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PREDICTION OF FOLDING SITES OF B-TREFOIL PROTEINS WITH IRREGULAR STRUCTURES

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Details of protein folding mechanism are still unknown. The solution to this problem is useful for elucidating the mechanism and treatment of diseases caused by misfolding. The relationship between the amino acid sequence and the structure of a protein is generally thought to be higher in structural similarity between proteins with high amino acid sequence identity. However, β-trefoil proteins are known to have a similar structure despite its low sequence identity among super families. In this study, we aim to obtain information on protein folding, targeting β-trefoil protein with a characteristic structure. We already clarified that the central unit is a folding core in β-trefoil protein with high structural symmetry in the previous. In this study, we predicted folding cores for β-trefoil proteins with irregular structures. The compact areas are predicted using a contact map based on inter-residue average distance statistics (average distance map). Then, high interaction residues are predicted by F-value analysis which calculates the contact frequency by using an effective potential derived from inter-residue average distance statistics. From these, we identify the points important in forming the 3D structure along given sequence. We also investigated the conservation of hydrophobic residues among sequences and attempted to clarify residues important for folding of β-trefoil proteins. Furthermore, the folding mechanisms of the β-trefoil proteins are simulated using the Go model and compared it with the obtained results by ADMs. Because of the ADM analyses, compact regions are found in the N-terminal unit and the C-terminal unit in a β-trefoil protein treated in this study. In the result of the F-value analyses, there is a peak of F-value plot in the central unit. After formation of units at both ends folding occurred, suggesting that the central unit interacts with them. Similar results were obtained in the results of the Go model simulations.

BIOGRAPHY

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