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2D IR Spectroscopy of Ubiquitin Unfolding Dynamics ZIAD GANIM, HOI SUNG CHUNG, ANDREI TOKMAKOFF, Department of Chemistry, Massachusetts Institute of Technology — The unfolding dynamics of ubiquitin have been studied using a combination of amide I 2D IR spectroscopy and spectral calculations drawing on structures from molecular dynamics simulations. Equilibrium temperature-dependent 2D IR spectra and transient 2D IR spectra following a nanosecond temperature jump are used to follow the unfolding of ubiquitin's β-sheet. The equilibrium 2D IR spectra show two features that arise from delocalized β-sheet vibrations of which differ by whether C=O oscillators vibrate parallel or perpendicular to its strands. Spectral changes in the transient difference spectrum start with an abrupt blue shift of the perpendicular diagonal region, which corresponds to the disruption of hydrogen bonds between water and solvent-exposed peptide groups. This change is followed over μs to ms time scales by a blue shift of the perpendicular region and disappearance of a cross peak, which reflect the gradual unfolding of the β-sheet of the protein. The experiments are compared with 2D IR spectra calculated from molecular dynamics trajectories of ubiquitin unfolding using a structure-based model for protein amide I spectroscopy.

Ziad Ganim
Department of Chemistry, Massachusetts Institute of Technology

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