



The CD Has Arrived in the X-Ray Facility

The Jasco 1500 CD spectrometer has been installed in the X-Ray Facility and is ready to use. The instrument has several configurations including, but not limited to:



- A temperature and mixing Peltier unit
- A diffuse reflectance sphere for solids
- A titration unit
- A micro-sampling disk
- A micro-capillary holder

Sign up for training on ChemFOM to learn how to use the CD for your research needs. Instrument rates are \$12.50/hr.

Microanalysis WORKSHOP

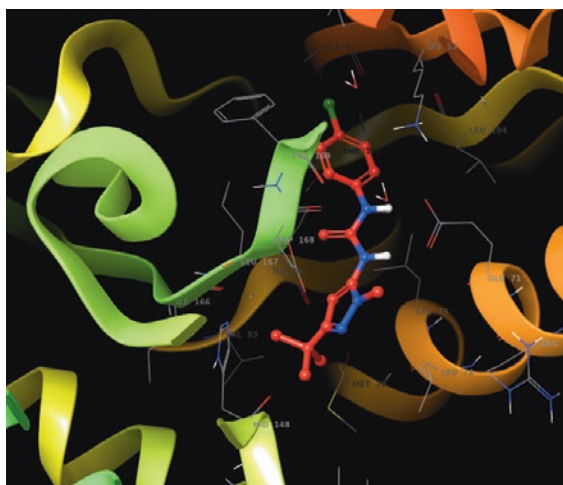
August 8 - 10

The Microanalysis Lab is holding a workshop on ICP analysis from August 8-10. This 3 day workshop will cover the fundamental principles, sample preparation, data collection, and data analysis for both ICP OES and MS techniques. The cost of the workshop will be \$40.28/person. If you are interested, contact Ashley Blystone (blystone@illinois.edu) for details and to sign up.

Please sign up by July 15, 2022

Note: a minimum of 4 students are necessary for the workshop to run.

COMING SOON: High-throughput Virtual Screening (HTVS)!



We are excited to announce that High-Throughput Screening Facility (HTSF) is planning to provide a virtual screening service to its users starting this summer. This will be a complementary approach to our conventional high-throughput screening service that utilizes physical collections of over 275,000 small molecules. Virtual screening taps into the large unused potential of synthetically feasible small molecules to enable users explore the chemical space currently inaccessible to experimental screening at a fraction of the cost and screen time. With billions of make-on-demand molecules available, the sheer size and diversity offered in virtual screening is unparalleled. We are planning to offer both structure-based and ligand-based virtual screening approaches for structure-determined and undetermined targets, respectively. The main methods employed will include docking with active learning, GPU shape screens and post-screening computational approaches such as Free Energy Prediction (FEP). While a crystal structure of the target is preferable for structure-based virtual screening, computationally predicted structures which have advanced considerably in recent years will also do. Users seeking to obtain hits for their targets of interest can discuss their virtual screening needs with HTSF. More updates on this will be forthcoming!



Meet the Newest Member of Electronic Services

Please join me in welcoming Dan Birge to the SCS. Dan is working in Electronic Services and will be developing a pump maintenance program over the next several months so be on the lookout for his emails. Some of you may have already heard from him to come and pick up a Welch 1400. - Danielle Gray