

REU Site: Research in Chemistry at West Virginia University

2022 Project Descriptions

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Separation-Based Characterization of Biological Therapeutics

Main faculty supervisor:

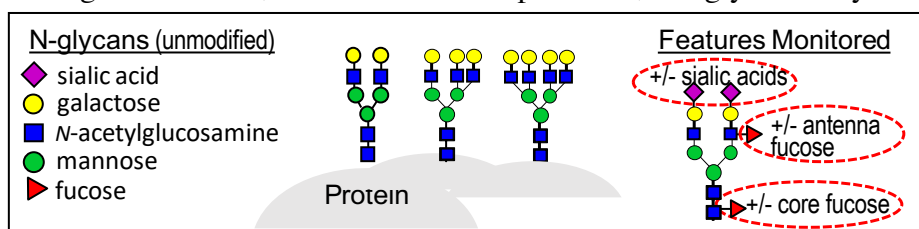
Lisa Holland (C. Eugene Bennett Department of Chemistry); <http://www.as.wvu.edu/~lholland/>

Goals of the project (for the summer)

Sequence and quantify post-translational glycosylation in an antibody therapeutic.

Project description

Biological therapeutics, which are protein-based drugs, are new and successful treatment strategies for cancer. Biotherapeutics are estimated to comprise \$125 billion of the annual global market by 2020. Glycans are post-translationally added to proteins and play critical roles in signaling and communication. Glycosylation on antibody therapeutics represent on 1.5% of the protein mass; yet, control the effectiveness of antibody-based strategies to mark cancer cells to be cleared by the immune system. Glycan analyses are challenging because the saccharide monomers that form them are structurally similar and can be combined in a wide variety of ways. Pharmaceutical manufacturers and regulators struggle to ensure that the protein glycosylation is appropriate for patented drugs and generics. Characterization of biotherapeutics through capillary electrophoresis methods benefit from small sample volume requirements, rapid analysis times, and high-resolution separations. The Holland lab has developed a novel separation additive called a nanogel to rapidly identify and quantify protein glycosylation. The student researcher will use this technique to characterize a biological drug. The research will be documented through the REU poster and will be included in a publication. The student will learn analytical figures of merit, fundamentals of separations, and glycan analyses.



Experimental/theoretical methods

- Capillary electrophoresis
- laser induced fluorescence
- glycan conjugation

Location of the project

Chemistry Research Labs (Rooms 351, 353), WVU Downtown Campus

Key references for further reading

- [1] G. Lu, L.A. Holland, Profiling the n-glycan composition of igg with lectins and capillary nanogel electrophoresis, *Anal. Chem.*, 91 (2019) 1375–1383.
- [2] Lu, C.L. Crieffield, S. Gattu, L.M. Veltri, L.A. Holland, Capillary electrophoresis separations of glycans, *Chem. Rev.*, 118 (2018) 7867–7885.

Collection of Mass Spectra to Support the Development of a New Mass-Spectral Comparison Algorithm

Main faculty supervisor

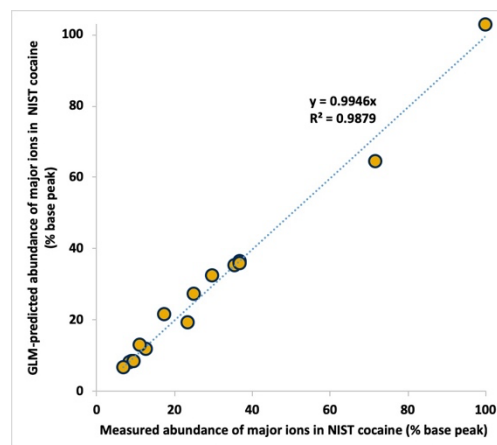
Dr. Glen P. Jackson (Forensic and Investigative Science and C. Eugene Bennett Department of Chemistry); <http://glen-jackson.eberly.wvu.edu/>

Goals of the project (for the summer)

The student will collect replicate spectra of a variety of drug standards on multiple instruments over several weeks. The student will then export the data and perform some preliminary data pre-processing to provide a suitable database of spectra for the project. This research will address a long-standing problem in forensic science in which analysts struggle to provide a level of confidence with their drug identifications. The data will be used to develop and test a new algorithm that will provide both probabilities of identifications with measures of false positive and false negative rates.

Project description

Current mass-spectral comparison algorithms attempt to provide probability-based scores for the identity of the substance providing the queried spectrum [1-3]. However, existing algorithms tend to provide a list of the closest matching spectra in a database rather than providing a probability of a certain compound. Our algorithm is different in that it accounts for non-random variance between replicate spectra and minimizes the uncertainty in ion abundance measurements. The result is that the new algorithm is far more precise than other algorithms and can enable the differentiation of stereoisomers like cocaine and pseudococaine. This project will enable a better understanding for the interpretation of evidence.



Experimental/theoretical skills that participant will acquire

- Calibration and tuning of a gas chromatography/mass spectrometer
- Sample preparation and analysis
- Data acquisition and interpretation
- Critical and analytical reasoning

Location of the project

Oglebay Hall 221 and 207, WVU Downtown Campus

Key references for further reading

- [1] F.W. McLafferty, D.A. Stauffer, S.Y. Loh, C. Wesdemiotis, Unknown Identification Using Reference Mass Spectra. Quality Evaluation of Databases, *J. Am. Soc. Mass Spectrom.* 10 (1999) 1229-1240.
- [2] S.E. Stein, D.R. Scott, Optimization and Testing of Mass Spectral Library Search Algorithms for Compound Identification, *J. Am. Soc. Mass Spectrom.* 5 (1994) 859-866.
- [3] S. Stein, Mass spectral reference libraries: an ever-expanding resource for chemical identification, *Anal. Chem.* 84(17) (2012) 7274-82.

Synthesis of Lipid Nanoparticles using Sound Waves in 3D-printed Microdevices

Main faculty supervisor

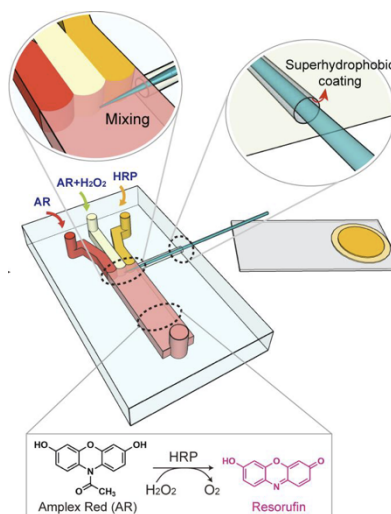
Dr. Peng Li (Assistant Professor); <https://penglab1.weebly.com/>

Goals of the project (for the summer)

The goal is to determine optimal design and operational parameters for synthesizing lipid nanoparticles. We are pursuing these specific aims: 1) Determine how the dimension of a microfluidic channel affects the size of lipid nanoparticles; and 2) Determine how the amplitude of sound waves affects the yield of nanoparticle synthesis

Project description

Lipid nanoparticles are a promising class of drug carriers for delivering biological therapeutics. It plays a critical role in efficient delivery of mRNA based COVID-19 vaccines. Despite the tremendous potential, synthesis of lipid nanoparticles still relies on traditional T-mixer with long mixing time and distance. As a result, controlling the size and loading efficiency of lipid nanoparticles is challenging. Our group has developed a highly efficient microfluidic mixer powered by high frequency sound waves, which has great potential to improve current lipid nanoparticle synthesis process. Combining sound waves with 3D printed microfluidic devices, we expect the new technology will enable precise size control of lipid nanoparticles with improved product yield, which will facilitate the further adoption and mass production of lipid nanoparticles.



Acoustic mixer in a 3D printed microchannel

Experimental/theoretical skills that participant will acquire

- Fluorescence microscopy and image processing
- Sample preparation and lipid nanoparticle synthesis
- Nanoparticle characterization techniques including dynamic light scattering and electron microscopy
- 3D printing technique and Solidworks 3D model design
- Microfluidic device operation

Location of the project

Chemistry Research Labs (Rooms 558 and 560), WVU Downtown Campus

Key references for further reading

- [1] Maeki et al., Understanding the formation mechanism of lipid nanoparticles in microfluidic devices with chaotic micromixers. Plos One, 2017, <https://doi.org/10.1371/journal.pone.0187962>
- [2] X. Li, Z. He, C. Li, P. Li, "One-step enzyme kinetics measurement in 3D printed microfluidic devices based on a high-performance single vibrating sharp-tip mixer." Anal Chim Acta. 2021, 1172, 338677.
- [3] Z. He, J. Wang, B. J. Fike, X. Li, C. Li, B. L. Mendis, P. Li "A portable droplet generation system for ultra-wide dynamic range digital PCR based on a vibrating sharp-tip capillary." Biosens Bioelectron. 2021, 191:113458. doi: 10.1016/j.bios.2021.113458.

Structure Characterization of Unique DNA and RNA Molecules

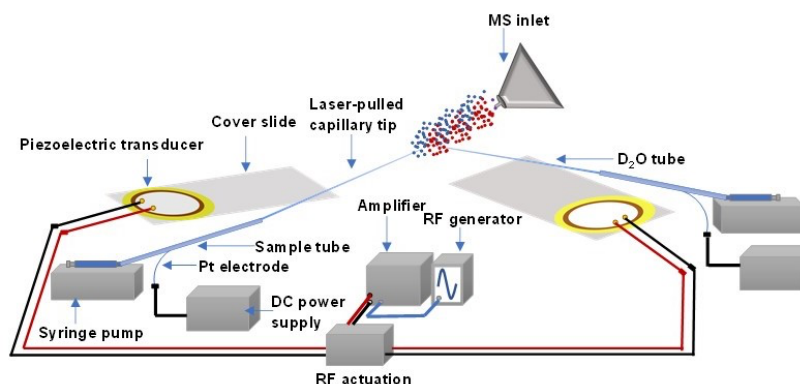
Main faculty supervisor

Dr. Stephen Valentine (C. Eugene Bennett Department of Chemistry);

<http://chemistry.wvu.edu/faculty-staff/faculty/stephen-valentine>

Goals of the project (for the summer)

We will develop tools for characterizing exotic DNA and RNA structures such as the quadruplex, i-motif, and triplex species. The tools will consist of in-droplet hydrogen deuterium exchange coupled with mass spectrometry. The summer work will focus on optimizing and testing the ion source design for DNA triplex characterization.



Schematic diagram of the Dual capillary vibrating sharp-edge spray ionization (cvSSI) setup to study DNA structures. Required component parts to perform *in-droplet* HDX-MS experiments are labeled. Briefly, droplets of analyte from aqueous samples are mixed with isotopic labeling solution (D₂O typically). Droplets coalesce and hydrogens exchange for deuteriums. The reaction is monitored by shifts in the mass of the analyte ions using mass spectrometry. Diagram is not drawn to scale

Project description

Arguably some of the least characterized biomolecular structures are exotic, non-canonical oligonucleotides. One example are DNA G-quadruplex species which are formed typically in guanine-rich tracts of DNA. Here the DNA backbone is arranged such that four guanine nucleoside bases form a planar hydrogen-bonded network termed a tetrad. Multiple, stacked tetrads stabilized by interdigitating metal ions are observed in a G-quadruplex species. These structures are important as it is believed they may provide druggable targets for diseases such as cancer. Recently we have employed a novel ionization source invented by Professor Peng Li at WVU to perform in-droplet hydrogen-deuterium exchange (HDX) as shown in the schematic diagram here. In-droplet HDX will be used to characterize these intractable (transient and/or fragile) biomolecular structures. Recent results have shown the approach is capable of distinguishing isobaric and isomeric ions by differences in reactivity.^{1,2} More recently, experiments have shown that the approach can reveal differences in reactivity for different quadruplex structures. Here, the approach will be extended to other unique oligonucleotide structures commencing with DNA triplex. Students will learn how to conduct state-of-the-art mass spectrometry measurements for examining biomolecular structure.

Experimental/theoretical skills that participant will acquire

- Analytical techniques associated with DNA sample preparation and native mass spectrometry
- Data acquisition with MS instrument
- Data manipulation and interpretation for HDX reactivity comparisons

Location of the project

Chemistry Research Labs (Rooms 381, 555, 551, and 553), WVU Downtown Campus

Key references for further reading

1. Majuta, S.; Li, C.; Jayasundara, K.; Karanji, A. K.; Attanayake, K.; Ranganathan, N.; Li, P.; Valentine, S. J. *J. Am. Soc. Mass Spectrom.* **2019**, *30*(6), 1102-1114.
2. DeBastiani, A.; Majuta, S. N.; Sharif, D.; Attanayake, K.; Li, C.; Li, P.; Valentine, S. J. *ACS Omega* **2021**, *6*(28), 18370-18382.

Atmospheric Oxidation of Conjugated Cyclic Ketones

Main faculty supervisor

Dr. Fabien Goulay (C. Eugene Bennett Department of Chemistry);

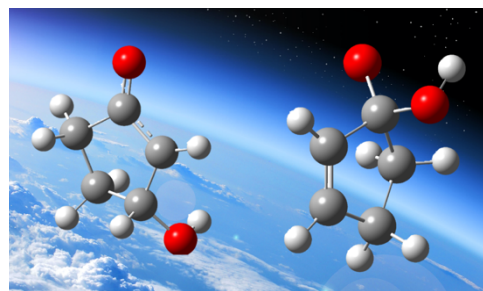
<https://fabiengoulay.faculty.wvu.edu/>

Goals of the project (for the summer)

Use laser photolysis and laser spectroscopy to measure the reaction rate coefficient of the OH radical with a series of conjugated cyclic ketones from room temperature to 700 K. The experimental data will be coupled to computational results in order to infer the most likely reaction mechanism.

Project description

Conjugated cyclic ketones are cyclic α,β -unsaturated carbonyl compounds (2-cyclopenten-1-one and 2-cyclohexen-1-one) which are formed in combustion and Earth's atmosphere from the oxidation of cyclic ketones such as cyclopentanone (C_5H_8O) and cyclohexanone ($C_6H_{10}O$). Once formed under oxidative conditions they can react with OH radicals and molecular oxygen to form peroxy radicals ($ROO\bullet$), therefore propagating the oxidation chemical scheme. However, addition of the OH radical to the β -carbon of a conjugated ketone leads to the formation of an OH-containing resonance-stabilized radical. Such radicals have enhanced stability and lower reactivity toward molecular oxygen. If the products are stabilized by resonance, the successive reaction with molecular oxygen to form the peroxy radical will be very slow, therefore halting the overall oxidation chemical scheme. Despite their expected chemical importance, the gas phase oxidation of conjugated cyclic ketones has not been investigated experimentally nor theoretically. The kinetic data coupled to computational studies will be used to infer the most likely reaction products.



Experimental/theoretical skills that participant will acquire

- Physical chemistry, developing experimental procedures
- Data acquisition and Labview programming
- Laser spectroscopy
- Vacuum techniques
- Introduction to Gaussian 16

Location of the project

Chemistry Research Labs (Rooms 473), WVU Downtown Campus

Key references for further reading

- [1] Caster, K. L.; Donnellan, Z. N.; Selby, T. M. and Goulay, F. *J. Phys. Chem. A* **2019**, *123*, 5692-5703.
- [2] Jin, H. F.; Liu, D. P.; Zou, J. B.; Hao, J. Y.; Shao, C.; Sarathy, S. M.; Farooq, A. *Combust. Flame* **2020**, *217*, 48-56.

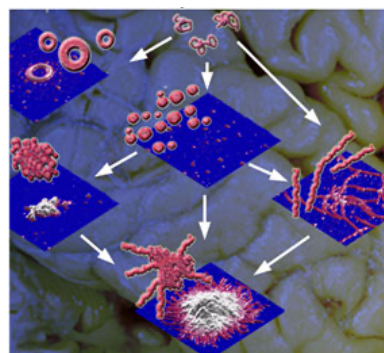
Manipulating htt Aggregation and Lipid Binding in a Model Organism as a Therapeutic Strategy

Main faculty supervisor

Dr. Justin Legleiter (Professor); <https://justinlegleiter.wixsite.com/mysite>

Goals of the project (for the summer)

The goal is to manipulate cellular interactions of huntingtin (htt) with itself and lipid membranes as a potential therapeutic strategy for Huntington's disease (HD). We recently discovered compounds that block the ability of htt to damage lipid membranes. We are interested in determining if these compounds can enhance the efficacy of traditional amyloid blocking compounds in treating neurodegeneration. We are pursuing these specific aims: 1) Determine the impact of amyloid blockers on mutant htt aggregation in a *C. elegans* model of HD; and 2) Determine if the addition of compounds that block htt/lipid binding improve the efficacy of amyloid blocker in the presence of lipids and in a *C. elegans* model of HD.



Htt protein aggregates imaged by AFM.

Project description

A common strategy in drug discovery for neurodegenerative diseases associated with protein aggregation (Alzheimer's, Parkinson's, and HD) is the development of aggregation blocking agents. However, these efforts have yet to yield an approved therapeutic. Many of the disease-related proteins directly interact with lipids, which can be targets for toxic mechanisms. As lipids promote unique aggregation pathways, many aggregation-blocking agents lose their effectiveness in the presence of membranes. Our lab has pursued a new therapeutic strategy aimed at blocking the protein/lipid interaction. Students will use a *C. elegans* model of HD to determine the impact of a variety of aggregation blocking agents on htt toxicity. To accomplish this, students will learn to culture *C. elegans* and perform viability assays, thrashing assays, and fluorescent microscopy to assess protein aggregation. They will also use scanning probe and a variety of vesicle-based assays to characterize and measure the endogenous interactions occurring between htt and membranes.

Experimental/theoretical skills that participant will acquire

- Biophysical chemistry, scanning probe microscopy, protein/peptide preparation.
- Data analysis and MatLab programming.
- Practical experience in culturing *C. elegans* and related assays.

Location of the project

Chemistry Research Labs (Rooms 251 and 556), WVU Downtown Campus

Key references for further reading

1. Beasley M., Stonebraker A.R., Hasan I., Kapp K.L., Liang B.J., Agarwal G., Groover S., Sedighi F., and Legleiter J. [Lipid Membranes Influence the Ability of Small Molecules To Inhibit Huntingtin Fibrillization](#). *Biochemistry* (2019) 58:4361-4373.
2. Adegbuyiro A., Sedighi F., Jain P., Pinti M.V., Siriwardhana C., Hollander J.M., and Legleiter J. [Mitochondrial membranes modify mutant huntingtin aggregation](#). *BBA-Biomembranes* (2021) 1863:186363.

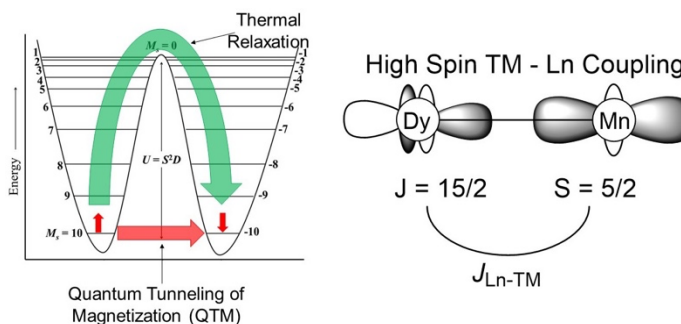
Transition Metal–Lanthanide Bonded Single Molecule Magnets Featuring High Spin Transition Metal Centers

Main faculty supervisor

Dr. Brian S. Dolinar (C. Eugene Bennett Department of Chemistry); <http://dolinar-lab.org>

Goals of the project (for the summer)

The undergraduate student will focus his/her time on the synthesis of novel metalloligands featuring a bulky amide or carbene attached to a first-row transition metal. The metalloligands will then be used to form high-spin transition metal – lanthanide bonds. If time permits, the single molecule magnetism of these compounds will be probed using SQUID magnetometry.



Project description

Single Molecule Magnets (SMMs) are molecular compounds that exhibit magnetic memory and have the potential to be utilized as magnetic bits in next generation information storage devices. SMMs are much smaller than the magnetic bits currently used in commercially available hard drives. Thus, SMMs have the potential to greatly improve storage density of information storage devices. In such molecules, magnetic anisotropy gives rise to a thermal barrier to magnetic relaxation, resulting in their magnetic memory behavior. Current, state of the art SMMs only exhibit magnet memory at cryogenic temperatures (< 80 K), limiting their commercial viability. This limitation arises largely from magnetic relaxation phenomena such as quantum tunneling of magnetization (QTM), which serves to circumvent the thermal barrier. Molecules featuring large magnetic exchange coupling offer an attractive way to combat QTM. The primary goal of this project is to develop transition metal-lanthanide SMMs that possess high degrees of magnetic exchange coupling and assess how the metal-metal bonding in these compounds influences the observed magnetic behavior of the compounds.

Experimental/theoretical skills that participant will acquire

- Organic and Inorganic synthesis
- Air-free synthetic techniques
- X-ray crystallography
- Electrochemistry

Location of the project

CRL 252, 254, 256 WVU Downtown Campus

Key references for further reading

1. Rinehart, J. D.; Long, J. R. Exploiting Single-Ion Anisotropy in the Design of f-Element Single-Molecule Magnets. *Chem. Sci.* **2011**, *2*, 2078.
2. Butovskii, M. V.; Kempe, R. Rare Earth-Metal Bonding in Molecular Compounds: Recent Advances, Challenges, and Perspectives. *New J. Chem.* **2015**, *39*, 7544.
3. Hicks, J.; Hoyer, C. E.; Moubaraki, B.; Manni, G. L.; Carter, E.; Murphy, D. M.; Murray, K. S.; Gagliardi, L.; Jones, C. A Two-Coordinate Manganese(0) Complex with an Unsupported Mn-Mg Bond: Allowing Access to Low Coordinate Homo- and Heterobimetallic Compounds. *J. Am. Chem. Soc.* **2014**, *136*, 5283.

Chemical Synthesis of Pharmacologically Active Molecules

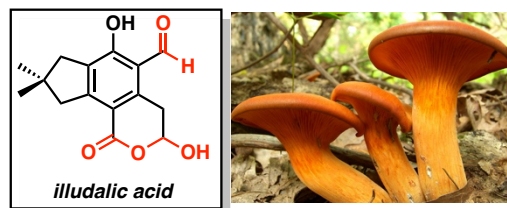
Main faculty supervisor

Dr. Gregory Dudley (C. Eugene Bennett Department of Chemistry);

<http://www.chemistry.wvu.edu/faculty-and-staff/directory/chair-and-leadership/gregory-dudley>

Goals of the project (for the summer)

Apply recent synthetic innovations from the Dudley lab to *design, prepare, and evaluate pharmacologically active compounds based on illudalic acid*, a natural product from the eastern jack o'lantern mushroom.



Project description

Our fundamental research goal is to devise, develop, and apply new ideas in organic chemistry to the efficient synthesis of interesting molecules, particularly natural products with medicinal applications. Illudalic acid is a potent and selective tyrosine phosphatase inhibitor, which has many implications for human health, but illudalic has been prohibitively difficult to make. Our lab recently validated a concise synthesis of illudalic acid and analogues. In collaboration with pharmacologists at WVU and the University of Utah, we are making and testing compounds with an eye toward improving the synthesis and pharmacology of selective phosphatase inhibitors. Students on this project will have opportunity to create new compounds, evaluate activity in various pharmacological assays, and then design new compounds based on their initial data.

Experimental/theoretical skills that participant will acquire

- Synthesis of organic and inorganic molecules
- Manipulation of air-sensitive materials
- Purification and separation of chemical mixtures
- Characterization of compounds by modern analytical methods
- Review of pharmacological data and effects
- Experimental design and scientific method

Location of the project

Chemistry Research Labs (Rooms 358 and 360), WVU Downtown Campus

Key references for further reading

- [1] Gaston, R., Jr.; Geldenhuys, W. J.; Dudley, G. B. Synthesis of illudinine from dimedone and identification of activity as a monoamine oxidase inhibitor. *J. Org. Chem.* **2020**, *85*, 13429–13437.
- [2] Tavakoli, A.; Dudley, G. B. Synthesis of 4,4-dimethyl-1,6-heptadiyne and alcyopterosin O. *Org. Lett.* **2020**, *22*, 8947–8951.
- [3] Fulo, H. F.; Rueb, N. J.; Gaston, R., Jr.; Batsomboon, P.; Ahmed, K. T.; Barrios, A. M.; Dudley, G. B. Synthesis of illudalic acid and analogous phosphatase inhibitors. *Org. Biomol. Chem.* **2021**, *19*, 10596–10600.

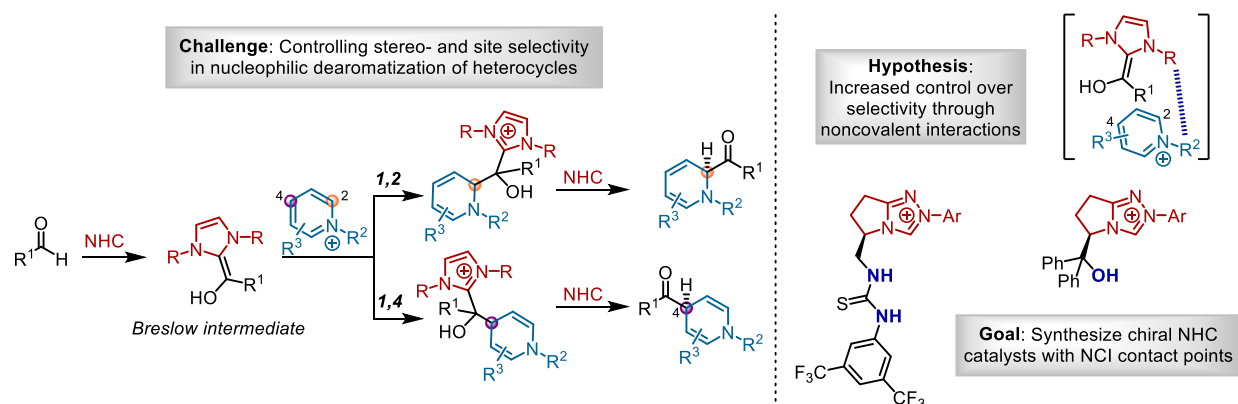
Development of Chiral NHC Catalysts for Nucleophilic Dearomatization of Heterocycles

Main faculty supervisor

Dr. Margaret Hilton (C. Eugene Bennett Department of Chemistry); www.mjhiltonlab.com

Goals of the project (for the summer)

Synthesize chiral NHC catalysts for the nucleophilic dearomatization of heterocycles.



Project description

The subtle power of noncovalent interactions (NCIs) to direct organic and organometallic transformations has been recognized for many years. Even though the community's understanding of these interactions has increased significantly, the a priori, intentional incorporation of NCIs into ligand and catalyst designs for control in the secondary sphere remains challenging. In order to study NCIs as design elements, the nucleophilic dearomatization of heterocycles, specifically pyridines, is proposed as a suitable setting, since i) pyridine derivatives are prevalent, valuable synthetic intermediates and end-products in organic chemistry, and ii) their enantio- and regioselective syntheses remains difficult. Thus, this project will *explore the influence of NCIs on selectivity issues in pyridine dearomatization via NHC catalyst development*.

Experimental/theoretical skills that participant will acquire

- Synthesis and purification of organic and inorganic molecules
- Manipulation of air-sensitive materials
- Characterization of compounds (NMR and HPLC)

Location of the project

Chemistry Research Labs (Rooms 362 and 373), WVU Downtown Campus

Key references for further reading

- [1] Flanigan, D. M., Rovis, T. *Chem. Sci.* **2017**, *8*, 6566.
- [2] Di Carmine, G., Ragno, D., Bortolini, O., Giovannini, P. P., Mazzanti, A., Massi, A., Fogagnolo, M. J. *Org. Chem.* **2018**, *83*, 2050.

Decarboxylation Reactions of Heteroaromatic Carboxylates

Main faculty supervisor

Dr. Jessica Hoover (C. Eugene Bennett Department of Chemistry);

<https://www.chemistry.wvu.edu/directory/associate-professor/jessica-hoover> and

<https://www.hooverlab.org/>

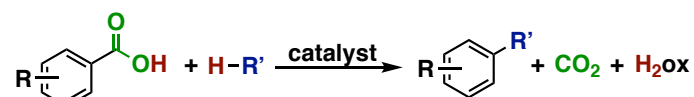
Goals of the project (for the summer)

We will explore the reactivity of heteroaromatic carboxylates in decarboxylation reactions through the synthesis and reactivity studies of well-defined metal-carboxylate complexes.

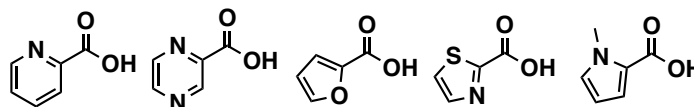
Project description

Our research focuses on the development and understanding of new catalytic methods for organic synthesis. Catalytic reactions are becoming more commonly used in the synthesis of complex structures - pharmaceutical molecules (medicines), polymers (plastics, clothing) and fuels - among others. In particular, our group has been interested in developing and understanding catalytic oxidative decarboxylative coupling reactions (Scheme a, below). These are reactions in which simple benzoic acids can be used as coupling partners to generate substituted arenes after the loss of CO₂. While substituted benzoic acids are efficient coupling partners in these reactions, the analogous reactions of heteroaromatic carboxylic acids are often challenging and poorly understood (Scheme b). Overcoming this limitation is important for the synthesis of medicinal compounds because heteroarenes are key structures in pharmaceuticals and biologically active molecules.

(a) Oxidative Decarboxylative Coupling Reaction of Benzoic Acids



(b) Select Heteroaromatic Carboxylic Acids for Decarboxylation



In this project, students will explore the decarboxylation reactivity of heteroaromatic carboxylic acids with the long-term goal of improving their cross-coupling reactivity. Students will synthesize metal-carboxylate complexes (coordination chemistry), monitor their decarboxylation reactions (NMR spectroscopy, HPLC analysis, reaction kinetics), and probe their reactivity in cross-coupling reactions (organic synthesis, catalysis).

Experimental/theoretical skills that participant will acquire

- Air-free synthetic methods such as Schlenk and glovebox techniques
- Spectroscopy (including ¹H and ¹³C NMR, IR, and mass spectrometry)
- Synthetic organic chemistry skills (including basic reaction set-up and workup procedures, TLC analysis, column chromatography, HPLC analysis, etc.)

Location of the project

Chemistry Research Labs (Rooms 550 and 583), WVU Downtown Campus

Key references for further reading

[1] A. P. Honeycutt, J. M. Hoover *ACS Catal.* **2017**, 7, 4596-4601.

[2] R. A. Crovak, J. M. Hoover *J. Am. Chem. Soc.* **2018**, 140, 2434-2437.

Difunctionalization of Alkenes with Boron and CO₂

Main faculty supervisor

Dr. Brian Popp (C. Eugene Bennett Department of Chemistry);

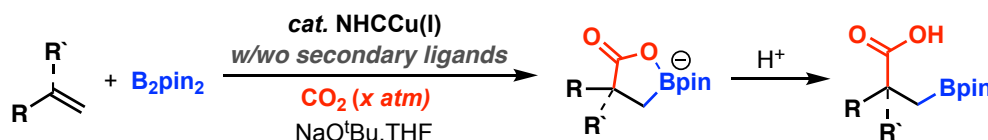
<http://community.wvu.edu/~bvpoppp/index.html>

Goals of the project (for the summer)

Prepare new highly functionalized organic molecules using homogeneous copper-catalysis.

Project description

Homogeneous transition-metal-catalyzed processes have supplied significant inspiration for the synthesis of many natural products and serve as methods to produce chemical feedstocks for nearly all consumer goods produced today. Unsaturated hydrocarbons, a byproduct of the catalytic cracking of petroleum, provide a route for the installation of functional groups that are more useful precursors to the synthetic community. Carbon dioxide (CO₂) also represents an important but underutilized chemical feedstock.¹ In 2016, we reported the first method to achieve 1,2-borylative-carboxylation (boracarboxylation) of an alkene (vinyl arene).² The mild method uses redox-neutral NHC-copper(I) catalysis and a single atmosphere of CO₂ to obtain boron-functionalized α -aryl carboxylic acids, including novel functionalized non-steroidal anti-inflammatory drugs (NSAIDs) such as bora-ibuprofen and bora-naproxen. The products can be further elaborated through a variety of reactions at the C–B bond. The participating student will join ongoing efforts to develop and expand boracarboxylation methodologies and/or downstream reactions.^{3,4}



Experimental/theoretical skills that the participant will acquire

- Learn standard techniques in synthetic chemistry (eg., column chromatography, extraction);
- Manipulate and isolate sensitive compounds and reactions (eg., work in a glovebox);
- Apply the fundamentals of organometallic chemistry and catalysis;
- Assess and critically interpret data (eg., NMR, IR, UV-vis spectroscopy and MS spectrometry);
- Develop useful teamwork, communication, and interpersonal laboratory skills.

Location of the project

Chemistry Research Labs (Rooms 453, 455, 462), WVU Downtown Campus

Key references for further reading

- [1] Liu, Q.; Wu, L.; Jackstell, R.; Beller, M. *Nat. Commun.* **2014**, *6*, 1.
- [2] Butcher, T. W.; McClain, E. J.; Hamilton, T. G.; Perrone, T. M.; Kroner, K. M.; Donohoe, G. C.; Akhmedov, N. G.; Petersen, J. L.; Popp, B. V. *Org. Lett.* **2016**, *18*, 6428.
- [3] Knowlden, S. W.; Popp, B. V. *ChemRxiv* **2022**; DOI: 10.26434/chemrxiv-2022-t31fm.
- [4] Baughman, N. N.; Akhmedov, N. G.; Petersen, J. L.; Popp, B. V. *Organometallics* **2021**, *40*, 23.