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Bio and materials solids NMR – solids DNP - MRI/S – (solution NMR)

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MRI/S – Dissolution DNP – Bio-solids NMR – metabolomics

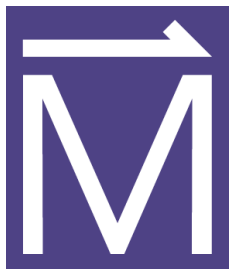
National High Magnetic Field Laboratory

FSU / UF / LANL



FLORIDA STATE
UNIVERSITY





NHMFL NMR/MRI User Programs

2014 Stats:



- **482 Users:**

- 229 Senior Personnel
- 64 Postdocs
- 165 Students
- 24 Technicians

337 Male
99 Female
39 Minority

- **100 Different Institutions**

- **106 Publications**
- in 50 different journals

- **Research Funding:**

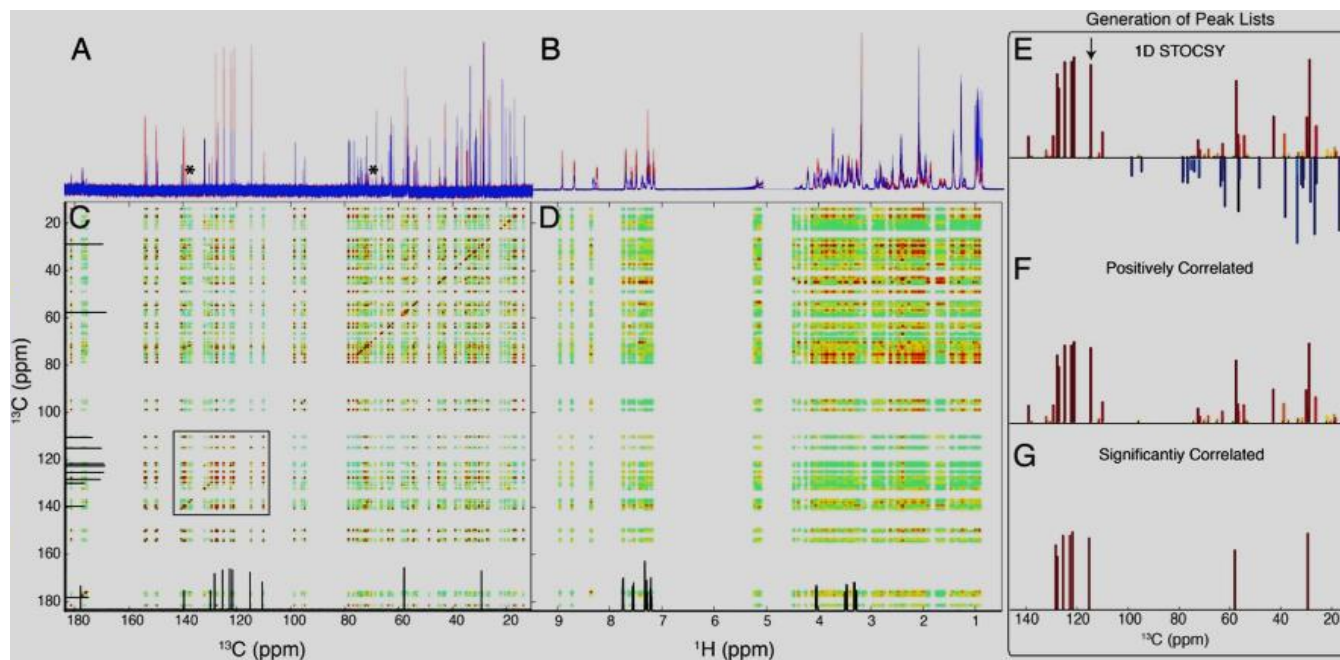
- NSF (8 Programs); NIH (10 institutes); DOE;
Army; NASA; NSERC; AHA; BSRP; EPA; etc.



HTS coils in NMR probes

University of Florida; National High Magnetic Field Laboratory

NSF DMR-1157490, State of Florida, NIH funded research

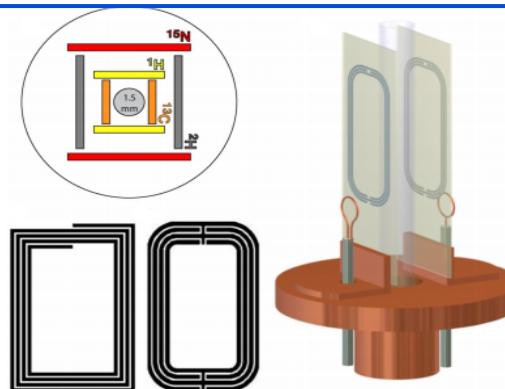


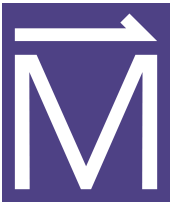
(A-D) 1D and 2D ^{13}C - ^{13}C and ^{13}C - ^1H correlations among samples provide more resolution than ^1H -based counterparts. This in turn gives better peak lists for the biomolecules in the samples, leading (E-G) to a more reliable compound identification.

^{13}C NMR Metabolomics:

Applications at Natural Abundance, C.S. Clendinen, B.Lee-McMullen, C. M. Williams, G.S. Stupp, K. Vandeborne, D. A. Hahn, G. A. Walter, and Arthur S. Edison, *Analytical Chemistry* 86 (18), 9242-9250 (2014)

The new 1.5 mm quadruply-tuned Maglab-built probe based on High Temperature Superconducting (HTS) coils, optimized for ^{13}C on small samples, is twice more sensitive than the best commercially-available counterpart





Short Hydrogen Bonds in the Influenza M2 Proton Channel Drug Target

Florida State University; National High Magnetic Field Laboratory;

NSF DMR-1157490, State of Florida, NIH AI 023007

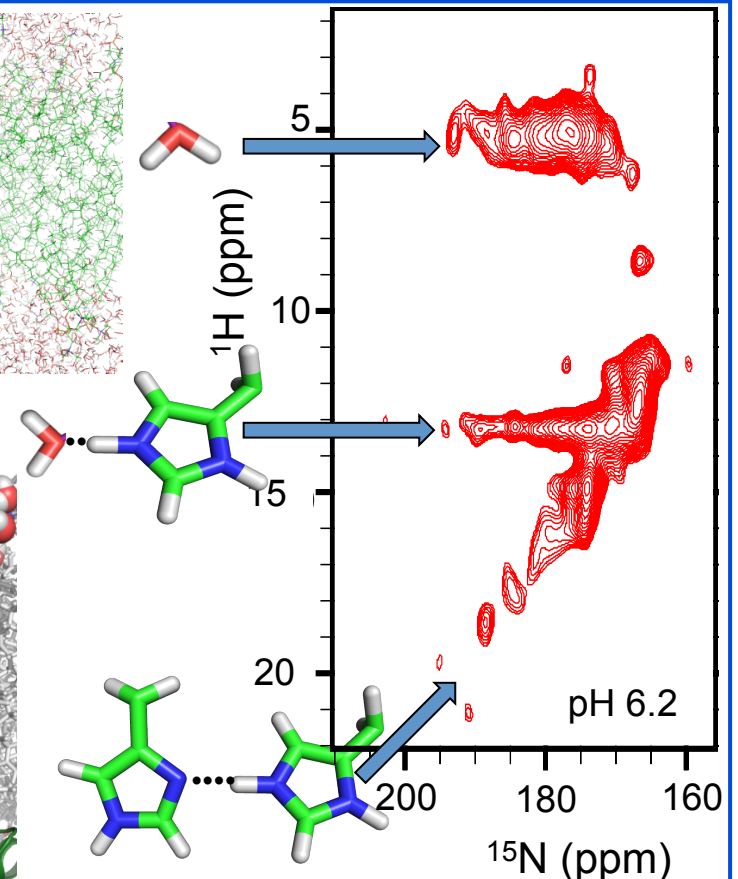
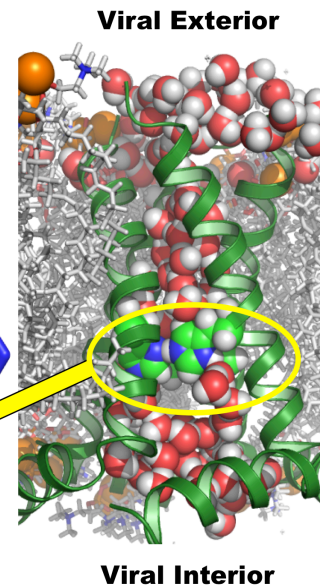
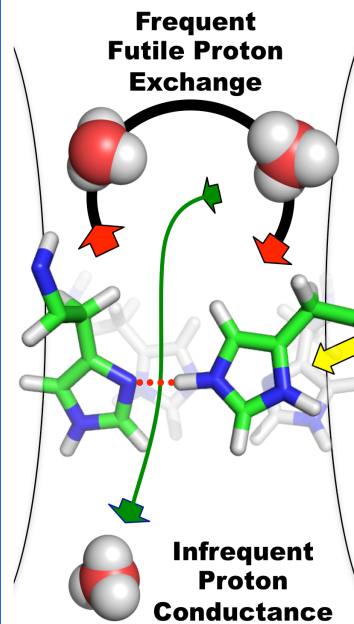
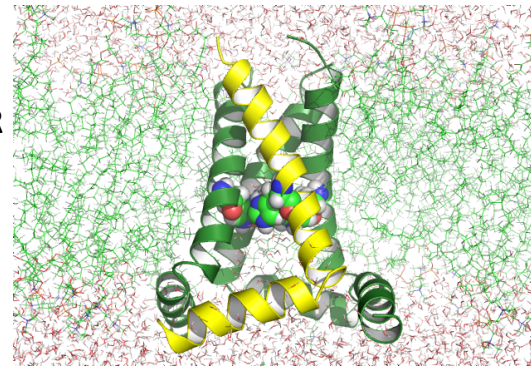


- Unique MAS solid-state NMR spectroscopy of the full length M2 protein has led to the subtle details of how protons are transported in the viral interior – a requirement for the viral life cycle.

Broader Impacts

- Knowing the proton conduction mechanism will facilitate drug development which to date has focused on only “plugging the pore.” Now more specific antiviral drugs can be designed.

The tetrameric M2 proton channel – ssNMR NMR structure obtained in a lipid bilayer environment.



The HN spectrum shows documents low barrier h-bonds (high ^1H frequencies), however these are not strong h-bonds, as water readily breaks them and water protons exchange with histidyl protons.

Magic Angle Spinning NMR Reveals Sequence-Dependent Structural Plasticity, Dynamics, and Spacer Peptide 1 Conformation in HIV-1 Capsid Protein Assemblies

Univ. of Delaware; National High Magnetic Field Laboratory;
Univ. of Pittsburgh, Pacific Northwest Laboratory, Agilent Technologies
Francis Bitter Laboratory

NSF DMR-1157490, NIH GM-082251, NIH RR-015588, NSF CHE-0959496, NIH EB-002026

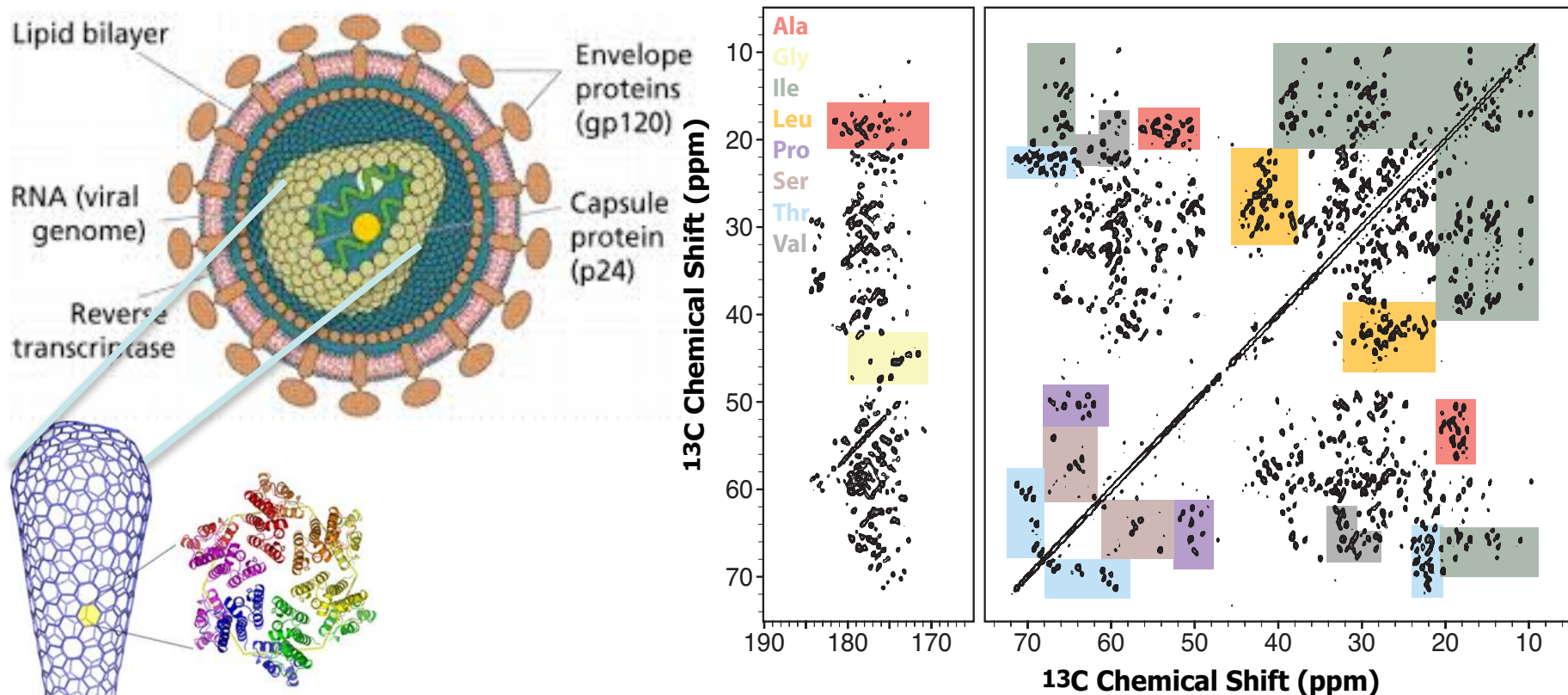
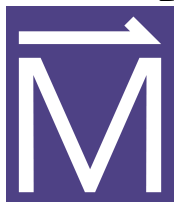
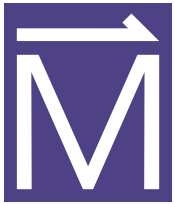


Fig. II.2: (Right) 2D ¹³C MAS NMR spectrum of the HIV-1 capsid protein assembly CA-SP1, highlighting correlations for different kinds of amino acids. (Left) Spectra like this reveal the tubular construct of CA-SP1 and its incorporation into the mature capsid, leading to potential new insights on how to target the HIV virus.

Y. Han, G. Hou, C. L. Suiter, J. Ahn, I.-L. Byeon, A. S. Lipton, S. Burton, I. Hung, P. L. Gor'kov, Z. Gan, W. Brey, D. Rice, A. M. Gronenborn, T. Polenova (2013) *J. Am. Chem. Soc.* 135:17793-17803.



Observation of *In vivo* metabolites facilitated by water suppression at high magnetic fields

Weizmann Institute of Science; National High Magnetic Field Laboratory;
Florida State University

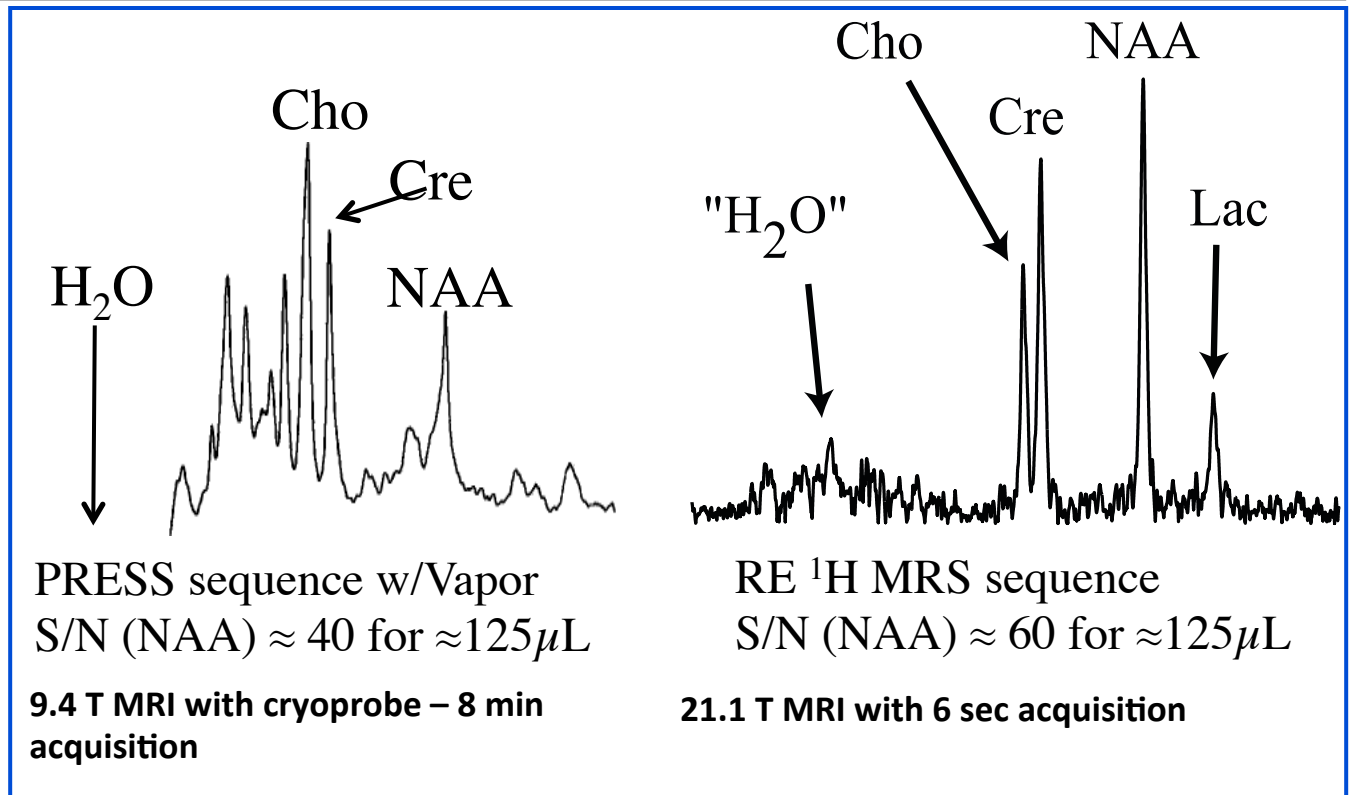


NSF DMR-1157490, NHMFL-UCGP, AHA 10GRNT3860040, ISF 1142/13, EC Marie Curie Action ITN METAFLUX 264780

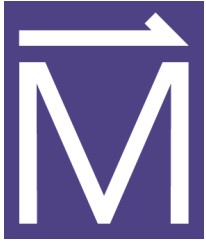
- ^1H MRS yields site-specific metabolic concentrations, biochemistry and kinetics.
- Suppression of the 55 Molar water signal is very challenging. However it is greatly enhanced at high field by the more favorable relaxation behavior of water and the greatly increased chemical shift dispersion.

Broader Impacts

These results demonstrate the revolutionary potential of ^1H MRS at ultra-high fields.



- 1) Shemesh N, Rosenberg JT, Dumez JN, Muniz JA, Grant SC, Frydman L., (2014) Metabolic properties in stroked rats revealed by relaxation-enhanced magnetic resonance spectroscopy at ultrahigh fields. *Nature Comm.* 5: 4958.
- 2) Shemesh N, Rosenberg JT, Dumez JN, Grant SC, Frydman L., (2014) Metabolic T1 dynamics and longitudinal relaxation enhancement in vivo at ultrahigh magnetic fields on ischemia. *J. Cerebral Blood Flow Metabolism* 34: 1810-7.



Remote Access

Spectroscopy from Your Office

Making our Facility Available World Wide:

The Last Two Slides Were Remote Access Spectroscopy

Bio Solids from Canada

Saving Tax Payer Dollars by Avoiding Travel Costs

However, an Initial Visit to the Facility is Recommended

Need Staff to Handle Samples and Provide Aid to the Users

Looking forward to Remote Probe Tuning



**FLORIDA STATE
UNIVERSITY**

