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Observation of Water-Protein Interaction Dynamics with Broadband Two-Dimensional Infrared Spectroscopy LUIGI DE MARCO, ANDREW HAKY, ANDREI TOKMAKOFF, The University of Chicago — Two-dimensional infrared (2D IR) spectroscopy has proven itself an indispensable tool for studying molecular dynamics and intermolecular interactions on ultrafast timescales. Using a novel source of broadband mid-IR pulses, we have collected 2D IR spectra of protein films at varying levels of hydration. With 2D IR, we can directly observe coupling between water's motions and the protein's. Protein films provide us with the ability to discriminate hydration waters from bulk water and thus give us access to studying water dynamics along the protein backbone, fluctuations in the protein structure, and the interplay between the molecular dynamics of the two. We present two representative protein films: poly-L-proline (PLP) and hen egg-white lysozyme (HEWL). Having no N–H groups, PLP allows us to look at water dynamics without interference from resonant energy transfer between the protein N–H stretch and the water O–H stretch. We conclude that at low hydration levels water-protein interactions dominate, and the water's dynamics are tied to those of the protein. In HEWL films, we take advantage of the robust secondary structure to partially deuterate the film, allowing us to spectrally distinguish the protein core from the exterior. From this, we show that resonant energy transfer to water provides an effective means of dissipating excess energy within the protein, while maintaining the structure. These methods are general and can easily be extended to studying specific protein-water interactions.

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