



NMR for Chemical Analysis, Mixture Analysis and Biomolecular Interactions

Nuclear Magnetic Resonance (NMR) spectroscopy provides a fundamental source of insight into chemical structure and molecular interactions. The four solution NMR spectrometers operating at 300, 400, 600 and 700 MHz are capable of observing a wide variety of nuclei, including proton, carbon, phosphorous, fluorine and boron, to name a few. In addition to chemical identification, the enhanced sensitivity of the 700 MHz spectrometer equipped with cryo-probe technology enables the analysis of biological molecules, including nucleic acids, proteins and cellular metabolites. A combination of experiments can be used to determine molecular structure along with the nature of interactions with other molecules. Rapid data collection is facilitated using NonUniform Sampling (NUS).

Services

The YSciCore NMR Facility at York University offers a wide range of NMR services:

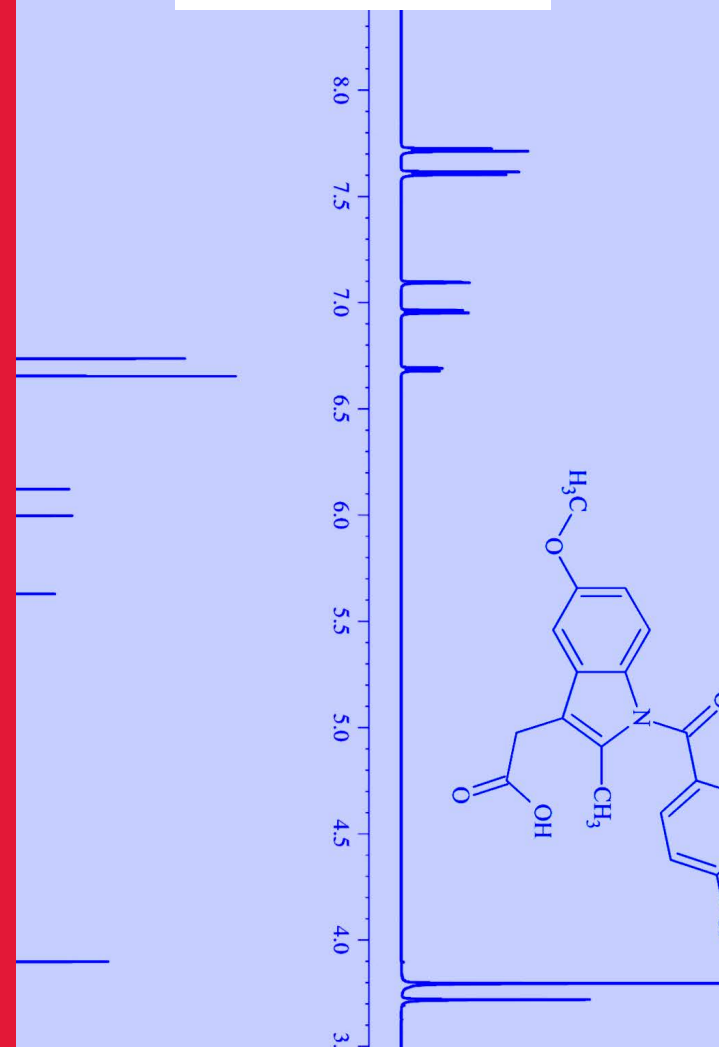
- Routine acquisition of 1D spectra
- Complete spectral analysis
- Quantitative analysis
- Impurity analysis
- NMR operator training
- Consultation
- Fast sample turn-around
- Reaction kinetics analysis

Contact Us

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YSciCore



Nuclear Magnetic Resonance Spectroscopy

science



Biological NMR Interactions

- **Protein Structure** — The 700 MHz NMR spectrometer is capable of collecting multi-dimensional spectra leading to protein structure determination. Deuterium decoupling is available for labelled samples.
- **Protein-Substrate Binding** — Using labelled samples and substrate titrations, binding interactions can be studied using ^1H - ^{15}N HSQC spectra. The nature of ligand binding to macromolecular receptors can also be evaluated using Saturation Transfer Difference (STD) spectroscopy.
- **Enzyme Kinetics** — Enzyme catalysis can be followed by monitoring the resonance intensity change over a period of time.
- **Metabolomics** — The enhanced resolution and sensitivity of the 700 MHz NMR spectrometer is optimal for identification and quantification of metabolites from cellular studies.

Chemical NMR Interactions

- **Routine Spectra** — ^1H and ^{13}C spectra can be provided for sample characterization.
- **Structure Determination** — Using a suite of 1D and 2D programs, spectra can be acquired to assist with chemical identification. Detailed analysis reports can be provided upon request.
- **Quantitative NMR** — Quantative NMR assays can provide purity analysis of compounds using various nuclei including proton, fluorine, phosphorous, carbon and other nuclei.
- **Mixture Analysis** — Component analysis of complex solutions can be identified and quantified.
- **Trace Analysis** — At 700 MHz impurities can be detected and quantified.

Capabilities

700MHz

- Three-channel ^1H , ^{13}C , ^{15}N , ^2H cryogenic probe for biological samples
- 1D, 2D, 3D ... nD acquisitions
- NonUniform Sampling

600MHz

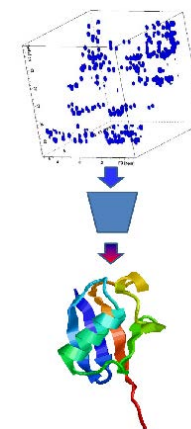
- Three-channel ^1H , ^{13}C , ^{31}P , ^2H probe
- Broad banded probe for multinuclear studies of low quantity samples
- HRMAS probe for gel-phase samples
- Flow probe for on-the-fly reaction monitoring

400MHz

- Two-channel broad banded automatic tune and match probe (including fluorine)
- Variable temperature
- Sample changer with full automation

300MHz

- Teaching and training instrument
- Two-channel broad banded automatic tune and match probe (including fluorine)
- Variable temperature
- Sample changer with full automation



NMR Applications Currently Assisting:

Biological Research

- Protein – Ligand Interactions
- Protein Structure
- Nucleic Acid Folding
- Metabolomics

Chemical Research

- Organic Synthesis Structure Verification
- Organo-metallic Synthesis
- Reaction Kinetics
- Catalysis Studies
- Gasification Effluent Analysis

Industrial Applications

- Pharmaceuticals
- Contract Manufacturing
- Industrial Chemical Quality Monitoring
- Lubricant Manufacturing
- Agricultural Products
- Environmental Studies

