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Computational Amide I Spectroscopy for Refinement of Disordered Peptide Ensembles: Maximum Entropy and Related Approaches
MICHAEL REPPERT, Massachusetts Inst of Tech-MIT, ANDREI TOKMAKOFF, University of Chicago — The structural characterization of intrinsically disordered peptides (IDPs) presents a challenging biophysical problem. Extreme heterogeneity and rapid conformational interconversion make traditional methods difficult to interpret. Due to its ultrafast (ps) shutter speed, Amide I vibrational spectroscopy has received considerable interest as a novel technique to probe IDP structure and dynamics. Historically, Amide I spectroscopy has been limited to delivering global secondary structural information. More recently, however, the method has been adapted to study structure at the local level through incorporation of isotope labels into the protein backbone at specific amide bonds. Thanks to the acute sensitivity of Amide I frequencies to local electrostatic interactions–particularly hydrogen bonds–spectroscopic data on isotope labeled residues directly reports on local peptide conformation. Quantitative information can be extracted using electrostatic frequency maps which translate molecular dynamics trajectories into Amide I spectra for comparison with experiment. Here we present our recent efforts in the development of a rigorous approach to incorporating Amide I spectroscopic restraints into refined molecular dynamics structural ensembles using maximum entropy and related approaches. By combining force field predictions with experimental spectroscopic data, we construct refined structural ensembles for a family of short, strongly disordered, elastin-like peptides in aqueous solution.

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