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Title:Terahertz spectroscopic analysis of peptides and proteins
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Abstract:Spectroscopic analysis using the Terahertz frequencies between 0.1-15 THz (3-500 cm⁻¹) has been underutilised by the biochemistry community but is starting to yield some scientifically interesting information. Analysis of structures from simple molecules like N-methylacetamide, to polyamides, peptides and relatively complex proteins provides different types of information dependant on the molecular size. The absorbance spectrum of small molecules is dominated by individual modes and specific hydrogen bonds, peptide spectra have peaks associated with secondary structure, while protein spectra are dominated by ensembles of hydrogen bonds and/or collective modes. Protein dynamics has been studied using Terahertz spectroscopy using proteins like bacteriorhodopsin, illustrating a potential application where this approach can provide complementary global dynamics information to the current nuclear magnetic resonance and fluorescence-based techniques. Analysis of higher-order protein structures like polyomavirus virus-like particles generate quite different spectra compared to their constituent parts. The presence of an extended hydration layer around proteins, first postulated to explain data generated using p-germanium spectroscopy may present a particularly interesting opportunity to better understand protein's complex interaction with water and small solutes in an aqueous environment. The practical aspects of Terahertz spectroscopy including sample handling, the use of molecular dynamics simulation and orthogonal experiment design are also discussed. © Springer Science+Business Media, LLC 2012.
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