Prediction of nearest neighbor effects on backbone torsion angles and NMR scalar coupling constants in disordered proteins.

Using fine-tuned hydrogen bonding criteria, a library of coiled peptide fragments has been generated from a large set of random polypeptides. This dataset was used for a comprehensive analysis of the nearest neighbor effects on torsion angles and NMR scalar coupling constants. The study revealed that certain motif types exhibit significantly different behavior from the fully random peptide population. This finding is important for understanding the structural dynamics of disordered proteins.

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