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Earle K. Plyler Prize for Molecular Spectroscopy and Dynamics Lecture: 2D IR Spectroscopy of Peptide Conformation

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Descriptions of protein and peptide conformation are colored by the methods we use to study them. Protein x-ray and NMR structures often lead to impressions of rigid or well-defined conformations, even though these are dynamic molecules. The conformational fluctuations and disorder of proteins and peptides is more difficult to quantify. This presentation will describe an approach toward characterizing and quantifying structural heterogeneity and disorder in peptides using 2D IR spectroscopy. Using amide I vibrational spectroscopy, isotope labeling strategies, and computational modeling based on molecular dynamics simulations and Markov state models allows us to characterize distinct peptide conformers and conformational variation. The examples illustrated include the beta-hairpin tripzip2 and elastin-like peptides.