Virtual NMR at the HFMRF

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High Field Magnetic Resonance Facility

provides state-of-the-art nuclear magnetic resonance (NMR) and electron paramagnetic resonance (EPR) instrumentation for determining molecular structures that impact environmental remediation and biological health effects.

**Instrumentation**

- Twelve NMR spectrometers (ranging from 900 to 300 MHz) and one pulsed EPR spectrometer, with capabilities in high-field liquid-state, solid-state and micro-imaging techniques
- Combined optical and magnetic resonance microscope
- Low temperature probes for metallo-protein chemistry and structure
- High temperature probe for catalytic materials
- Virtual NMR capability to enable use and collaboration with EMSL scientists by remote users

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Science Areas

Solution-state

• Structural Genomics
• Biomolecular complexes
  • Nucleic Acids/Protein
  • Protein-Protein complexes
  • Protein-Lipid complexes

EPR

• Metalloproteins
• Membrane proteins and redox chemistry mechanisms
• Catalytic RNA’s

Solid-state

• Metalloproteins
• Solid-state materials research
  • catalytic, ceramics, amorphous materials.
  • emerging in biological solid-state research.
• Environmental chemistry
• Actinide chemistry

MR Imaging/ Microscopy

• Imaging and metabolic “signatures” of cells/tissues and organisms.
• Flow and transport
• Polymer aging
• Methods development
  • Slow-MAS
  • confocal microscopy
High Field Magnetic Resonance Facility

Proposal Process

The primary objective is to facilitate the best possible science.

- Open call twice a year (1800 recipients)
- Submitted online via the EMSL User System
- Proposals reviewed
  - EMSL staff
  - External panel
- Review criteria:
  - Scientific Merit
  - Appropriateness of the requested instrumentation
  - Relevance to the EMSL/DOE Mission
  - Contribution staff can have in bringing that science to fruition

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<th>April</th>
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Virtual NMR Access at HFMRF

- Secure, remote operation of spectrometers via internet
- Live consultations using collaboration tools
- Reduced travel costs and more flexible scheduling
- ~20% of facility users elect to use remote access tools

Publications:


Virtual NMR Access at HFMRF

U. Washington - G. Varani
Structure of telomerase RNA and telomeric proteins

Montana State U. - Valerie Copie
Three Dimensional Solution Structure of NoSL

Burnham Institute - K. Ely
Adaptor Proteins Implicated in Breast-Cancer Cell Drug Resistance

Wayne State U. - J. Wang
Structure of Apo-Lp III/HDL Particles

Cornell - Chih-hsin Cheng
Properties of Surface Functional Groups of Black Carbon

Princeton - F. Hughson
Intracellular Protein Transport

CWRU - F. Sonnichsen
100 KDal Membrane-Bound Enzyme Complex

U. Central Florida - L. An
Amorphous SiAlCN Ceramics

Arizona State U. - R. Nieman
Structure and Function of the Membrane Protein OEP16

Los Alamos National Laboratories - Ryszard Michalczyk
Studies of Ligand-Induced Conformational Changes in CD44 Receptor

U. Kansas - C. Larive
Wichita State - W. Carper
Fulvic Acid-Heavy Metal Complexes

Pacific Northwest National Laboratory
Operated by Battelle for the U.S. Department of Energy
High Field Magnetic Resonance - Summary

- HFMRF: 12-NMR spectrometers, 1-pulsed EPR
- 900 MHz NMR
  - High Resolution liquids – structure of complexes
  - Solid State – optimal for quadrupolar nuclei and biological solids
  - 63 mm bore – optimal for solid-state/ imaging projects
- Cold probes
  - 2 - 600 MHz now available to users
  - 800 MHz delivery (9/15/05)
- Next call for proposals (due 01/15/06)
- Remote access to operate instruments with staff