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Two-dimensional infrared spectroscopy of the thermal unfolding of proteins ANDREI TOKMAKOFF, MIT, HOI SUNG CHUNG, MUNIRA KHALIL, ADAM SMITH, ZIAD GANIM — Steady-state and transient conformational changes upon the thermal unfolding of ubiquitin were investigated with femtosecond infrared spectroscopy of the amide I vibrations. Equilibrium temperature-dependent 2D IR spectroscopy reveals the unfolding of the β-sheet of ubiquitin through the loss of cross peaks formed between transitions arising from vibrations of the β-sheet. Transient unfolding following a nanosecond temperature jump is monitored with vibrational echo spectroscopy, a projection of the 2D IR spectrum. While the equilibrium study follows a simple two-state unfolding, the transient experiments observe complex relaxation behavior that differs for various spectral components and spans time scales from nanoseconds to milliseconds. By modeling the amide I vibrations of ubiquitin, this observation is explained as unfolding of the less stable strands *III-V* of the β-sheet prior to unfolding of the hairpin that forms part of the hydrophobic core.

Andrei Tokmakoff
MIT

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