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**Automated Interpretation of NMR Data using Structures Derived from X-ray Crystallography.** Ling-Hong Hung, Ram Samudrala, Microbiology, Univ. of Washington, UW Micro Box 357242, Seattle, WA 98195 USA.

Apart from sample preparation, the major bottleneck for the determination of solution structures is the interpretation of NOE spectra. NOE data comes in the form of crosspeaks, whose coordinates represent the chemical shifts of two protons close in space. Higher dimensional experiments further narrow the possible combinations by providing limits to the chemical shifts of the heteroatoms attached to one or both of the proton pairs. Traditional NOE interpretation relies heavily upon identifying crosspeaks where these chemical shift restrictions can only be satisfied by a unique pair of protons. Heuristic rules based upon conserved distances found in known structures and low resolution structures obtained from this data can then be used to resolve ambiguities and iteratively lead to the assignment of more crosspeaks.

We take the opposite approach and start by enumerating proton contact patterns found in 2000 protein crystal structures and deriving initial estimates of proton contact probability. The NOE crosspeak data is then used to limit the possible proton pairs and using Bayesian inference, refine the initial estimate of contact probabilities. The resulting posterior probabilities are used to generate structures which can be used to further derive new probability estimates and iteratively refine the interpretation of the NOE data. This approach bypasses the need for crosspeaks to uniquely identify proton pairs. As a further consequence, complete chemical shift information is no longer necessary before structures can be obtained, thus relieving two bottlenecks to the determination of NMR structures.