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Title:	Mapping NMR chemical shift anisotropy parameters of backbone nuclei onto secondary structure elements in proteins
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Abstract:	There has been much recent progress in using NMR chemical shift anisotropy (CSA) parameters to gain information about secondary structure content in proteins. This paper focuses on the comparison of CSA tensors of different backbone nuclei (namely 13Ca, 13C′, 15N,1Ha, 1HN) of all twenty amino acids appearing in well-defined secondary structures such as helices and sheets. Dihedral angle information of these backbone nuclei in different secondary structure elements has been extracted from experimentally determined structures of proteins deposited in the protein databank. The CSA tensors of these backbone nuclei have been computed for the corresponding dihedral angles using ab initio quantum chemical methods. It is shown that 2D correlated plots of a novel set of CSA parameters (ρ,τ), that define the magnitude and shape of the anisotropy, are extremely useful in identifying secondary structure content. Further, multinuclear correlations between these CSA parameters can clearly distinguish between various secondary structure elements such as helices and sheets.
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