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Investigating protein structure and folding with coherent two-dimensional infrared spectroscopy CARLOS BAIZ, CHUNTE PENG, MICHAEL REPPERT, KEVIN JONES, ANDREI TOKMAKOFF, Massachusetts Institute of Technology — We present a new technique to quantitatively determine the secondary structure composition of proteins in solution based on ultrafast two-dimensional infrared (2DIR) spectroscopy. The percentage of residues in alpha-helix, beta-sheet, and unstructured conformations is extracted from a principal component analysis of the measured amide-I 2DIR spectra. We benchmark the method against a library of commercially-available proteins by comparing the predicted structure compositions with the x-ray crystal structures. The new technique offers sub-picosecond time resolution, and can be used to study systems that are difficult to study with conventional methods such as gels, intrinsically disordered peptides, fibers, and aggregates. We use the technique to investigate the structural changes and timescales associated with folding and denaturing of small proteins via equilibrium and transient temperature-jump 2DIR spectroscopy.

Carlos Baiz
Massachusetts Institute of Technology

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