Protein Folding Topology from Conformation Networks

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We introduce a network approach to capture the statistical properties of the structure of conformational space of proteins. This approach accommodates the multidimensionality of protein folding that is generally lost when projecting the energy landscape onto a few order parameters. Here, conformations are represented as nodes of the network, while links are transitions via rotations around backbone dihedral angles. This network representation preserves the structure and captures the dimensionality of conformation spaces, and at the same time creates a framework for a statistical description of their structural properties. Thus, allowing us to identify the key statistical features needed to recover generic properties of folding dynamics. Self-avoidance such as excluded volume of a polypeptide chain introduces degree correlations in the conformation network, which in turn lead to energy landscape correlations. Folding can be interpreted as a biased random walk on the conformational network. Furthermore, the folding pathways along energy gradients organize themselves into scale free networks, thus explaining previous observations made via molecular dynamics (MD) simulations. The microscopic origin of scale-free character and connectivity exponent of protein folding networks mapped from MD simulations of short peptides are also discussed. We have used MD simulations of helical peptide to show that the structure of the folding network fundamentally changes at high temperatures.