The Nuclear Magnetic Resonance Spectroscopy Core at the University of Virginia

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Abstract

The NMR Spectroscopy Core has six NMR spectrometers: one 500 MHz, four 600 MHz, and one 800 MHz. A 600 MHz and the 800 MHz spectrometers have cryogenically cooled probes for NMR signal sensitivity enhancement. Another 600 MHz spectrometer has an automatic sample changer which will accept 384 samples. The Core is used by a large group of scientists, located throughout UVa and other institutions, for molecular structure determination and study of the dynamics of small and large molecules in solution. Recently published research describes drug discovery, the function of several proteins involved in cancer, transmembrane transport, membrane fusion, infection by ebola virus, and interactions between bacterial and human cells. Other recent research includes discovery of new or more efficient synthetic routes to desired molecular products. The spectrometers are also used for undergraduate courses taught by the UVa Chemistry Dept.

Provision of solution NMR services at UVa is centralized in one laboratory. The number of lab staff per NMR spectrometer is at the low end of a peer group of academic NMR labs. Centralization of services allows one to efficiently obtain, use, and maintain expensive, state of the art instrumentation as well as to provide instrumentation to researchers that could not be purchased by most individual labs.

Front - Bruker Avance III 800 MHz NMR Spectrometer with cryoprobe
Rear - Bruker Avance III 600 MHz NMR Spectrometer with cryoprobe

Recent work supported by the NMR spectroscopy core

Cancer drug discovery
Illendula, A. et al. (Bushweller lab) (2015) A small-molecule inhibitor of the aberrant transcription factor CBFβ-SMMHC delays leukemia in mice. *Science* **347**, 779.

Description of differences in protein structure and dynamics which cause changes in protein function
Regen. M.C. et al. (Bushweller lab) (2013) Structural and dynamic studies of the transcription factor ERG reveal DNA binding is allosterically autoinhibited. *Proc. Natl. Acad. Sci. USA* **110**, 13374.

Engineering of transmembrane protein channels
Zhuang, T. et al. (Tamm lab) (2014) Control of the conductance of engineered protein nanopores through concerted loop motions. *Angew. Chem. Int. Ed*. **53**, 5897.

Mechanism of Ebolavirus function
Gregory, S.M. et al. (Tamm lab) (2014) Ebolavirus entry requires a compact hydrophobic fist at the tip of the fusion loop. *J. Virol.* **88**, 6636.

Mechanism of membrane fusion during signal transmission between peripheral nerves

Liang, B. et al. (Cafiso and Tamm labs) (2014) The SNARE motif of synaptobrevin exhibits an aqueous−interfacial partitioning that is modulated by membrane curvature. *Biochemistry* **53**, 1485.

Exploration of host – pathogen interactions
Fox, D.A. et al. (Columbus lab) (2014) Structure of the Neisserial Outer Membrane Protein Opa60: Loop Flexibility Essential to Receptor Recognition and Bacterial Engulfment. *J. Amer. Chem. Soc*. **136**, 9938.

High resolution structure of an Ebolavirus protein domain
Dziubanska, P.J. et al. (Derewenda lab) (2014) The structure of the C-terminal domain of the Zaire ebolavirus nucleoprotein. *Acta Cryst*. **D70**, 2420.

Conversion of simple alkanes to trifluoroacetate esters
Konnick, M.M. et al. (Gunnoe lab and others) (2014) Selective CH functionalization of methane, ethane, and propane by a perfluoroarene iodine(III) complex. *Angew. Chem. Int. Ed*. **53**, 10490.

Oxidation of simple alkanes
Fortman, G.C. et al. (Gunnoe lab and others) (2014) Selective Monooxidation of Light Alkanes Using Chloride and Iodate. *J. Amer. Chem. Soc*. **136**, 8393.

Stereospecific chemical synthesis
Lankenau, A.W. et al. (Harman lab) (2015) Enantioenrichment of a Tungsten Dearomatization Agent Utilizing Chiral Acids. *J. Amer. Chem. Soc*. **137**, 3649.

Synthesis of a compound for tumor imaging
Samonina-Kosicka, J. et al. (Fraser lab and others) (2015) Luminescent Difluoroboron β-Diketonate PEGPLA Oxygen Nanosensors for Tumor Imaging. *Macromol. Rapid Commun*. **36**, 694.

Synthesis of chiral alcohols
Pu, L. (Pu lab) (2014) Asymmetric Functional Organozinc Additions to Aldehydes Catalyzed by 1,1′-Bi-2-naphthols (BINOLs). *Acc. Chem. Res.* **47**, 1523.

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