Abstract

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A Framework for Protein Structure Prediction by energy minimization

Protein structure prediction (PSP) is one of the most important and challenging problems in bioinformatics today. Protein structure can be experimentally determined using either X-ray crystallography Nuclear Magnetic Resonance (NMR). However, these empirical techniques are very time consuming. This paper focuses on computational paradigm which depends on the chemical and physical properties of the amino acids called ab initio approach. This approach gives an explanation to the protein folding process. In fact, not all ab initio algorithms have the same performance, so the general success keys for any of such algorithms are presented. Also, this paper proposes 3 phases framework to predict protein tertiary structure. In phase I, database is prepared while phase II predicts the secondary structure finally phase III predict protein tertiary structure by ing the best protein secondary structure conformation through an energy function criteria. The proposed framework is tested using three benchmark data sets and produces average accuracy 80.45%. This result is considered as an enhancement over existing ab initio prediction methods.