Supplementary data

Table S1: Calculation times for spectra simulations on an Intel Xeon E5405 2.0 GHz server.

	protein	**ubiquitin**	**DsbA**	**VDAC**
	number of residues in pdb-file	76	188	288
	PDB ID	2JZZ	2LEG	2JK4
1	Chem. shifts: ShiftX2 prediction Correlations: C-C intraresidue, depth “all”, nr of bonds “all”	17.160s 17.735s 17.672s	31.366s 30.701s 29.712s	32.272s 32.209s 32.209s
2	Chem. shifts: Sparta+ prediction Correlations: C-C intraresidue, depth “all”, nr of bonds “all”	10.147s 10.150s 9.074s	19.475s 19.526s 19.531s	19.523s 17.740s 17.822s
3	Chem. shifts: ShiftX2 prediction Correlations: N(i)-C(i-1) interresidue, depth “all”	14.903s 15.343s 15.258s	27.343s 26.961s 26.870s	29.305s 28.838s 28.925s
4	Chem. shifts: Sparta+ prediction Correlations: N(i)-C(i-1) interresidue, depth “all”	9.121s 8.880s 8.945s	17.914s 17.878s 17.913s	21.157s 15.925s 16.163s
5	Chem. shifts: ShiftX2 prediction Correlations: Through-space, atom mode “C-C”, mode “intramolecular”, dist. threshold “0.0 Å”, dist. cut-off “5.5 Å”	43.042s 43.704s 42.614s	108.015s 115.210s 118.914s	152.219s 141.990s 131.972s
6	Chem. shifts: Sparta+ prediction Correlations: Through-space, atom mode “C-C”, mode “intramolecular”, dist. threshold “0.0 Å”, dist. cut-off “5.5 Å”	44.079s 39.627s 44.406s	97.951s 98.960s 92.043s	122.462s 114.161s 111.559s