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Nearest Neighbor Interactions Affect the Conformational Distribution in the Unfolded State of Peptides SIOBHAN TOAL, REINHARD SCHWEITZER-STENNER, Drexel University, KARIN RYBKA, HARDOL SCHWALBE, Johann Wolfgang Goethe University — In order to enable structural predictions of intrinsically disordered proteins (IDPs) the intrinsic conformational propensities of amino acids must be complimented by information on nearest-neighbor interactions. To explore the influence of nearest-neighbors on conformational distributions, we preformed a joint vibrational (Infrared, Vibrational Circular Dichroism (VCD), polarized Raman) and 2D-NMR study of selected GxyG host-guest peptides: GDyG, GSyG, GxLG, GxVG, where x/y={A,K,LV}. D and S (L and V) were chosen at the x (y) position due to their observance to drastically change the distribution of alanine in xAy tripeptide sequences in truncated coil libraries. The conformationally sensitive amide' profiles of the respective spectra were analyzed in terms of a statistical ensemble described as a superposition of 2D-Gaussian functions in Ramachandran space representing sub-ensembles of pPII-,β-strand-, helical-, and turn-like conformations. Our analysis and simulation of the amide I$'$ band profiles exploits excitonic coupling between the local amide I$'$ vibrational modes in the tetra-peptides. The resulting distributions reveal that D and S, which themselves have high propensities for turn-structures, strongly affect the conformational distribution of their downstream neighbor. Taken together, our results indicate that Dx and Sx motifs might act as conformational randomizers in proteins, attenuating intrinsic propensities of neighboring residues. Overall, our results show that nearest neighbor interactions contribute significantly to the Gibbs energy landscape of disordered peptides and proteins.

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