

Dear CORES Users,

Happy 2021! We are all looking forward to a new year with new opportunities to support your research needs.

This past year saw the new Bruker 600 NMR starting to come online (automation has not yet been installed), the availability of some ion mobility experiments in Mass Spec, the availability of charge density experiments in X-ray, and new imagers in High Throughput. With these instruments and new experiments to CORES, this year is ripe with new experimental possibilities.



All the Best for 2021,  
Danielle Gray  
Associate CORES  
Director  
dgray@illinois.edu



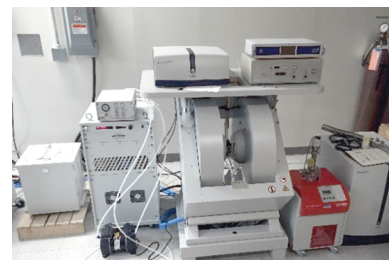
## New Low-Volume Isothermal Calorimeter in the Microanalysis Lab

The TA Affinity LV-ITC (Low-volume Isothermal Calorimeter) is a highly sensitive analytical tool that measures the affinity of binding between two or more molecules, such as macromolecules, proteins, DNA and lipids. The obtained titration curves provide thermodynamic data ( $K_a$ ,  $\Delta H$ ,  $\Delta S$ ,  $n$ ) that is characteristic of the binding interaction. It is equipped with automated cleaning system & protocols to ensure that no traces of samples are left in the titration cell.

Presently, it is set-up for aqueous solutions, which is commonly used. However, if users require testing in organic solutions, they can request for the system to be set-up for that. This will require a several day reservation for conversion, experimental use and conversion back to aqueous mode.

## Instrumentation Available in the EPR Facility

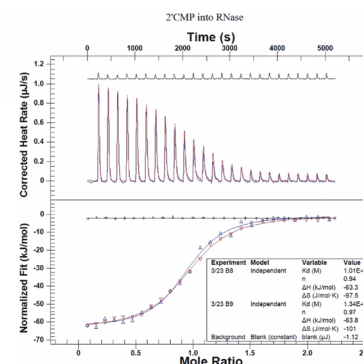
The **EMXPlus** is an X-band (9.8 GHz) spectrometer that users can be trained to operate themselves. It can be equipped with a liquid nitrogen finger dewar for data collection at 77 K or a helium cryostat for data collection between 5 and 300 K. The EMXPlus has a high-sensitivity resonator that can measure spin concentrations as low as 10 micromolar, even lower for some types of samples. The high-sensitivity resonator is an ideal choice for performing spin-trapping experiments, which attempt to determine if your reaction involves a transient radical intermediate. With the proper spin trap, transient radicals with extremely short lifetimes can still be detected. A dual-mode resonator that can record spectra in both the typical perpendicular mode and in parallel mode is also available for the EMXPlus. Parallel mode can be quite useful for integer spin systems which have a tendency to be EPR silent in perpendicular mode.



The **E-580** spectrometer is the EPR lab's multi-frequency spectrometer that is equipped with a helium cryostat for data collection between 5 and 300 K. It can be configured for S-band (3 GHz), X-band (9.8 GHz), or Q-band (35 GHz). Q-band frequency is useful for increasing resolution – signals that overlap at X-band frequency can often be resolved as separate signals at Q-band frequency. The lower frequency S-band configuration can be useful for observing weak hyperfine splitting patterns. The spectral line widths at S-band tend to be narrower than at the higher frequencies, allowing resolution of splitting patterns that would be obscured by the signal line width at higher frequencies.



For more information or to discuss possible EPR experiments, please contact Toby Woods at [tobyw@illinois.edu](mailto:tobyw@illinois.edu).



Typical titration curve obtained from the ITC (taken from TA website):