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Study of the compact denatured state of a protein by molecular dynamics simulation | Issledovanie kompaktnogo denaturirovannogo sostoianiia belka metodom imitatsii molekuliarnoi dinamiki.

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Abstract

The native state can be considered as a unique conformation of the protein molecule with the lowest free energy of residue contacts. In this case, all other conformations correspond to the denatured state. The degree of their compactness varies significantly. Under folding conditions, the compact denatured state rather than the random coil is in equilibrium with native protein. The balance between the main forces of protein folding, the solvophobic interactions and conformational entropy, suggests that some properties of the compact denatured state are close to those of native protein, whereas other properties are close to those of the random coil. To investigate the molecular structure of the compact denatured state, the method of molecular dynamics simulation seems to be very useful.