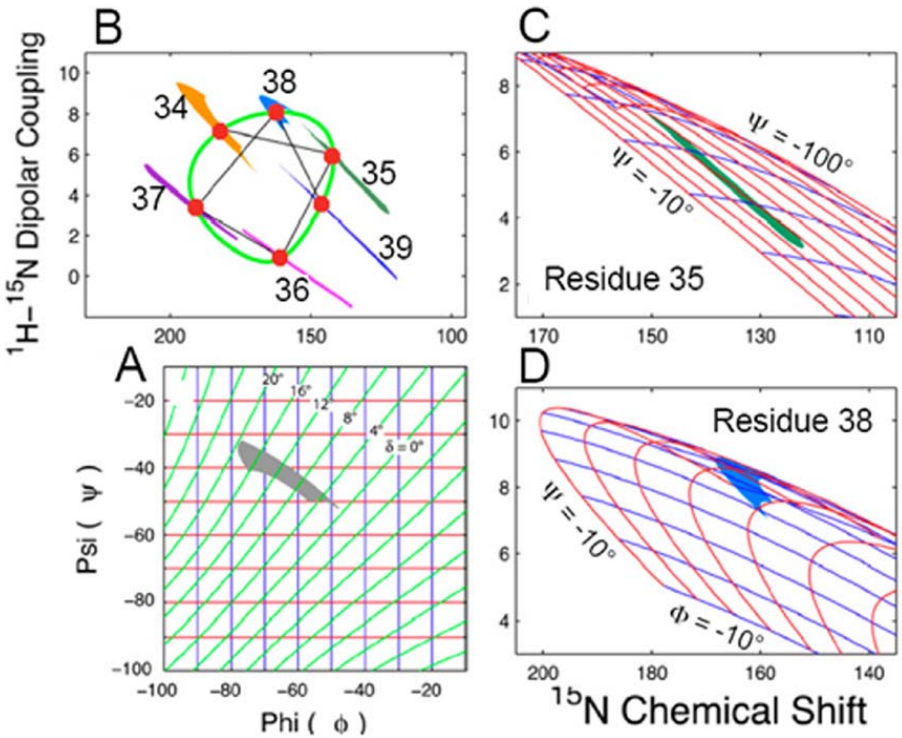
Spectral Mapping of Protein Torsion Angles

National High Magnetic Field Laboratory

NMR Spectroscopy and Imaging Facility, Florida State University

Nuclear Magnetic Resonance spectroscopy permits the observation of all atoms within complex biological macromolecules. Assigning the signals (resonances) to specific sites is an essential step prior to chemical and structural characterizations of these molecules. Here, in recording signals that are dependent on the orientation of the atoms with respect to the magnetic field, we have shown for the first time that a transform of the parameters that characterize protein structure to spectral frequencies can be achieved, for example, a transform from torsion angles to anisotropic chemical shifts and dipolar interactions. The result is that initial NMR spectra can provide structural insights prior to the determination of resonance assignments.

Page, R.C.; Kim, S. and Cross, T.A., ***Structure***, 16 (5), 787-797 (2008)



A. Allowed Φ and Ψ torsion angle space for an alpha helical protein structure B. Modeled data for an alpha helix of a protein structure - amino acids 34-39 and torsion angle space mapped onto the spectral space. C&D. For amino acids 35 and 38 maps of the torsion angle space on the NMR spectra.

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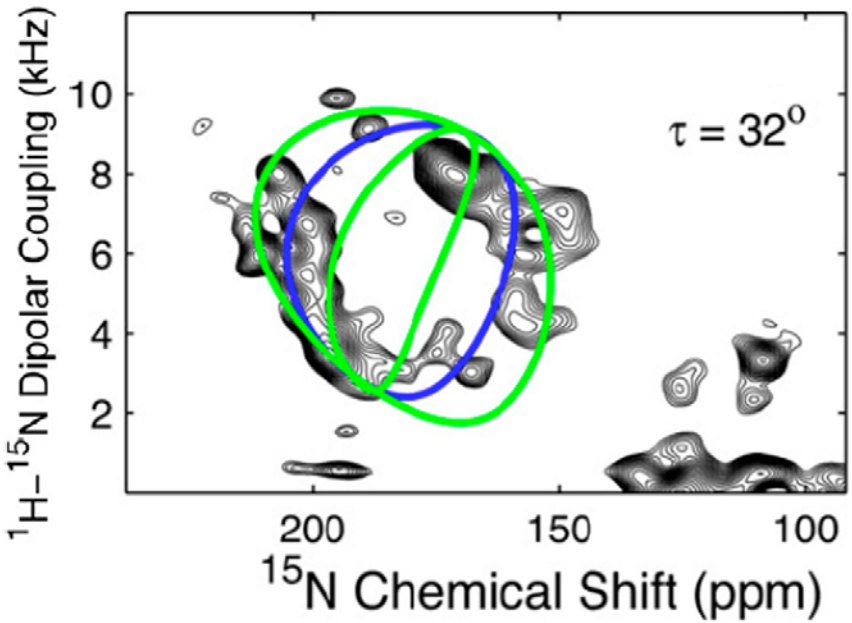

Experimental data for the M2 protein from Influenza A virus with the antiviral drug Amantadine bound. The circles represent lines of constant torsion angle value. The blue circle is for an ideal helical structure, the green circles represent the outer limits of the fit to the experimental data with torsion angles that differ from the blue circle by just ±10°.

The structural characterization of proteins that occur on the surface of cells, known as membrane proteins is important for understanding cellular metabolism and for the development of antibiotics and antiviral drugs.

NMR spectroscopy is a unique tool that permits the characterization of these structures in the presence of a membrane environment. This is critically important as the membrane protein structure is influenced not only by the amino acid sequence (what text books say), but also by the membrane environment. Here we are now able to obtain this structural data much more easily than before.