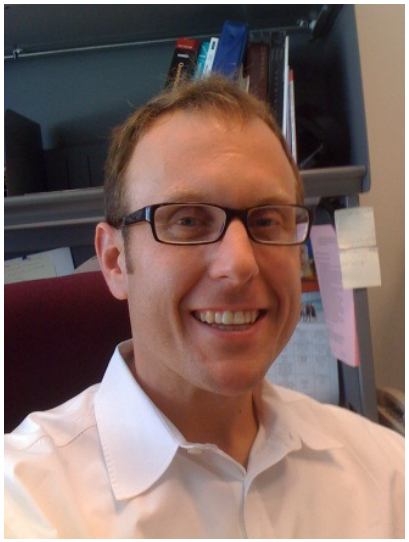
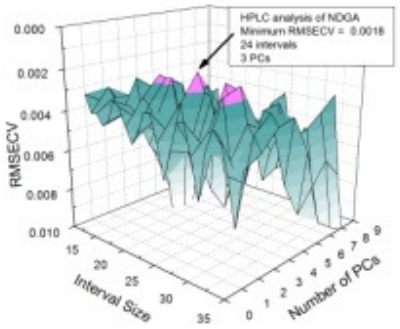
Dr. Robert D. Luttrell – Analytical Chemistry



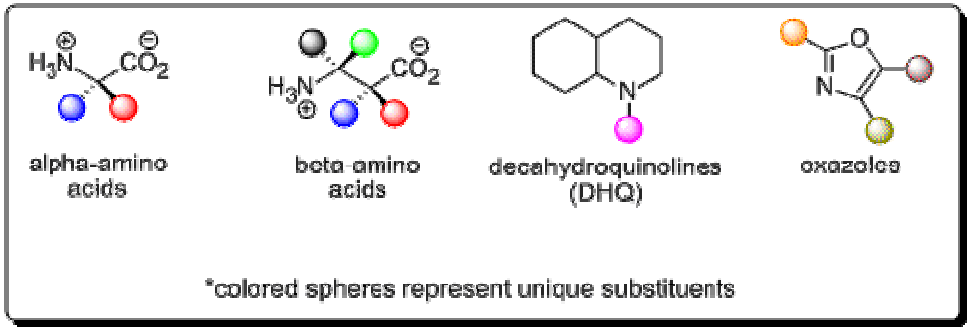
My students and I develop new computational methods to improve the understanding of information obtained from chemical instrumentation. This interdisciplinary field of chemistry, known as chemometrics, is an exciting blend of chemistry, mathematics, and computer science. Currently, we are working on a project which enhances the quantitative analysis of high performance liquid chromatography (HPLC) data.



The figure on the right is a 3-dimensional error surface which is used for optimizing the stacked principal component regression analysis (SPCR) of the HPLC data acquired for the biochemical molecule, NDGA.

Dr. Stephen A. Habay – Organic Chemistry

In my laboratory we are interested in designing new and efficient chemical reactions for the purpose of making important organic building blocks that can be used as pharmaceuticals or molecular tools for biology. In particular, we are interested in making molecules that interact with the brain and can be used to study sleep and anxiety disorders. My research students will learn how to safely perform



Dr. Fredrick Kundell – Physical/Computational Chemistry

For the last eight years I have been using computational chemistry to examine the origin of life on Earth. This work led to an article entitled “A suggested Pioneer Organism for the Wachershauser Origin of life Hypothesisi” published online in the journal “Origin of Life and Evolution of Biospheres” during the Spring of 2010. This article suggests that an initial RNA was formed on the growing edge of small pyrite crystals. The next step in this project is the computational examination of a growing pyrite crystal surface as a catalytic source for other biologically important compounds.

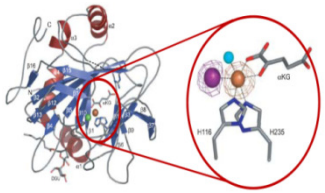
Dr. Ed Senkbeil – Biochemistry/Chemical Education

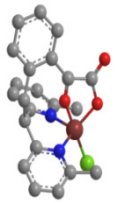
My students and I are developing a Chemistry Outreach Program for the surrounding area. Science students who participate will learn to perform numerous chemical demonstrations and "hands-on" activities. Our goal is for students and audience alike to gain a deeper appreciation of science / chemistry, while still having FUN!! Students will develop a variety of knowledge skills including selection of demonstrations, understanding of the relevant chemistry of the demonstrations, practical knowledge of the chemicals used with an emphasis on safety and disposal, mechanics of performing the demonstration, and reflection / assessment of the effectiveness of the demonstration.

Dr. Seth Friese – Organic Chemistry

My research is centered around designing new molecules and ligands that can be used to help us answer interesting chemical questions. For example, one project is inspired by the halogenase enzyme SyrB2. The new molecules that we make will be used as model complexes of SyrB2. By studying the reactivity of these new complexes we hope to learn about how this reaction works and the chemical characteristics of intermediates. Alternatively, we are also investigating how we can use ligands to increase the separation efficiency of environmentally relevant metals.

Pictures on the right show the active site of SyrB2 and the target model complex we are pursuing.

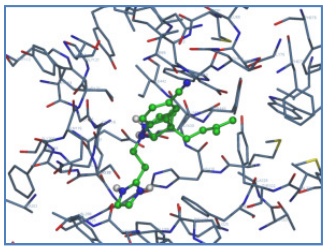




Dr. Miguel O. Mitchell – Organic Chemistry

In my research lab, we invent new medicinal agents with the potential to treat a variety of diseases: tuberculosis, various drug-resistant bacterial infections, Alzheimer's disease, and cancer. We also discover new chemical reactions that can help chemists be better molecular engineers, making compounds more efficiently and with less environmental impact. Students combine both organic chemistry, creating compounds from scratch, with biological or biochemical testing, seeing first hand if their compounds work to kill bacteria, stop cancer cell replication, or inhibit a dangerous enzyme.

The figure on the right shows a potential inhibitor (in green for carbon, blue for nitrogen, and white for hydrogens) docking by computer simulation into the active site of human butyrylcholinesterase (BChE), one of the enzymes whose activity is responsible for memory loss in Alzheimer's disease. In the future, inhibitors like this one could lead to better treatments for Alzheimer's disease.



Dr. Anita Brown – Physical/Computational Chemistry

Have you ever wondered why two molecules might "stick together?" or whether a molecule would prefer to "hang out" with one substance over another? If so, then you may be interested in computational chemistry research with Dr. Brown. Using computer programs, we build models of individual molecules. Then we use principles of physics to predict how those molecules will behave. Currently Dr. Brown's group is investigating pi-pi and pi-cation interactions in biomolecular systems. One of these projects involves the possible inhibition of an enzyme in tuberculosis.