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.

Recent work supported by the NMR spectroscopy core

Engineering of transmembrane protein channels

Mechanism of Ebolavirus function

Mechanism of membrane fusion during signal transmission between peripheral nerves

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 Envelopment. J. Amer. Chem. Soc. 136, 9938.

High resolution structure of an Ebolavirus protein domain

Conversion of simple alkanes to trifluoroacetate esters

Oxidation of simple alkanes

Stereospecific chemical synthesis

Synthesis of a compound for tumor imaging

Synthesis of chiral alcohols

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