Nuclear Magnetic Resonance

umass.edu/ials/nmr

Located on the 3rd and 6th floors in the Conte Polymer Research Building and in the basement of the Lederle Graduate Research Tower the NMR facility houses 5 state-of-the-art instruments to study structure, dynamics and interactions of small molecules and biological macromolecules such as proteins, nucleic acids, lipids, and their complexes.

The facility accepts samples and will perform requested analysis. We offer training to users who want to conduct their experiments independently. We charge a fee for a service for both internal and external researchers, academic or industry based. Following an initial consultation, training and setting up of experiments is arranged through the director.

ACCESS

To request access, training, or additional information please contact Weiguo Hu at weiguoh@polysci.umass.edu for solid state and small organic molecule samples. For biomolecular NMR assistance contact Jasna Fejzo at jfejzo@umass.edu.

Our rates are competitive and tiered based on needs and usage. Visit our website at *umass.edu/ials/nmr* for current listing.

TRAINING

Training for new users consists of:

- lab safety training,
- operation of the instrument and associated software,
- use of data analysis software,
- exporting or presenting data,
- clean up and shutdown of the instrumentation.

Once the training is complete, researchers may schedule their experiments through the director of Nuclear Magnetic Resonance (Weiguo Hu or Jasna Fejzo) or online through FOM (Facilities Online Manager) at *fom.umass.edu/fom*

UMassAmherst | Core Facilities

Institute for Applied Life Sciences
University of Massachusetts Amherst
Life Science Laboratories
240 Thatcher Road
Amherst, MA 01003

Research and Innovation to Translate Basic Science into Product Candidates

PARTNER WITH US!

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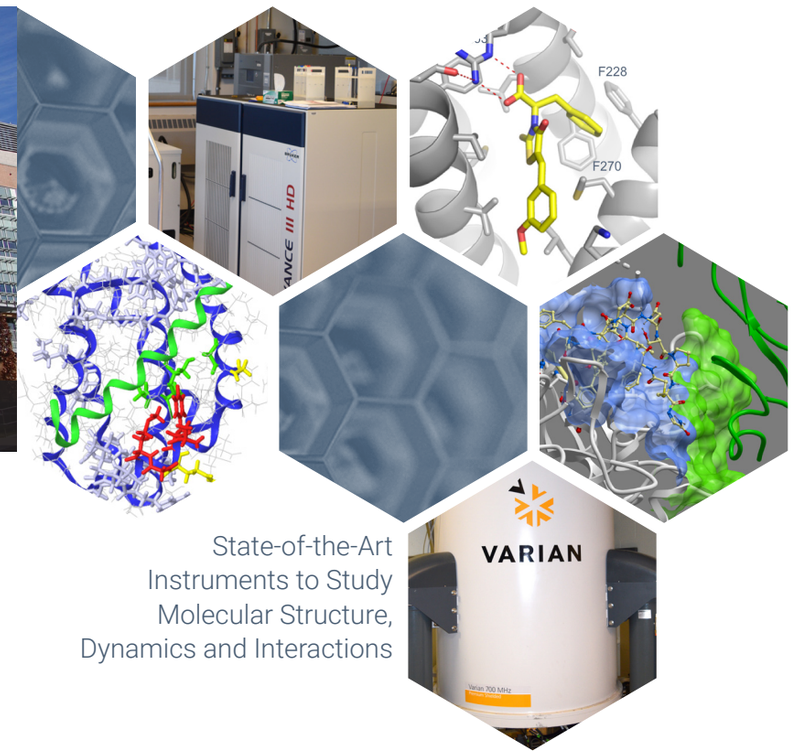
Revision (08/08/18)

UMassAmherst | Core Facilities

Nuclear Magnetic Resonance

Institute for Applied Life Sciences
University of Massachusetts Amherst



State-of-the-Art Instruments to Study Molecular Structure, Dynamics and Interactions

APPLICATIONS OF NMR

Solid State NMR

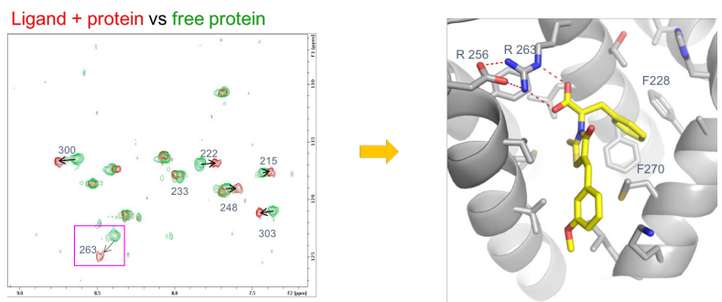
- Chemical structure of polymers and inorganic molecules
- Polymer morphology and molecular dynamics
- Membrane peptides and proteins

Liquid State, High-Resolution NMR

- Microstructure of polymers
- Constitution, conformation and dynamics of small molecules
- Biomolecular NMR:
  - ◊ Structure determination of biomacromolecules
  - ◊ Characterization of dynamics and mobility, enzyme kinetics, protein folding
  - ◊ Ligand binding and molecular interactions in solution
- Metabolomics – Study of metabolites & metabolic pathways in cells, tissues and body fluids

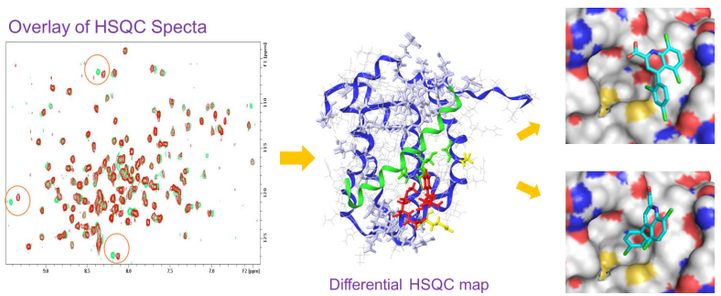
RESEARCH CAPABILITIES

Probing Specific Interactions Between Ligands and Macromolecules

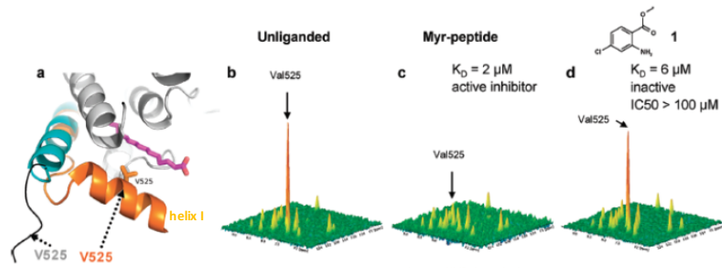


Testing interactions between the ligand and Arg residues on the partner protein.

NMR Can Determine Binding Mode of Ligands in Solution

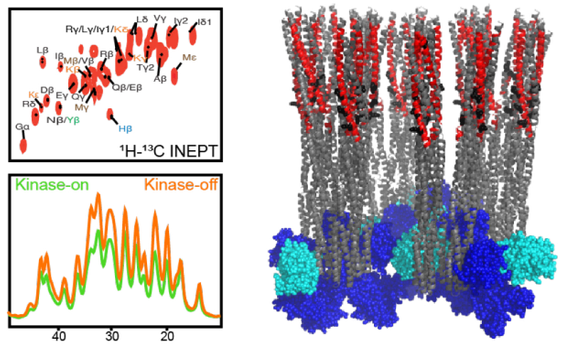


Binding or Bending – NMR Conformational Assay



NMR could be used as a conformational assay to distinguish between ligands that induce conformational change (functional antagonists) and those that do not (agonists – inactive inhibitors).

Identifying Signaling-Related Dynamics by NMR

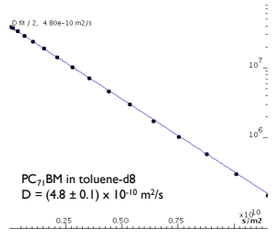


We Offer Early Drug Discovery Project Support:

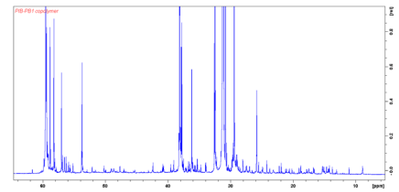
NMR in Drug Discovery

- Fragment based screening (FBS)
  - ◊ Primary screening of mixtures and mixture deconvolution
  - ◊ FBS Follow up
- Hit validation (from HTS; from literature) & binding specificity determination
- Ligand binding mode determination:
  - ◊ NMR constraints determination
  - ◊ NMR guided molecular modeling
- Epitope mapping of biological drugs
- Assistance in biochemical & biophysical assay design

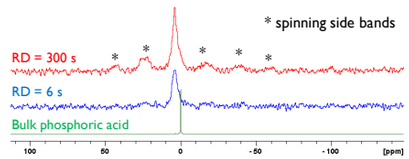
Polymer Microstructure, Morphology, and Diffusion



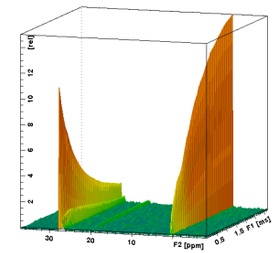
DIFF30 probe provides precise determination of diffusion for large assemblies.



Superior resolution and sensitivity of ^{13}C NMR spectra reveals detailed microstructure of polymers.



Solid-state ^{31}P NMR spectra of PBO fiber showing the physical behavior of trace phosphorous.



Change of reactant and product observed real time by a ^{31}P kinetics NMR experiment.

SPECTROMETERS

- Bruker Avance III 400 MHz, 500 MHz, 600 MHz (high-resolution), 600 MHz (solid-state and diffusion)
- Agilent 700 MHz

PROBES AND ACCESSORIES

- Cryoprobes (600 MHz and 700 MHz)
- Prodigy® Cryoprobes (400 MHz and 500 MHz)
- 1.9mm solid-state probe with ^{1}H, ^{19}F, ^{13}C and ^{15}N
- 4mm CP/MAS HX solid-state probe, capable of detecting ^{1}H and ^{15}N – ^{31}P
- 4mm CP/MAS E-Free solid-state probe, specialized for salty biological samples
- Diff30 probe, ideal for diffusion of polymers/assemblies
- Autosamplers enable high throughput NMR experiments

MASSACHUSETTS LIFE SCIENCES CENTER

A significant portion of core equipment has been purchased through MLSC grant funding support.

TESTIMONIAL

"The NMR Facility has been instrumental in not only analyzing the structures of our polymers, but also in investigating their self-assembly, stimulus-induced changes in morphology and dynamics, as well as studying intermolecular interactions."

– Prof. S. Thayumanavan, Chemistry