



STRUCTURAL NMR RESOURCE

Albert Einstein College of Medicine

Ullmann Building Room B-8

WEB SITE: <http://www.bioc.aecom.yu.edu/labs/girvlab/nmr/>

OVERVIEW

The Structural NMR Resource provides AECOM with state of the art facilities for the analysis of molecular structure, dynamics, and interactions by NMR. The local resource in Ullmann B-8 consists of one 300 and two 600 MHz spectrometers with several off-line graphics workstations, providing the instrumentation, computational resources, and expertise for the determination of molecular structures and dynamics by nuclear magnetic resonance techniques.

FACILITIES – BRUKER 300 MHZ NMR



BRUKER 300 MHZ SPECTROMETER

Small molecules are routinely analyzed on the 2 channel 300 MHz instrument. Multinuclear 5 mm (quad - $^1\text{H}^{13}\text{C}^{19}\text{F}^{31}\text{P}$ and inverse broadband) and 10 mm broadband probes are available.

APPLICATIONS (SEE PUBLICATIONS ON WEB SITE):

The DRX300 is a “walk-up” instrument available to anyone at AECOM.

- routine 1D and 2D ^{13}C , ^{15}N , ^{31}P and ^{19}F NMR experiments for the analysis of organic compounds and small biomolecules including lipids, carbohydrates, peptides, substrates, products, and natural products
- screening and optimization of sample conditions for high field NMR studies
- pH titration for the determination of pKa values
- isotope effects on chemical shifts and equilibrium constants for the study of enzyme mechanism.

FACILITIES – BRUKER & VARIAN 600 MHZ NMR



BRUKER & VARIAN 600 MHZ SPECTROMETERS

Macromolecular structure and dynamics are studied using the 600 MHz spectrometers. These 4-channel systems can simultaneously manipulate ^1H , ^{13}C , ^{15}N and ^{31}P spins in isotopically labeled samples in 1D through 4D experiments. Excellent water suppression and artifact elimination are provided by x,y,z-axis pulsed field gradients. The cryogenic probe on the new Varian 600 increases sensitivity by 3-4 fold, making it especially useful for samples of low concentration.

APPLICATIONS (SEE PUBLICATIONS):

The 600 MHz spectrometers are scheduled 1-2 two weeks in advance, to accommodate longer studies.

- Structural studies of peptides, proteins, nucleic acids, and carbohydrates
- Dynamics studies of macromolecules
- pH titration for the determination of pKa values in proteins and bound ligands
- site-specific interactions and interaction interfaces in biomolecular complexes

CONTACT INFORMATION

For further information or to schedule time on the NMR instruments:

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FACILITIES – The New York Structural Biology Center



NEW YORK STRUCTURAL BIOLOGY CENTER

AECOM is a full member of the New York Structural Biology Center consortium, located at the City College Campus on 133rd and Convent Ave. We currently have regular access to the one 900MHz spectrometer, three 800 MHz NMR spectrometers (with cryogenic probes) and one 700 MHz spectrometer (with cryogenic probe). These instruments are especially useful for large macromolecules and complexes (> 35 kD).

SERVICES AND FEES

Planning, assistance, and training are available and encouraged. The Resource Staff are always available to discuss experiments, assist setting up experiments and processing data, and for training on the instruments.

300 MHz spectrometer	\$ 5.00 per hr
600 MHz spectrometer, conventional probe	\$ 7.50 per hour
600 MHz spectrometer, cryogenic probe	\$10.00 per hour
800 MHz Spectrometer, NYSBC	\$16.00 per hour
Service Spectra - collected, processed and plotted	\$25.00 per hour