PROTEIN STRUCTURE AND DYNAMICS PROBED BY NONLINEAR IR SPECTROSCOPY

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The three-dimensional structure of proteins and their dynamics are essential properties responsible for the extremely high specificity of biological reactions. Utilizing intense femtosecond IR pulses we have recently demonstrated a series of novel nonlinear IR spectroscopic techniques to develop new multidimensional spectroscopic tools to study the structure and the dynamics of proteins. Experimental examples of these techniques, their underlying principles and their application will be discussed. Through these examples, we hope to demonstrate the utility of nonlinear IR spectroscopy in studying a variety of physical, chemical, and biological problems. As a detailed description, in case of 2D vibrational spectroscopy of a cyclic penta-peptide in solution, spectrally resolved cross peaks occur in the off-diagonal region of the 2D IR spectrum of the amide-I region, analogous to those in 2D NMR spectroscopy. These cross peaks measure the coupling between the different amide groups in the structure. Their intensities and polarizations relate directly to the three dimensional structure of the peptide. With the help of a model coupling Hamiltonian, supplemented by density functional calculations, the spectra of this penta-peptide can be regenerated from the known solution phase structure. This 2D-IR measurement, with an intrinsic time resolution of less than 1ps, could be used in all time regimes of interest in biology. We believe that multidimensional IR spectroscopy will potentially complement multidimentional NMR spectroscopy in probing the dynamics of biomolecules and determining their structures.

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