Title:	Identifying secondary structures in proteins using NMR chemical shift 3D correlation maps
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Keywords:	NMR spectroscopy Isotropic chemical shifts Dihedral angle database 3D correlation maps
Issue Date:	2013
Publisher:	Elsevier
Citation:	Journal of Molecular Structure, 1041, pp.200-212.
Abstract:	NMR chemical shifts are accurate indicators of molecular environment and have been extensively used as aids in protein structure determination. This work focuses on creating empirical 3D correlation maps of backbone chemical shift nuclei for use as identifiers of secondary structure elements in proteins. A correlated database of backbone nuclei chemical shifts was constructed from experimental structural data gathered from entries in the Protein Data Bank (PDB) as well as isotropic chemical shift values from the RefDB database. Rigorous statistical analysis of the maps led to the conclusion that specific correlations between triplets of backbone chemical shifts are best able to differentiate between different secondary structures such as α-helices, β-strands and turns. The method is compared with similar techniques that use NMR chemical shift information as aids in biomolecular structure determination and performs well in tests done on experimental data determined for different types of proteins, including large multi-domain proteins and membrane proteins.
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