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J R Quine* (quine@math.fsu.edu), Department of Mathematics, Florida State University, Tallahassee, FL 32306-4510, and Jeffrey K Denny and Timothy A Cross. Transmembrane protein structure from NMR, mathematical analysis. Preliminary report.

Transmembrane proteins are an important part of the genome and knowledge of their structure and function is of great use in understanding the mechanisms of cells. The structure of membrane proteins is difficult to obtain by x-ray crystallography because they are difficult to crystallize, and by solution NMR since they are not easily solubilized. An experimental method has been developed to use solid-state NMR to explore these transmembrane structures. Resonance patterns observed in 2D solid-state NMR from a transmembrane alpha helix have been demonstrated to yield structural details of the protein. The PISEMA (polarization inversion spin exchange at magic angle) experiment correlates anisotropic dipolar and chemical shift interactions for ¹⁵N labeled proteins and the patterns observed have been termed PISA wheels. These wheels are useful in determining the orientation of the helix with respect to the magnetic field, and with high resolution data can be used to compute the structure of the backbone. The mathematical algorithm uses the values of tensors found from NMR observables to find the orientation with respect to the magnetic field direction of discrete Frenet frames along the protein backbone. (Received October 01, 2000)