1020-00-151 **Di Wu*** (di.wu@wku.edu), Department of Mathematics, Western Kentucky University, 1906 College Heights Blvd#11078, Bowling Green, KY, **Robert Jernigan**, Department of Biochemistry, Biophysics, 123 Office & Laboratory, Iowa State University, Ames, IA , and **Zhijun Wu**, Department of Mathematics, 370 Carver, Iowa State University, Ames, IA. *NMR Protein Structure Refinement with Mean Force Potentials.*

NMR (Nuclear Magnetic Resonance Spectroscopy) determined protein structures are not as fixed and detailed as those by X-ray crystallography, due to insufficient distance data available from NMR experiments. Therefore, the applications of NMR determined structures are severely limited in some important fields, such as homology modeling and rational drug design. A knowledge-based approach is introduced here to refine NMR-determined structures by using database derived mean-force potentials. It shows that the structures are improved significantly in terms of several standard criteria when a selected set of distances are optimized with corresponding mean-force potentials. (Received August 30, 2006)