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Impact of the water environment on protein folding

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Fuzzy oil drop model in contrast to discrete oil drop introduces the gradual decrease of hydrophobicity from the center of protein molecule (the highest concentration of hydrophobicity) reaching zero level on the surface of protein body. The 3D Gauss function is assumed to represent the idealized hydrophobicity distribution in protein molecule. The real hydrophobicity distribution may differ since it is the result of residues distribution and the pair-wise hydrophobic interaction depending on the intrinsic hydrophobicity of each residue. The difference between idealized distribution and observed one can be measured quantitatively applying the Kullback-Leibler divergence entropy. It measures the distance between observed versus idealized hydrophobicity distribution in the protein as a whole and is able to identify the fragments of high and low similarity. In consequence the localization of high and low stability may be identified since hydrophobic core is assumed to be responsible for tertiary structure stabilization. The directing hydrophobic residue toward the center of protein is the effect of external force field (water environment) during folding process. The balance between external force field (water) and internal force field (non-bonding interaction between toms in protein) is assumed to be the mechanism of protein folding. Local disorder of hydrophobic core (versus idealized one) is quite often related to biological activity (ligand/substrate binding-local hydrophobicity deficiency, protein-protein complexation-local excess of hydrophobicity).

Biography

Irena Roterman-Konieczna has completed her PhD from Nicolaus Copernicus Medical Academy Krakow, Poland and Postdoctoral studies from Cornell University, Ithaca, USA in Harold Scheraga Group. She is the Director of Department of Bioinformatics and Telemedicine at Jagiellonian University, Medical College. She has published more than 25 papers in reputed journals and has been serving as an Editorial Board Member of reputed. Her field of interest is the protein structure and folding simulation as well as systems biology. She is the Chief Editor of the journal *Bio-Algorithms and Med-Systems* (de Gruyter).

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