Supporting Information for Publication

Contact Model for the Prediction of NMR N-H Order Parameters in Globular Proteins

F. Zhang and R. Brüschweiler*

Eq. (1) is implemented on our public webserver <http://spinportal.magnet.fsu.edu/s2/s2.html>, which accepts Protein Data Bank files as input and returns the predicted S^2 order parameter profile. The Python program `s2predict.py`, which performs the same task, can be downloaded from <http://spin.magnet.fsu.edu>.

References:

Zhang, Z.; Brüschweiler, R. *J. Am. Chem. Soc.* **2002**, *124*, 12654-12655.