Title:	Using the chemical shift anisotropy tensor of carbonyl backbone nuclei as a probe of secondary structure in proteins
Authors:	Kumari, Amrita (/jspui/browse?type=author&value=Kumari%2C+Amrita) Dorai, K. (/jspui/browse?type=author&value=Dorai%2C+K.)
Keywords:	3D clusters Ab initio method Backbone carbonyl
Issue Date:	2010
Publisher:	American Chemical Society.
Citation:	Journal of Physical Chemistry A, 114 (18), pp. 5830-5837.
Abstract:	This study seeks to establish that the chemical shift anisotropy (CSA) tensor of the backbone carbonyl (13C) nucleus is a useful indicator of secondary structure elements in proteins. The CSA tensors of protein backbone nuclei in different secondary structures were computed for experimentally determined dihedral angles using ab initio methods and by calculating the CSA tensor for a model peptide over the entire dihedral angle space. It is shown that 2D and 3D cluster plots of CSA tensor parameters for 13C' nuclei are able to distinguish between different secondary structure elements with little to no overlap. As evidenced by multinuclear 2D plots, the CSA of the 13C nucleus when correlated with different CSA parameters of the other backbone nuclei (such as Cα or 1Hα) is also useful in secondary structure identification. The differentiation of α-helix versus β-sheet motifs (the most populated regions of the Ramachandran map) for experimentally determined values of the carbonyl CSA tensor for proteins ubiquitin and binase (obtained from the literature) agrees well with the quantum chemical predictions.
Description:	Only IISERM authors are available in the record.
URI:	http://pubs.acs.org/doi/abs/10.1021/jp9113199 (http://pubs.acs.org/doi/abs/10.1021/jp9113199)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/290/4/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/123456

Show full item record (/jspui/handle/123456789/290?mode=full) (/jspui/handle/123456789/290/statistics)