**Carmen Azevedo 2015 From: Durham, CA**

Advisor: Robert Thompson

**Description:** The Thompson lab is working on refining experiments for instrumental analysis that are performed routinely in forensic laboratories. The goal is to produce a laboratory manual describing a set of experiments and crime scenarios for chemical analysis faculty elsewhere to use in their courses and curricula. This summer, we are working on improving and finalizing experiments for the detection of drugs in urine and characterization of bulk drug samples. Bulk drugs are powders whose identity and purity must be determined, mimicking confiscated drugs and unknown substances found on crime scenes. For the analysis of urine samples, solid phase extraction with mixed-mode chromatography isolates the analyte of interest, followed by qualitative and quantitative analysis by liquid chromatography mass spectrometry. Characteristic retention times and mass/charge ratios provide identifying characteristics of the drugs and/or their metabolites—amphetamine, methamphetamine, cocaine, benzoylcegonine, morphine, 6-acetyl morphine—and isotope labels for internal standards aid in quantification of the amount of compounds in urine. IR and Raman spectroscopy are also used to analyze bulk drugs. Characteristic absorbance peaks indicate the identities of the drugs and their cutting agents. The molar percent of the drug in the mixture can be determined by examining spectral features. Spot tests verify the identity of the drug; the presence of each drug of interest is indicated by a characteristic color change.

**Other Interests:** Studying French, hiking, cooking, running

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**Eric Bell 2015 From: Hamilton, OH**

Advisor: Jesse Rowsell

**Project: “3D Printing of Molecular Models”**

**Description:** I am currently researching different software pathways that convert crystallographic data into 3D-printing coordinates (G-Code) as well as hardware improvements to create more complex and aesthetically clean molecular models. For the software, I am currently using the Chimera suite for model editing, Netfabb Basic and Blender for modifying and verifying the 3D meshes, and Slic3r to convert meshes into G-Code. Jobs are then completed within Oberlin’s new 3D Printing Facility. I have been learning more about 3D printer functionality and maintenance during efforts to optimize print quality.

**Other Interests:** Playing horn, video games, and music production
**Project:** "Colormetric Metal Ion Binding Coatings"

**Description:** Melanin, a widely recognized biological pigment, is a prevalent but poorly understood biomolecule. Melanin and its analogs are able to bind to metals such as lead and copper, which could lead to applications in water purification and metal detection. In the past, our lab has developed metal-binding discs coated using catechols, one type of synthetic melanin analog. Upon binding, these discs produce a discernable color change. By analyzing the colorimetric properties of these discs, we are exploring the binding affinity of the catechols for a variety of metal ions. This summer we are hoping to optimize the responsiveness and selectivity of the discs for desired metals.

**Other Interests:** Likes to dance, run, and go adventuring outside of chemistry.

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**Project:** "Synthesis of Lead Oxide Carboxylate Single Crystals and Nanostructures"

**Description:** Lead oxide carboxylates are hybrid inorganic-organic compounds in which Pb^{2+} ions are coordinated by both oxide anions and carboxylate ligands. Our laboratory recently synthesized and structurally characterized several new compounds in this family containing functionalized benzoate ligands. The hybrid compounds include one-dimensional inorganic substructures based on edge-sharing Pb_4O tetrahedra, making them candidates for exfoliation into wires. The goals of this summer’s work include exploring solution processing methods to prepare lead oxide carboxylate nanostructures as well as synthesizing novel members of this family of compounds. We will characterize materials using single crystal and powder X-ray diffraction, scanning electron microscopy, and thermogravimetric analysis.

**Other Interests:** Is a member of Koreo, a hiphop dance group on campus. I also enjoy running and breakdancing.
Adam Hammer 2017  From: Thousand Oaks, CA  
Advisor: Matt Elrod

**Project:** "Nucleophilic Addition of Atmospherically Relevant Anions to Aldehydes on Secondary Organic Aerosol"

**Description:** Gas-phase aldehydes are known to be significant intermediates in atmospheric reaction pathways. Addition of polar functional groups to aldehydes is known to produce less volatile products, which may condense on secondary organic aerosol (SOA). The composition of SOA in the atmosphere has been shown to influence weather patterns and the Earth's albedo, and thus addition reactions to aldehydes are linked to the issue of global climate change. The nucleophilic hydration of aldehydes to form less volatile gem-diol products has been well studied. Recent work has suggested that nucleophiles present in the atmosphere other than water may attack carbonyl carbons. We will measure equilibrium constants and rate constants for the addition of chloride, sulfate, and nitrate to aldehydes via nuclear magnetic resonance analytical methods. This work will allow for a more detailed quantitative modelling of SOA in the atmosphere.

**Other Interests:** Enjoys hiking, soil, cute bugs, kindness, impressionism, and gender nonconformity.

Justin Kang 2015  From: Salem, OR  
Advisor: Jesse Rowsell

**Project:** Crystal Engineering with H-Acid

**Description:** I am currently pursuing the isolation of a lithium compound of the aromatic sulfonate "H-Acid", an important dye intermediate. Having successfully created other H-acid crystals with magnesium, potassium, calcium, barium, and other Groups 1 and 2 metals, the lithium crystal proves to be elusive because of its substantial solubility in water and rapid degradation. Using a variety of crystallization techniques, I hope to produce a lithium crystal large enough to collect single crystal x-ray diffraction data in order to further understand its crystal structure and compare it to those of the other compounds.

**Other Interests:** Piano, Pipe Organ, Hiking (and the general great outdoors), Food.
Project: "Design and Synthesis of Porous Molecular Crystals"

Description: The crystal structure of 1,3,5-tris(4-carboxyphenyl)benzene (tcpb) is microporous and retains its crystallinity even after solvent evaporation. The distinctive packing of tcpb that gives the molecular crystal its extrinsic porosity is largely determined by two intermolecular forces: aromatic stacking between phenyl rings and hydrogen bonding between carboxylic acids. Recent work in our group demonstrated that the crystal packing, pore volume, and surface polarity of the channels can be modified by functionalizing the central benzene ring. Current work is focused on understanding the effect of different functional groups on the crystal packing of tcpb, performing solid-state post-synthetic modifications of the new materials, and exploring potential applications in gas sorption.

Other Interests: Percussion, Running, Talking, Love Poems.

Project: “Colormetric Metal Ion Binding Coatings.”

Description: Melanin, a widely recognized biological pigment, is a prevalent but poorly understood biomolecule. Melanin and its analogs are able to bind to metals such as lead and copper, which could lead to applications in water purification and metal detection. In the past, our lab has developed metal-binding discs coated using catechols, one type of synthetic melanin analog. Upon binding, these discs produce a discernible color change. By analyzing the colorimetric properties of these discs, we are exploring the binding affinity of the catechols for a variety of metal ions. This summer we are hoping to optimize the responsiveness and selectivity of the discs for desired metals.

Other Interests: Reading, running, and watching "Doctor Who".
Sarel Loewus 2016 From: Pullman, WA
Advisor: Manish Mehta

Project: "In situ Monitoring of the Spontaneous Co-Crystallization of Caffeine and Malonic Acid using Solid State NMR"

Description: The co-crystallization of active pharmaceutical ingredients (APIs) with non-toxic co-formers has become a topic of interest in the pharmaceutical science community because it can lead to greater control over the stability and bioavailability of APIs. Traditionally pharmaceutical co-crystals have been synthesized using solvent-based approaches, solid phase grinding, or liquid-assisted grinding. However, it was recently discovered that some API-coformer combinations, such as caffeine and malonic acid, spontaneously co-crystallize when simply mixed together in stoichiometric amounts. The mechanism for this spontaneous co-crystallization is not very well understood, but it is thought to involve submerged eutectics, an amorphous intermediate, and/or deliquescence. In this project we will use 13C magic angle spinning solid state NMR to better understand the underlying mechanism of spontaneous co-crystallization. The transformation of caffeine and malonic acid into the co-crystal will be monitored in situ in an NMR rotor by a decrease in intensity of the caffeine and malonic acid resonances and an increase in intensity of the slightly shifted co-crystal resonances. Since 13C solid state NMR relies only on the chemical environment of the carbon atoms in a solid, and not whether the solid itself is crystalline, it will allow us to detect any amorphous intermediates that form during the spontaneous co-crystallization of malonic acid and caffeine.

Other Interests: Running, German, biking.

Venkata Mandala 2015 From: New Delhi, India
Advisor: Manish Mehta

Project: "Investigating spontaneous cocrystallization of pharmaceutical compounds with diacid co-formers using PXRD"

Description: Cocrystals are compounds that are composed of two or more distinct chemical species, packed in a repeating lattice that is different from the crystal structure of the individual components. Cocrystals of active pharmaceutical ingredients (APIs) and API-mimics with carboxylic diacids are of interest to the pharmaceutical industry as cocrystals can have physical and chemical properties different from the API itself. For example, cocrystallization has been shown to increase the stability and solubility of APIs, leading to favorable characteristics for developing drugs based on the API. Cocrystals can be grown from a suitable solvent by evaporation, or by mechanochemical methods such as neat and liquid-assisted grinding. In addition to these methods, caffeine (CA) and malonic acid (MA) have been found to form a cocrystal spontaneously, that is, simply upon mixing of crystals of CA and MA. Studies have shown that particle size affects the kinetics of the cocrystallization of CA and MA: smaller particles react faster. We are studying the effects of particle size, humidity, and storage vessel on the CA-MA system using powder X-ray diffraction (PXRD). Preliminary results indicate that increased humidity, smaller particles, and tighter packing enhance the rate of cocrystal formation. We are also investigating spontaneous cocrystallization in cocrystals of CA with different diacids such as oxalic acid and glutaric acid, as well as the cocrystallization of other pharmaceutical ingredients such as theophylline and nicotinamide with the same diacids. PXRD data collected shows that several other cocrystals form spontaneously at high humidity (75%RH), although kinetics and percent conversion to cocrystal vary significantly from system-to-system.

Other Interests: Playing soccer and biking.
**Conor Narovec  2015  From: Frazeysburg, OH**  
**Advisor:** Rebecca Whelan  

**Project:** "Development of a Colorimetric Assay for CA125 Cancer Biomarker Using Gold-Nanoparticles and DNA Aptamer"  
**Description:** Regular monitoring of CA125 levels is an important method in the detection and diagnosis of ovarian cancer in high risk groups. Traditional assays which rely on anti-bodies are expensive, time consuming, and possibly underrepresent CA125 levels. Single-stranded DNA aptamers, which are much less expensive and potentially more sensitive than antibodies, have been designed, using SELEX, to bind CA125. Gold nanoparticles in colloidal solution are red, but salt induced aggregation causes a color change to a dark purple. Single-stranded DNA coats nanoparticles, protecting them from aggregation, and thus preventing a color change. Using the color of a solution as a measure of aggregation, the concentration of aptamer, and thus CA125 can be inferred.  

**Other Interests:** Track, hiking, camping.

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**Claudia Nunes  2017  From: Swarthmore, PA**  
**Advisor:** Catherine Oertel  

**Project:** Ion-Exchange Synthesis and Structural Characterization of Complex Niobium and Tantalum Oxides.  
**Description:** Complex niobium and tantalum oxides are of interest for their potential as photocatalysts with applications including water-splitting. The Oertel lab has successfully hydrothermally synthesized potassium niobium and potassium tantalum oxides with the defect pyrochlore structure. This structure has the general formula $\text{A}_2\text{M}_2\text{O}_6\text{O'}$, with variable occupancy possible in both the A and O' sites. Previous work in the Oertel lab has demonstrated the potential for cation exchange at the A site under relatively mild reactive conditions. Current work seeks to carry out further cation exchange reactions in these compounds and structurally characterize the products to look for changes in the lattice parameters, site occupancies, and unit cell symmetry. Synthesis techniques include solvothermal synthesis in a Parr bomb and room-temperature ion exchange reactions. The products are characterized primarily with powder X-ray diffraction, complemented by energy dispersive spectroscopy, thermogravimetric analysis, and Fourier-transform infrared spectroscopy and with structural refinement done using the Rietveld method.  

**Other Interests:** Reading fantasy novels, watching too much TV, knitting, baking.
Jonathan Quirke 2016  From: Miami, FL  Advisor: Jason Belitsky

Description: Melanins are some of the least understood biopolymers, but they have the potential to have a significant positive impact, potentially acting as water purification tools and organic semiconductors. Of the three different kinds of melanin, the type being studied in the Belitsky lab is eumelanin, the form that gives rise to black and brown coloration in hair and skin. Currently, the Belitsky lab is carrying out a series of reactions on functionalized indoles (such as DMI or DHI), compounds that when trimerized likely emulate the characteristics of eumelanin. Unlike eumelanin, these compounds are relatively easy to work with, meaning that they function as useful analogs of the biopolymer. This reaction series will hopefully help us better understand efficient synthetic pathways for this trimerization. Specifically, we are currently working on modifications of the Suzuki-Miyaura coupling reaction, such that we achieve coupling at the desired sites on the indoles.

Other Interests: Likes collecting and playing board/card games.

Eric Rappeport 2016  From: Randolph, NJ  Advisor: Rebecca Whelan

Description: Bowerbirds are creatures endemic to southeast regions such as New Guinea and Northern Australia. They are well known for their elaborate mating displays in which a male builds a large structure (a bower) and decorates it with a variety of brightly colored objects, as well as rubbing a paste onto it. Recently, a partnered team from the University of Maryland has found a positive correlation between the interest a female expresses in the paste and the likelihood of the display being successful. My project thus focuses on the employment of gas chromatography coupled with mass spectrometry (GC-MS) to identify the primary compounds present in this paste.

Other Interests: Violin, movies and hiking.
Harry (won Hee) Ryu  2016  From: Seol, South Korea  
Advisor: Jason Belitsky

Project: "The Development of Synthetic Pathways Towards Melanin Analogs"
Description: Melanins are some of the least understood biopolymers, but they have the potential to have a significant positive impact, potentially acting as water purification tools and organic semiconductors. Of the three different kinds of melanin, the type being studied in the Belitsky lab is eumelanin, the form that gives rise to black and brown coloration in hair and skin. Currently, the Belitsky lab is carrying out a series of reactions on functionalized indoles (such as DMI or DHI), compounds that when trimerized likely emulate the characteristics of eumelanin. Unlike eumelanin, these compounds are relatively easy to work with, meaning that they function as useful analogs of the biopolymer. This reaction series will hopefully help us better understand efficient synthetic pathways for this trimerization. Specifically, we are currently working on modifications of the Suzuki-Miyaura coupling reaction, such that we achieve coupling at the desired sites on the indoles.

Other Interests: Guitar and movies. Is also a Math major.

Santino Stropoli  2018  From: Manhattan, NY  
Advisor: Matt Elrod

Project: "Nucleophilic Reactions of Amines with Epoxides on Secondary Organic Aerosol"
Description: The reactions of gas phase epoxide intermediates are known to play an important role in secondary organic aerosol (SOA) formation, and are thus linked to the issues of air pollution and global climate change. Previous work has shown that water, alcohols, sulfate, nitrate are important nucleophiles in the reactions of epoxides on SOA. Recent work has suggested that amines are also possible nucleophilic addition agents for these reactions. We will measure the rate constants for the reactions of a number of epoxides using various amines via nuclear magnetic resonance analytical methods. This work will allow for a more detailed quantitative modeling of SOA in the atmosphere.

Other Interests: I am a double degree in chemistry/music. I study violin in the conservatory, but I am also very interested in jazz guitar and flamenco ukulele.
**Will Thomas 2015  From: Cleveland, OH**  
**Advisor:** Matt Elrod  

**Project:** "Gas Phase Oxidation Kinetics and Mechanisms for Atmospherically Relevant Pinene Derivatives"  
**Description:** Pinene is the second most abundant biogenic non-methane hydrocarbon present in the atmosphere. This volatile bicyclic alkene, produced mainly by coniferous trees, undergoes gas phase reactions to form epoxide intermediates. The oxidation of α-pinene to the epoxide α-pinene oxide is related to both tropospheric ozone and secondary organic aerosol (SOA) formation, and thus linked to issues of air pollution and global climate change. We are interested in determining the mechanism and rate constants for the reactions of atmospherically relevant α-pinene aldehyde derivatives with OH radicals. Specifically, we are investigating the daytime OH radical initiated process using our lab's unique turbulent flow chemical ionization mass spectrometer (TF-CIMS). These measurements will allow a determination of the efficiency of the gas phase reactions of these α-pinene derivatives, and the role these reactions have on the production of tropospheric ozone and SOA.

**Other Interests:** Likes writing, drawing and playing various instruments.

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**Ruben Ulloa 2015  From: Chicago, IL**  
**Advisor:** Robert Thompson  

**Description:** The Thompson lab is working on refining experiments for instrumental analysis that are performed routinely in forensic laboratories. The goal is to produce a laboratory manual describing a set of experiments and crime scenarios for chemical analysis faculty elsewhere to use in their courses and curricula. This summer, we are working on improving and finalizing experiments for the detection of drugs in urine and characterization of bulk drug samples. Bulk drugs are powders whose identity and purity must be determined, mimicking confiscated drugs and unknown substances found on crime scenes. For the analysis of urine samples, solid phase extraction with mixed-mode chromatography isolates the analyte of interest, followed by qualitative and quantitative analysis by liquid chromatography mass spectrometry. Characteristic retention times and mass/charge ratios provide identifying characteristics of the drugs and/or their metabolites—amphetamine, methamphetamine, cocaine, benzoylecgonine, morphine, 6-acetylmorphine—and isotope labels for internal standards aid in quantification of the amount of compounds in urine. IR and Raman spectroscopy are also used to analyze bulk drugs. Characteristic absorbance peaks indicate the identities of the drugs and their cutting agents. The molar percent of the drug in the mixture can be determined by examining spectral features. Spot tests verify the identity of the drug; the presence of each drug of interest is indicated by a characteristic color change.
**Project:** "Chiral Channels in Molecular Co-Crystals: Unexpected Structures on the Synthetic Path to Tris(carboxyphenyl)arenes"

**Description:** Porous organic materials are unique because of the interchangeability of molecular units and functional groups that permit nanoporous crystal structure pore scaleability and specialization. 1,3,5-Tris(4-carboxyphenyl)benzene (tcpb) is a porous organic material that has connected channels that run through its crystal structure, potentially useful for gas entrapment or separation. I am synthesizing, crystallizing, and co-crystallizing synthetic intermediates of tcpb derivatives, specifically 2,4,6-tris(4-methylphenyl)pyridine and 2,4,6-tris(4-methylphenyl)pyrylium tetrafluoroborate. These intermediates were chosen to study how competitive intermolecular interactions modifies the structure. In addition to characterizing these intermediates, I am attempting to template trimesic acid crystallization using a suite of aromatic acids.

**Other Interests:** Cycling and bicycle mechanics, optical photography, cello.

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**Project:** Research Intern at Nanotech Innovations

**Description:** Synthesize carbon nano tubes on a quartz wool and combine them with melanin in order to produce a water filter.

**Other Interests:** Football and lacrosse, movies, board games and hanging out.