Chemistry Research

The chemistry department values active student participation in original research projects. Here are some of the many research areas in which our faculty are involved.

Salisbury UNIVERSITY

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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 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 involved in tuberculosis infections.

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Dr. Alison Dewald • Biochemistry

One project in the Dewald lab focuses on the folding of outer membrane proteins into liposomes. Outer membrane proteins are found in many bacteria, chloroplasts and mitochondria. They play an important role in pathogenesis, but are incredibly difficult to study because they must first be "folded" into something resembling a cell membrane. This project aims to streamline the study of membrane proteins by identifying protein and environmental characteristics that facilitate folding. A second project is to test and characterize the function of novel proteins whose three-dimensional structures have been determined. Some proteins are predicted to have a specific enzymatic function based on their similarity to other, known, enzymes. The Dewald lab uses bioinformatics to make such predictions then classic biochemistry to study the enzyme's function.

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Dr. Seth Friese • Organic Chemistry

Research in Dr. Friese's lab is centered on designing and making new molecules and ligands that can be used to help answer interesting chemical questions. One area of study that has important implications in the nuclear energy cycle has students making novel N-donor ligands that will be tested for their separation selectivity and efficiency of Ln/An ions. A second project has students working on an alternative method for the synthesis of compounds which contain the dihydroisobenzofuran substructure using an intramolecular cyclization reaction. These students are currently exploring the versatility of this method in order to adapt this new cyclization to the making of natural products, with special interests toward a recently isolated natural product, pestacin.

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Dr. Stephen A. Habay • Organic Chemistry

Students in Dr. Habay's laboratory are designing new and efficient chemical reactions used to produce important organic molecules used in the construction of pharmaceuticals and molecular tools for biology. In one project, Dr. Habay's students have developed a new ring-forming reaction that will be used to produce thrombin inhibitors, thereby preventing platelet aggregation and blood clotting. In a more recent project, students discovered a new chemical process to produce building blocks useful in the production of a variety of polymers and non-natural amino acids. Students in Dr. Habay's laboratory work as molecular architects, designing and building molecules from smaller chemical fragments. Applying principles of organic chemistry from the classroom, students use advanced laboratory techniques and collaborative problem solving to build better molecules more quickly and efficiently.

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Dr. Jose Juncosa • Organic/Medicinal Chemistry

Dr. Juncosa and his students work in the area of medicinal chemistry. In general, they try to do one of three things: produce new drug candidates for treatment of disease, improve on current treatments for disease or find new ways to treat a disease. In particular, their research focuses on neurotransmitters, specifically dopamine, serotonin and D-serine. Dr. Juncosa's students aim to create molecules that can mimic the neurotransmitters' normal function, but only in specific conditions or with specific results. For example, their goal with serotonin is to create molecules that can differentiate between learning and hallucinations caused by activating the serotonin 2A receptor, whereas with D-serine, they want to halt its production so that neurons don't die from unneeded overactivity. For this purpose, they use computer simulations to design molecules, which they then synthesize in our lab; once they get test results for them, they improve their models and repeat the process until their goal is met.

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Dr. David Keifer • Analytical Chemistry

Dr. Keifer and his students do mass spectrometry-related simulations. Currently, we simulate the charging behavior of nanoparticles, proteins and even viruses that are analyzed by mass spectrometry (MS). In a typical MS experiment, an analyte is launched into the gas phase and picks up a bunch of charges, and its mass-to-charge ratio (*m/z*) is measured so its mass can be figured out. But Dr. Keifer believes that the more information you can get out of one measurement, the better, so by simulating how these analytes pick up charge as a function of their shape and size, we can use the z part of the *m/z* measurement to learn more about these analytes. Students working with Dr. Keifer not only get to learn about MS, they also will learn the invaluable skill of programming.

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Dr. Robert D. Luttrell • Analytical Chemistry

Dr. Luttrell and his students develop and apply new computational methods that improve the understanding of data generated by chemical instrumentation. This interdisciplinary field of analytical chemistry, known as chemometrics, is an exciting blend of chemistry, mathematics and computer programming. Dr. Luttrell's group is involved in several chemometrics-based research projects. Currently, they are analyzing complex infrared spectra using innovative regression fusion techniques. Regression fusion allows us to determine which sections of the spectra are more strongly related to analyte concentration. By placing additional emphasis on these sections, they are able to decrease the error associated with the final quantitative results. Their next goal is to apply "Moving Window" regression fusion to further improve these results.

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Dr. Katherine Miller • Biochemistry

Research in Dr. Miller's lab focuses on the analyzing the diversity of microbial communities in wetlands in an effort to understand how various wetland functions such as denitrification are influenced by anthropomorphic and environmental factors. Influences such as sample depth, season, geographic location and nearby land use can impact microbial communities. By extracting microbial DNA and RNA, and using DNA fingerprinting, gene cloning and DNA sequencing techniques, students in Dr. Miller's lab can analyze the genetic diversity of a community as well as determine which of these genes are expressed under the sampling conditions.

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Dr. Joshua Sokoloski • Biochemistry

Research in Dr. Sokoloski's lab involves studying structure-function relationships in protein-nucleic acid interactions and developing new biophysical tools and techniques to monitor these interactions. The primary projects Dr. Sokoloski is pursuing now involve using fluorescent dyes to detect and monitor changes in protein-nucleic acid binding as well as to measure the uptake or release of Mg2+ ions during formation of protein-nucleic acid complexes. Future projects will include exploring the role of protein-protein interactions in regulating the functions of helicases, key enzymes involved in DNA replication, recombination and repair. Students in Dr. Sokoloski's lab will learn basic molecular biology and biochemical techniques in addition to learning about fluorescence measurements in biology and chemistry.

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