Dynamics of Protein Structure Networks

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The protein structures have been represented as networks of non-covalent connections, which are weighed on the basis of the strength of interaction. It has been shown that the degree distribution profiles of structure networks are complex, ranging from a random Gaussian–like to exponential-like behaviour, depending on the strength of interaction(1). The size of the largest cluster undergoes a transition like behaviour at a critical strength of interaction, which appears to be related to the process of protein folding. The dynamics of protein structure networks have been investigated by combining the methods of molecular dynamics simulation and the structure network analysis. The network dynamics in equilibrium is investigated by simulating the protein, Methionyl t-RNA sythetase at 300K. The advantage of the network analysis in understanding the dynamics of different domains at the level of side-chain interaction will be discussed. The unfolding simulations of Lysozyme are carried at 500K and the process of unfolding has been investigated through structure networks (2). The transition from folded to unfolded states have been monitored through changes in the network of side-chain interactions. Correlations between the dynamical nature of the network and experimental findings on protein stability and folding have been observed.

References:

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