

Services Offered

500, 600, and 800 MHz NMR spectrometer time.

Consultation on all aspects of using NMR spectroscopy for elucidation of molecular structure and dynamics.

Expertise Available

The laboratories of John Bushweller and Lukas Tamm in Molecular Physiology and Biological Physics, Sepideh Khorasanizadeh in Biochemistry and Molecular Genetics, and Robert Bryant, David Cafiso, and Linda Columbus in Chemistry have considerable experience with the application of NMR spectroscopy to biologically interesting molecules (primarily proteins and nucleic acids).

The manager and only staff member of the BioNMR Core, Jeffrey Ellena, has 25 years of experience in the application of NMR spectroscopy to molecular structure determination.

Instrumentation

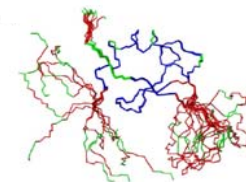
State of the art 500, 600 (3), and 800 MHz NMR spectrometers. All spectrometers will perform the wide range of experiments typically used for elucidation of protein and nucleic acid structure and dynamics. Two of the 600 and the 800 MHz spectrometers are equipped with cryogenically cooled probes for optimum sensitivity. Two spectrometers (the 500 and one 600) have automated sample changers for unattended data collection from multiple (up to 50) samples. All spectrometers are located in the Chemistry Building on McCormick Rd.



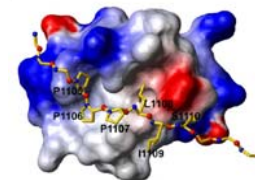
**Bruker 800 MHz
NMR Spectrometer**

**For more information contact Jeffrey Ellena,
ife@virginia.edu 434-924-3163**

NMR spectroscopy yields high resolution molecular structure information which allows one to correlate structure with function.



Structural Basis for Recognition of SMRT/N-CoR by the MYND Domain and Its Contribution to AML1/ETO's Activity
Liu et al. (Bushweller Lab)
Cancer Cell **11**, 483-497, (2007)



NMR spectroscopy yields quantitative information on amplitudes and rates of atomic motion in molecules.

CBF β Allosterically Regulates the Runx1 Runt Domain Via a Dynamic Conformational Equilibrium
Yan et al. (Bushweller Lab)
Nature Structural and Molecular Biology **11**, 901-906, (2004)

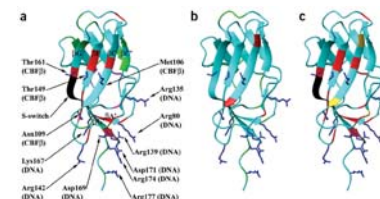


Figure 4 Ribbon representations of the structure of the Runt domain (PDB entry 1H0D) colored according to dynamic behavior. The side chains of residues energetically important for binding to CBF β and DNA are shown and structural elements mentioned in the text are labeled. (a) Runt domain colored according to the dynamic behavior of the Runt domain in the Runt domain-DNA complex; residues fit to model 1 (5°) or not analyzed, cyan; residues fit to models 2 (5° and 10°) and 5 (5° , 5° and 10°), green; residues fit to model 3 (5° and R_{ex}), red; residues fit to model 4 (5° , 10° and R_{ex}), magenta. (b) Runt domain colored according to the dynamic behavior in the CBF β -Runt domain-DNA complex using the same color scheme as for (a). (c) Runt domain colored according to the calculated changes in R_{ex} for residues that were fit in both complexes; residues that show a decrease in R_{ex} going from the Runt domain-DNA complex to the CBF β -Runt domain-DNA complex, red; residues that show an increase in R_{ex} in the same transition, gold.

Solution NMR techniques can be used to obtain high resolution structural and dynamic information about membrane proteins.

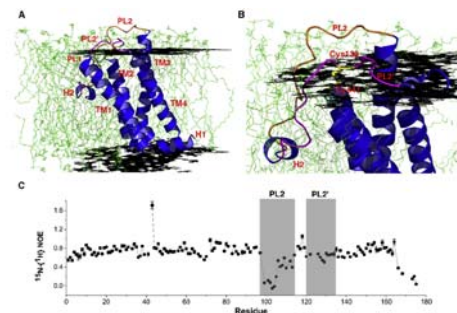


Figure 3. Docking of DsbB(C55C) into a POPC Lipid Bilayer and Periplasmic Loop Dynamics
(A) Structure of DsbB(C55C) docked into a POPC bilayer using EPR measurements. Black planes represent the level of the phosphate head group and green are individual phospholipid molecules from a molecular dynamics simulation.
(B) Close-up view of DsbB(C55C) docked into a POPC bilayer.
(C) Plot of ^{15}N - ^1H heteronuclear NCEs versus the primary sequence. PL2 (res 107-115) and PL2' (res 120-135) are indicated with gray shadow. Depressed values in the N-terminus of PL2 (res 99-105) indicate increased mobility in this region.

NMR Solution Structure of the Integral Membrane Enzyme DsbB: Functional Insights into DsbB-Catalyzed Disulfide Bond Formation