Ab-initio protein structure prediction of Leucosporidium antarcticum antifreeze proteins using I-TASSER simulations

ABSTRACT

Organisms living in cold environment produce some Antifreeze Protein (AFP) which exhibit special functions as a result of cold adaption. AFP is currently being identified in many organisms such as bacteria, plants, fish, and fungi that exposed to freezing stress. Due to the limited structural information from fold library, it gave a big challenge in its structure prediction. Therefore, this study seeks to predict the three-dimensional (3D) model of the Leucosporidium antarcticum antifreeze protein by using homology modeling, threading and ab-initio methods. As low of percentage of sequence identity, not more than 25% (ótwilight zoneö) and poor results in threading methods, the search proceeded with ab-initio method by using I-TASSER simulations, where 5 predicted models were obtained. All the models were then evaluated with PROCHECK and Verify3D servers. Ramachandran Plot showed that the residues in most favored regions were 75.2% with only 4 residues in disallowed regions (Ser21, Phe29, Ala100 and Ala114). For the Verify3D, the structurally and functionally important residues in AFP have scored from 0.30-0.60. These results suggest that ab-initio methods as I-TASSER may soon become useful for low-resolution structure prediction for proteins that lack of close homologue of known structure.

Keyword: Antifreeze proteins (AFP); Leucosporidium; Homology modeling; Fold recognition/threading; Ab-initio; I-TASSER