

Symmetric Features of Structure Formation in Molecular Biological and Model Chiral Systems

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Abstract: One of the most actual fundamental problems of natural sciences is the problem of protein folding. Elucidation of the mechanisms of the "correct" folding of the polypeptide chain into the native conformation is not so much a biological problem as a physical one. The structure of a protein determines its function and role in the biosystem. However, despite the abundant data on the different proteins' functions, some of them remain unclear.

In this work, we present the analysis of the symmetry characteristics of the protein structures of the following classes: hydrolases, isomerases, oxidoreductases, chaperones, structural proteins, viral proteins, electron transport proteins, exocytosis/endocytosis proteins. We analyzed the arrangement of secondary structures (α -helices, β -sheets, 3₁₀-helices, irregular structures) and coiled coil structures in polypeptide chains. Common and individual features of studied protein classes are revealed.

Another aspect of this work is related to the symmetric mechanical features of structure formation. The mechanical properties of α -helices during the formation of coiled coil superhelices are considered, taking into account the chirality of the initial structures. The coiled coil structure was described geometrically in 1953 by F. Crick, and later this description was improved and refined. In this work, we calculated the moduli of tension and force arising during the formation of right-handed and left-handed superhelices from right-handed α -helices in the model system. Thus, it was shown that during the formation of a right-handed supercoil from right-handed α -helices, the modulus of strength and tension is larger than during the formation of a left-handed supercoil from right-handed α -helices. Mechanically, it is easier to form a left-handed supercoil from right-handed α -helices, which is observed in native structures.

The results of this study can be used to develop the concept of a protein as a molecular machine.

Keywords: chirality; proteins; secondary structure; helix; coiled coil

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