorimetric experiments on previously identified cocrystals and their cofomers. We use bomb calorimetry to determine enthalpy of formation and differential scanning calorimetry for standard molar entropy. We will combine these data with findings from laboratory work conducted in 2016 and 2017 by students in CHEM 349 (Statistical Thermodynamics) to calculate the Gibbs energy of formation for each of the cocrystal systems under study. This project has expanded to include modification of the procedure used for Oberlin's differential scanning calorimeter to optimize efficiency and data quality.

The second project involves prospecting novel cocrystal systems composed of amino acid derivative cofomers. We are in the early stages of developing methodology, currently investigating the efficacy of gel-based crystal growth compared to our previously used methods of solvent precipitation and mechanochemistry. We are beginning our tests with derivatives of small non-polar amino acids. Characterization techniques include powder x-ray diffraction, single-crystal x-ray diffraction, and nuclear magnetic resonance spectroscopy.



**Emma Eisenbraun '19**  
*from Albany, NY*

**Major:** Chemistry & Biochemistry

**Other Interests:**  
Reading, Hiking, Cooking

### **Analysis of the Binding Affinity of DNA Aptamers to HE4 Using APCE**

*advisor* Rebecca Whelan

The survival rates for ovarian cancer are significantly improved with early detection, before metastasis has occurred. Given this relationship, the Whelan lab is working to develop novel affinity probes capable of binding to identify new ovarian cancer biomarkers. Application of such affinity probes that may enable earlier detection. The HE4 gene has been identified as more highly expressed in ovarian cancer epithelium than in noncancerous ovarian tissue. Recently, the Whelan lab has used a Systematic Evolution of Ligands by EXponential enrichment (SELEX) method involving magnetic beads to identify potential aptamers for HE4. Aptamers are single-stranded oligonucleotides that bind to a specific target molecule with high high affinity.

My current work characterizes the binding affinity of various DNA aptamers to HE4 proteins using Affinity Probe Capillary Electrophoresis (APCE). In this method, the fluorescently-labeled aptamers are incubated with the protein of interest, here HE4. The solution is then sent through a capillary through across which a voltage is applied, resulting in different migration rates of the free aptamers and aptamers-protein complexes. From this data, an isotherm can be generated and the dissociation constant (K<sub>d</sub>) of the aptamer-protein interaction can be calculated.



**Grace Ge '19**  
*from Suzhou, China*

**Major:** Chemistry

### **Find DNA Aptamer of Ovarian Cancer Biomarker by Galaxy**

*advisor* Rebecca Whelan

The Bioinformatics tool Galaxy is used to analyze the sequencing dataset resulted from performing cell-SELEX on possible DNA aptamers of MUC16. The enrichment of each aptamer over 10 rounds is calculated and compared to select best several candidates for the further study in lab. Motif analysis, clusters aptamer nucleotide analysis and G-quartet prediction may also be used to better interpret the data and the possible binding and structure properties of the selected aptamers.



**Arden Hammer '18**  
*from Thousand Oaks, CA*

**Major:** Chemistry & Biochemistry

**Other Interests:**

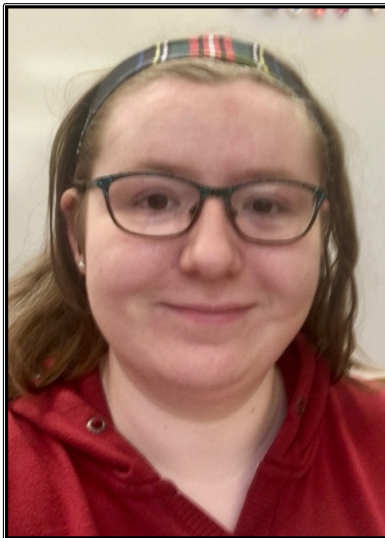
dogs, bats, geology, the sun, nice people, science puns, classical music

### **Synthesis and Structural Chemistry of Lead Oxide Carboxylates with Isomeric 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 will synthesize novel lead oxide carboxylates with isomeric 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.





**Kirsten Heuring '20**  
*from Toledo, OH*

**Major:** undeclared

### **Computational Analysis of DNA Aptamers**

*advisor Rebecca Whelan*

For my Winter Term project, I am processing data on DNA aptamers. These aptamers are single-stranded pieces of DNA which fold up on themselves and can bind with proteins. Specifically, I am looking at aptamers which bind to the HE4 protein. This protein is abundant in the bloodstream when ovarian cancer cells are in the body. I am finding which aptamers can bind to these proteins the best using an online program called Galaxy. This program specializes in bioinformatics and can process information on vast amounts of data including the massive number of aptamers used in the testing process.



**Mikaila Hoffman '18**  
*from Pittsburgh, PA*

**Major:** Chemistry  
Cognitive Science

**Other Interests:**

Getting way more books than I have time to read, painting, getting very invested in sports, Bananagrams, and crossword puzzles

### **Investigating Cocrystal Formation Mechanisms using Solid-State NMR**

*advisor Manish Mehta*

Previous work in the Mehta laboratory has tracked the formation of the caffeine and malonic acid co-crystal in situ using carbon-13 CP-MAS solid-state NMR. I am looking to build on that work and search for further mechanistic insight using similar in situ runs. My experiments will use isotopically enriched malonic acid in order to increase sensitivity. I will investigate the effect of elevated temperatures on the formation reaction, and search for evidence of a vapor or liquid phase mechanism.



**Daniel Katz '19**  
*from Washington, D.C.*

**Major:** Chemistry

**Other Interests:**  
Fishing and swing dancing

### **Analysis of Nutraceuticals Marketed to Treat BPH**

*advisor Robert Thompson*

Nutraceuticals, such as pygeum bark, are marketed to treat benign prostatic hyperplasia (BPH), but are considered “dietary supplements” and are therefore not regulated by the FDA. Several compounds found in pygeum products are thought to be effective in treatment of BPH. The Thompson lab is developing a method to determine the levels of these compounds in nutraceutical products using Liquid Chromatography–Triple Quadruple Mass Spectrometry (LC-TQMS). Once the method is complete, it will be used to analyze twelve products that claim to treat BPH in order to determine whether they actually contain the compounds of interest.



**Raif Khan '19**  
*from Dallas, TX*

**Major:** Biochemistry

**Other Interests:**  
Reading and listening to music

### **Using Computational Tools to find DNA Aptamers for Ovarian Cancer Biomarkers**

*advisor Rebecca Whelan*

Ovarian Cancer is a disease that is best treated as early as possible but is often caught after it has done severe damage to a patient. In order to catch Ovarian Cancer early we have to develop new ways of detecting cancer no matter the stage of progression it is at. One way of doing this is using DNA Aptamers that bind strongly to the biomarkers that are presented on the surface of ovarian cancer cells. Mesothelin is one such protein, and Professor Whelan and her lab have identified possible aptamers that bind to this protein, using a process called Cell SELEX. SELEX is a process by which aptamers are exposed to a protein, Mesothelin in this case, based on binding. The strong binders are amplified and run through this process a number of times. Cell SELEX is this same process, but the aptamers are exposed to live cells with the protein displayed on their surface. This process was successful but returned hundreds of gigabytes of data that was hard to make sense of. Using Galaxy Bioinformatics Suite, I am identifying possible aptamers that are especially promising binders to Mesothelin and would be useful to test in Professor Whelan's lab in future.



**Jasper Perry-Anderson '20**  
*from Philadelphia, PA*

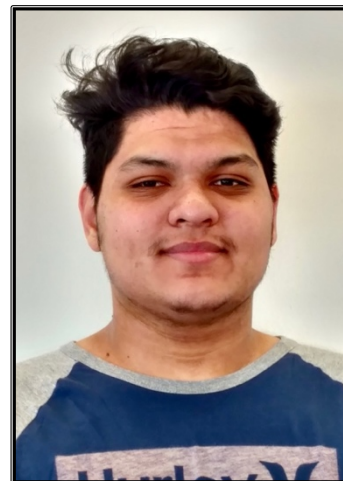
**Major:** Biochemistry

### **CA125 Aptamer Computational Identification**

*advisor* Rebecca Whelan

CA125 is a protein biomarker of ovarian cancer, and the ability to test its levels would help with diagnosis and with future research. Aptamers are small strands of DNA and RNA that can bind with high affinity and specificity to molecules of interest, including proteins. To identify aptamers, many researchers use the Systematic Evolution of Ligands by Exponential Enrichment method, a form of in-vitro evolution in which researchers alternate selection steps (separating the DNA bound to the protein from the DNA not bound to the protein) and enrichment steps (cloning the DNA bound to the protein). By starting from samples of many DNA sequences and selecting DNA that binds well to the protein of interest, researchers can identify aptamers that bind well to proteins and can thus be used to detect them in clinical applications.

In this project, I'm re-analyzing data from past research students in the Whelan lab's experiments to find more possible aptamers to test for how well they bind to CA125. High-throughput sequencing makes it possible to use different data analysis methods to identify aptamers that bind well to the protein but did not quickly become the most prevalent in the sample.



**Roberto Ramos '21**  
*from Santa Ana, CA*

**Major:** undeclared

**Other Interests:**  
Playing music, video games

### **Galaxy Aptamer Selection for HE4**

*advisor* Rebecca Whelan

Ovarian cancer is a very deadly disease that is unfortunately often not diagnosed until its late stages. The chances of long term survival after being diagnosed with ovarian cancer quickly decrease as the disease progresses. Biomarkers are biological molecules which can be used to determine the state of a biological organism. As far as ovarian cancer, the presence of certain biomarkers in a patient's body can be used to determine whether the patient has ovarian cancer. My project focuses on the protein HE4 as a potential biomarker to better detect ovarian cancer at earlier stages; previous members of the Whelan lab have gone through a process called SELEX in which aptamers (single stranded DNA) are selected with a bias for binding with HE4. I will be using an online-based bioinformatics data analyzer called Galaxy to analyze data collected by previous members of the Whelan lab. The data fed into Galaxy consists of about 7 million aptamer sequences. In the lab, the sequences underwent multiple rounds of selection in hopes of the best binding aptamers being abundant at the end of the last selection round. Using Galaxy, I will track the trends of the sequences, looking for sequences that increased in abundance with each round. At the end of my project, I hope to find a set of aptamers which greatly increased in abundance for future Whelan lab members to confirm their affinity for HE4.



**He Ren '20**  
*from Chengu, China*

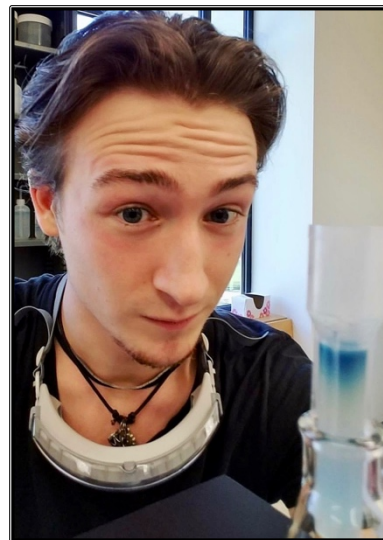
**Major:** Biochemistry

**Other Interests:**  
cooking and eating

### **Synthesis of a fluorocarbamate library for profiling reactivity across the serine hydrolase family**

*advisor William Parsons*

Serine hydrolases represent one of the largest classes of enzymes in the body and play critical roles in many physiological processes including lipid metabolism and neurotransmission. In this winter term, my goal is to start synthesizing a small library of fluorocarbamates which can be used as probes to study the reactivity of this family of enzymes and ultimately interrogate their functions.



**Daniel Russo '19**  
*from Ivoryton, CT*

**Major:** Biology

**Other Interests:**  
Drumming, the Outdoors, D&D, Frisbee

### **Developing Natural Product Isolation Protocols & Continuing HE-4 Biomarker Analysis**

*advisors William Parsons & Rebecca Whelan*

Natural product isolation experiments (the isolation of pure chemical matter from raw organic materials, such as foods) are very useful in teaching the extraction and characterization of chemicals. In order to incorporate these experiments into Oberlin's chemistry lab curriculum, I am working in Professor Parsons' lab to develop lab experiments for CHEM 205 and 327. These experiments involve isolating pure organic compounds from common household foods and spices such as cloves, oranges, cinnamon, and spinach.

I am also working in Professor Whelan's lab, continuing research on aptamers (short functional strands of oligonucleotides) for the Ovarian cancer biomarker protein HE-4. I will be testing a variety of different candidates using a technique known as fluorescence anisotropy. This involves irradiating samples of aptamer and protein with polarized light, which will emit polarized fluorescence based on how much the protein and aptamer are complexing. This measurement can be used to help determine binding affinity, showing us which aptamers are strong candidates for continued research.





**Neil Ruthen '20**  
*from Carlisle, MA*

**Major:** Biochemistry

**Other Interests:**  
Tennis, Skiing, A cappella, Alto  
Saxophone

### **Computational Analysis of DNA Aptamer Selection Data for Cancer Biomarker MUC 16**

*advisor* Rebecca Whelan

With the rise of high-throughput sequencing techniques and a multitude of companies that have automated such techniques, DNA sequencing has never been easier, faster, nor more affordable. Researchers now have the means to carry out inherently data-rich approaches but they lack the tools to analyze the resulting big data. The burden of this problem has fallen to the big data industry and computational biologists/chemists to invent new tools to handle the unprecedentedly large and complex datasets of modern research. Such are the challenges faced by the Whelan Lab with regard to its DNA aptamer datasets. Over the past six years, Dr. Whelan has advanced and carried out an aptamer selection process for finding good binders to ovarian cancer biomarkers over many rounds of enrichment and selection--producing large quantities of sequencing data that need to be analyzed. For this Winter Term, I am joining a bioinformatics team in the hopes of extracting new information from the DNA aptamer sequencing data through computational methods. Harnessing a new sequencing data manipulation platform, Galaxy, my project is to sift through the MUC 16 (an ovarian cancer biomarker) dataset for the best-binding DNA aptamers through enrichment analysis--a method to determine and compare the representation of sequences over each round of aptamer selection.



**Farzad Sarkari '21**  
*from Sugar Land, TX*

**Major:** undeclared

**Other Interests:**  
mathematics, chemistry, dance,  
music, video games, cleaning,  
shoes, cars, food, movies,  
technology, any kind of outdoor  
activities; part of the Oberlin  
Swimming and Diving Team

### **Aptamer biomarkers for OV CA**

*advisor* Rebecca Whelan

I am helping out with the data analysis part of aptamer selection process by using a powerful and user-friendly web-based tool called Galaxy Bioinformatics. I am analyzing 1 out of the 8 sets of data and the name of my set is: HE4 Magnetic SELEX Illumina (ACBKL6ANXX).





**Brendan Sheehan '18**

*from Middleton, WI*

**Major:** English, Biochemistry

### **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.



**Santino Stropoli '18**

*from Manhattan, NY*

**Major:** Chemistry &  
Violin Performance

**Other Interests:**  
classic rock-style guitar,  
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 in the southeastern United States have identified epoxide intermediates as key species in the formation of isoprene-derived SOA. Additionally, recent field work has suggested that isoprene-derived dimers constitute a significant fraction of SOA in the southeastern United States. We use nuclear magnetic resonance (NMR) techniques to study acid catalyzed oligomerization of the isoprene-derived epoxide, IEPOX-4, in order to rationalize field observations of isoprene-derived dimers.



**Andrew Sugarman '19**

*from Phoenix, MD*

**Major:** Biochemistry

**Other Interests:**

Baseball, Snowboarding, Music,  
Computers, Exercise

**Computational Structural Biology**

*advisor Zoey Hua*

Spleen Tyrosine Kinase (SYK) is a non-receptor tyrosine kinase residing in the cytoplasm of hematopoietic 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 done in VMD.



**Zachary Vaughn '20**

*from Vacaville, CA*

**Major:** Chemistry

**Other Interests:**

Tennis, hiking, contemporary art,  
Beat poetry, literature.

**Inorganic Synthesis and Characterization**

*advisor Catherine Oertel*

Ion exchange synthesis of silver niobium oxide using hydrothermal methods and powder x-ray diffraction (PXRD) characterization.



**Leo Wu '20**  
*from China*

**Major:** Chemistry

### **Metal Oxide Synthesis Research**

*advisor Catherine Oertel*

Make deuterated version of niobium and silver compound and determine its crystal structure by using powder X-ray diffraction.



**Shuangyi Xu '19**  
*from Qingdao, China*

**Major:** Biology & Biochemistry

**Other Interests:**  
reading, swimming, watching movies

### **Synthesis of a 4-haloisocoumarin library as candidate inhibitors for PARL**

*advisor William Parsons*

PARL is a serine hydrolase that is thought to play a critical role in mitochondrial maintenance as well as the pathogenesis of both type 2 diabetes and Parkinson's disease. The function of PARL is not yet well studied due to the lack of a suitable selective inhibitor. My project involves synthesizing a library of 4-haloisocoumarin compounds as candidate PARL inhibitors. To access these compounds, I will be performing metal-catalyzed coupling reactions followed by a cyclization reaction to obtain the final 4-haloisocoumarin scaffolds. The cyclized products can then be tested using competitive SDS-PAGE-based assays to determine their ability to inhibit PARL activity.





**Raul Zaorski '21**  
*from Wellesley, MA*

**Major:** undeclared

**Other Interests:**  
Clarinet and Short Track  
Speedskating

## **Using computational tools to find DNA aptamers for ovarian cancer biomarkers**

*advisor* Rebecca Whelan

Human Epididymis protein (HE4) is a protein that is used as an early biomarker for ovarian and endometrial cancer. An aptamer selection process for HE4 in the Whelan lab is currently at the step where a large dataset needs to be processed. I am using the Galaxy Bioinformatics suite—a new web-based tool designed for the purpose of examining sequence data from aptamer selection efforts—to sort through and analyze that dataset. The ultimate goal of my winter term is to determine which aptamers are worth testing in the lab.