Protein Structure Reduction in Protein Fold Recognition

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Abstract: The protein structure is a result of interactions between its residues in three dimension space. One of the main problems in structural bioinformatics is to decipher and decode the structure of the complex network of interactions in proteins that contribute to the 3D structure. Despite the large number of high-resolution protein structures, the coding of a protein structure has not been fully decoded yet. It is generally assumed that the native structure has the lowest free energy among all the possible conformations of an amino acid sequence [1]. The total potential energy of a protein structure is considered as the summation of all pairwise interaction energies. Knowledge-based potentials (KBP) are one type of the energy functions which derived from databases of known protein conformations [2]. They are derived from a non-redundant set of protein X-ray structures by measuring the probability of a special feature such as distance, relative to a reference state. Although several knowledge-based potential functions exist, the impact of different types of amino acids in the scoring functions has not been studied yet. Previously, we have reported the importance of nonlocal interactions in scoring function (based on Delaunay tessellation) in discrimination of native structures [3]. In this study, a Reduced Structure Model is introduced to reduce protein structure of P into S. S is considered as a reduced structure of only some amino acids and all their interactions. The model was tested using four criteria and the results show that only thirty percent of interactions on average is sufficient in discrimination of native structure.

Keywords: protein native structure; decoy set; knowledge-based potential.

References

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