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Meet the Staff

Goodbye 2021... Hello 2022!

2021 is soon coming to an end and with the first semester back on campus wrapping up, it has been great to see new and old faces more regularly these past few months. Good luck to all in the next few weeks as you finish up your semester and get ready for the holiday season.

The Shared Instrumentation Facility will be open for you to use during the holiday break between December 24th, 2021, to January 3rd, 2022 provided you have building access. A staff member might be on site briefly for required weekly system maintenance, but assistance and training will not be available during this time period. If you plan on working during the holiday break, think ahead and obtain the necessary instrument training if needed.

Stay safe and healthy everyone! Relax and enjoy your well deserved break.

Dr. Chin Lin, Dr. Chunhua Hu,
Dr. Trinanjana Mandal, and Dr. Joel Tang
It has been a VERY long wait, but the Bruker 500 NMR spectrometer in Brown 353A was finally upgraded this past September. The system now boasts a new AVANCE NEO console with new technology that enhances your NMR experience. The system is equipped with a 5mm X-Optimized Double Resonance Cryo Probe for high sensitivity, a 60 position autosampler for high throughput analysis, and a low temperature accessory that can cool sample temperatures to approximately 0°C.

The Bruker ELEXSYS E500 EPR spectrometer was also upgraded this past October to accommodate transient (trEPR) experiments in addition to standard continuous wave (CW-EPR) experiments. trEPR is a continuous-wave EPR method where photoexcited paramagnetic species, such as molecular multiplet states and radical pairs, are examined in a time-resolved manner following pulsed laser excitation. Kinetic information on a nanosecond timescale and longer can be determined, unperturbed by any spectrometer dead time. The upgrade included the addition of a Flexline splitting probe and cryostat, improved SuperX FT-EPR microwave bridge, and a ColdEdge Stinger cryogen-free low temperature system.

The Bruker AVANCE III 400 NMR spectrometer located in Brown 252 was also upgraded in October to add a three channel gradient amplifier and a 5mm broadband+19F double resonance probe with XYZ gradients. This setup will allow users to apply gradients along the XYZ directions of a sample and can be used in experiments such as 3D microimaging or diffusion studies.
The TA Instrument Nano Differential Scanning Calorimeter (Nano-DSC) is designed to characterize the molecular stability of biomolecules in solution with very low concentration. This instrument uses the innovative capillary design which attenuates the onset of sample aggregation until after unfolding is complete. The system has an active cell volume of 300 µL, typically requiring 450-600 µL sample volume. As little as 2 µg of protein can be analyzed and still be able to obtain quantitative results. Solid-state thermoelectric elements are used to precisely control temperature and a built-in precision linear actuator maintains constant or controlled variable pressure in the cell. The scanning temperature range is from -10 °C to 130 °C with a scan rate of 0.001 °C to 2 °C/min.

The Nano low volume isothermal titration calorimeter (ITC) provides maximum sensitivity and flexibility to study biomolecular binding. Protein-ligand binding constants are critical to understand protein structure and function.

Solid state thermoelectric heating and cooling systems are used to precisely control temperature and flexible injection syringe assemblies provide efficient and accurate delivery of titrant. True instrument’s sensitivity and flexibility for an ultrasensitive ITC analysis of biological samples in-solution.

The scanning temperature range is from 2°C to 80°C with a minimum detectable heat of 0.05 µJ and a maximum measurable heat of 5000 µJ. The active cell volume is around 190 µL and the minimum injection volume is 0.06 µL. The low volume reduces the amount of time required to complete a titration by as much as 50% while using 80% less sample. The 2X improved sensitivity versus standard volumes will generate accurate and reproducible results.
Software and Video Resources

There are six different workstations located throughout the SIF which are setup to process and analyze your data after it has been acquired. This is to free up time on the instrument computers. Listed below are the locations of the workstations and the available software:

<table>
<thead>
<tr>
<th>Workstation</th>
<th>Location</th>
<th>Software</th>
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</thead>
<tbody>
<tr>
<td>1</td>
<td>Brown 357 (next to 800 NMR)</td>
<td>• MestreNova 10 (NMR and MS) • Topspin 3.5 (NMR) • OMNIC 8.3 (FTIR) • Zetasizer 7.11 • TQ Analyst 8.5</td>
</tr>
<tr>
<td>2</td>
<td>Silver 720 (next to LCMS-SQ)</td>
<td>• MestreNova 14 (NMR and MS) • Topspin 3.5 (NMR) • FreeStyle 1.6 (MS) • OpenLab ChemStation C.01.07 offline (MS)</td>
</tr>
<tr>
<td>3</td>
<td>Silver 714</td>
<td>• MestreNova 14 (NMR and MS) • Topspin 3.5 (NMR) • ChemOffice 2004</td>
</tr>
<tr>
<td>4</td>
<td>Silver 720 (next to LC-TOF)</td>
<td>• FlexAnalysis 3.4 (MALDI) • Agilent MassHunter Qualitative Analysis B.03.01 (LC-TOF)</td>
</tr>
<tr>
<td>5</td>
<td>Brown 357 (in front of 357C)</td>
<td>• MestreNova 14 (NMR) • Topspin 3.5 (NMR)</td>
</tr>
<tr>
<td>6</td>
<td>Silver 720 (end of LCMS-TSQ workbench)</td>
<td>• MestreNova 14 (NMR and MS) • Topspin 3.5 (NMR) • SoftMaxPro 5.4.6 (FlexStation) • TA NanoAnalyze 3.4 (ITC/DSC) • OMNIC for Dispersive Raman (Raman) • ChemOffice 2004 • Origin Pro 2015</td>
</tr>
</tbody>
</table>

We also have MestreNova licenses for processing and spectra prediction available for purchase. This can be used on your lab/office/personal computers to analyze NMR data. Due to limited number of licenses, these are only available for Department of Chemistry users. Contact Dr. Joel Tang for more details.

If you are unable to come and use one of our workstations, the SIF website also provides a list of software for NMR, MS and optical spectroscopy analysis that can be downloaded and installed on your personal computers. Most of the software listed are FREE!

Need a refresher on how to use one of the instruments? On the SIF website, there are a series of videos that demonstrate how to acquire and process data for many of the instruments. NOTE: These are not to be used in lieu of training. For proper training and access to the instruments, contact one of SIF staff members.
Dr. Chin Lin has been the Director of the Shared Instrumentation Facility since 2001. Initially having a background in biological NMR spectroscopy, Dr. Lin has built-up his scientific knowledge through the various instrumentation upgrades and acquisitions over the years. He is very knowledgeable on the variety of instruments in the SIF and their capabilities. He is a valuable asset to the department and can be extremely helpful with your research.

Find out more about Dr. Lin at: [LinkedIn] [ResearchGate]

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In the Shared Instrumentation Facility, we are fortunate enough to have many top of the line scientific research instruments available for our community to use. Over the years there have been some interesting and groundbreaking results discovered using the SIF instruments. To help demonstrate the capabilities of these instruments, we would like to start featuring the spectra/images/results that you have acquired here. If you would like to share any published data that is interesting or demonstrates the unique capabilities of the instruments in the SIF please contact Dr. Joel Tang and it will be highlighted in a future newsletter.

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We are here to help. Feel free to contact us if you have any questions.

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