2021-2022 school year has begun and we want to welcome all the new undergraduate, graduate and postdoc researchers that have started their new tenure at NYU. Come by and introduce yourself to the SIF staff. We are here to help enhance your research using the instruments we have available for you to use.

Please don’t mind the mess around the SIF. We are in the middle of a series of upgrades and installations that have been delayed or difficult to schedule due to the pandemic. As well as room shuffling of some of the instruments. We are trying our best to get these resolved as quick as possible and hope it will not disrupt the workflow of the facility too much. Let us know of any questions or concerns.

Now that we have students back to in-person learning, research labs are at full capacity and campus activities begin to increase, we should still be mindful of everyone’s well-being. Stay safe and healthy everyone!

Dr. Chin Lin, Dr. Chunhua Hu,
Dr. Trinanjana Mandal, and Dr. Joel Tang
Facility Update: Solid-State NMR

Have you ever wondered about certain characteristics or properties of your compound as a solid? Did you ever want to analyze your compound using NMR spectroscopy but is not soluble in any solvent? Well now you can with the newly installed solid-state NMR (SSNMR) probe on the 800 MHz NMR spectrometer located in Brown 353A.

SSNMR is used in various scientific fields such as chemistry and materials science, biology and even art conservatory. In addition to structure elucidation, other analyses include chemical composition, local motions, kinetics, porosity and molecular level interfacing.

In solution, molecules randomly tumble and produce narrow lines in an NMR spectrum. Crystallites in powder samples are stationary and biological compounds in suspensions are not as mobile as small molecules. The lack of tumbling allows many NMR interactions, such as dipolar coupling and chemical shift anisotropy, to exist and broaden signals. SSNMR can be used to rotate the sample at a magic angle to average out these interactions and significantly narrow the linewidths.

Rotating the sample at fast spinning speeds, up to 40 kHZ in our facility, and having a dedicated $^2$H lock channel for biological samples such as peptides and proteins to stabilize magnetic field drifts, solution-like NMR spectra can be acquired. Our SSNMR probe is quite unique because it has the capabilities to perform quadruple resonance experiments (HFXY). This will allow users to perform experiments using up to four channels: for example, observe $^{13}$C and decouple $^1$H, $^{19}$F and $^{15}$N resonances at the same time.

We would like to thank Cindy Ridenour from Phoenix NMR for installing the probe and teaching us about its capabilities and maintenance.

**Phoenix HFXY Premium Probe Highlights:**

- 1.6 mm sample rotor (8 µL active sample volume)
- Sample rotation between 8.0 and 40.0 kHz
- Multiple channel configurations:
  - HFXY, HFX, HXY, FXY, HF, HX, FX.
  - **X:** $^{31}$P to $^{15}$N or $^{31}$P to $^{13}$C, **Y:** $^{23}$Na to $^{15}$N
- Dedicated $^2$H lock channel
- Frost and condensation free variable temperature system.
- VT range: -125 to +125 °C
Raman Spectroscopy tracks how the photons from incident light *inelastically scatter* after interacting with the molecules present in a specimen. When the photon loses energy to the molecules, it is termed as Stokes Raman Scattering and when it gains energy from the molecules it is termed as anti-Stokes Raman Scattering. The observed raman shift is the difference between the wavenumbers of the incident and the scattered lights. Unlike fluorescence spectroscopy, in Raman, the incident radiation does NOT need to match the difference in vibrational energy levels, in fact most commonly in Raman the molecule is excited away from it’s electronic absorption region to avoid interference from Fluorescence. **FT-IR and Raman are often considered complimentary** techniques; symmetric vibrations lead to relatively strong Raman signals and no IR signal whereas asymmetric and bending vibrations lead to strong IR signal and much weaker raman bands. It is a non-destructive method of analysis that provides both qualitative and quantitative information. If you are working with organic or inorganic crystals, polymers, thin films, graphene or carbon nanotubes raman microscopy may be a useful tool to you.

The Thermo-DXR2 Raman Microscope, located in Silver 720, is an easy to use point-and-shoot instrument that is equipped with auto-alignment and calibration tool for accurate measurements. Some of the exciting features of the instrument are highlighted below:

- Equipped with two user-interchangeable diode lasers (532 nm and 785 nm), gratings and filters.
- Four long distance Olympus objectives 10x, 20x, 50x and 100x and brightfield darkfield illuminator.
- Real-time spectral preview, automated fluorescence correction, autoexposure, and cosmic ray rejection by OMNIC software.
- Macro sampling adapter for solution based samples.
- Hyperspectral raman mapping and image analysis by OMNIC Atlus.
- Polarized raman coupled with sample rotation for determining sample orientation.
- Linkam stage and Linksys software for variable temperature measurements.
Meet the Staff

Dr. Trinanjana (Trina) Mandal joined SIF as technical support for the Microscopy Facility in 2015. During the academic year she shares time between teaching undergraduate courses on Analytical and General Chemistry and providing Microscopy support. She has extensive experience in Scanning Electron Microscopy, Atomic Force Microscopy and Raman Microscopy amongst other instrumental techniques. She is passionate about teaching next generational chemists the wonders of chemistry and promoting diversity in STEM laboratories.

Find out more about Dr. Mandal at: LinkedIn ResearchGate

SIF Safety Protocols

As some of you may be new to the facility, below are the current safety protocols in place while using the SIF:

1. Masks are required to be worn at all times within the facility.
2. Physical distancing is not required for those who have been fully vaccinated. For those who are not fully vaccinated, it is your responsibility to maintain physical distancing.
3. Please sanitize instrument and local areas that have been touched
   • Wipe down keyboard covers and mouse covers and instruments before and after use
   • Sanitize sample doors and areas that have been touched on the instruments and counters
   • Wipe NMR sample spinners, EPR sample screw caps, etc. before and after use.
4. Follow these detailed instructions for cleaning the microscopes after each use.

Thank you all for your cooperation and keeping the facility safe for all to use.

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

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