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2D IR Spectroscopy of Protein Conformation, Folding, and Binding KEVIN JONES, ANDREI TOKMAKOFF, ZIAD GANIM, JOSHUA LESSING, C. SAM PENG, MIT Department of Chemistry — 2D IR spectroscopy is an increasingly powerful tool for investigation of protein structure and dynamics. As an ultrafast spectroscopy, it provides information on protein structure and conformational variation with high time resolution, providing a tool to study the dynamics of folding and binding. Some of the unique characteristics of 2D IR result from the powerful structure based modeling that is available for amide vibrations. This talk will cover recent examples from our group in which different forms of protein 2D IR and computational spectroscopy are used to reveal conformational heterogeneity in peptides, the folding and binding of proteins, and protein-water interactions. When combined with temperature-jump experiments, the formation and interchange of these structures is probed.

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