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شبكة المعلومات الجامعية

التوثيق الالكتروني والميكروفيلم

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لم ترد بالأصل

Ain Shams University
Faculty of Computers and information Science
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A Hybrid Model for Protein Structure Prediction

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By

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Abstract

Proteins are considered the source of life. They handle a bunch of activities in all known organisms, from replication of chromosomes to carrying oxygen, and are generally responsible for controlling the cellular machinery ultimately, the phenotype of an organism. Proteins carry out their function by three-dimensional (3D) tertiary and quaternary interactions between various substrates such as DNA and RNA, and other proteins.

Protein folding is the physical process by which the one-dimensional protein structure assumes its functional conformation by transforming into its three-dimensional structure. If the 3D structure is defective, it affects the protein's expected function in the cells and body. The malfunctioning of the protein due to the misfolding is one of the main causes of some diseases, such as Alzheimer, mad cow and some types of cancer. Thus, knowing the structure of a protein is a prerequisite to gain insight into the protein's function**.**

Protein structure prediction "PSP" derives the 3D structure of a protein from its amino acid sequence. PSP is considered one of the most hunted topics by bioinformatics, it is involved in medical fields such drug design, and in biotechnology, such as the design of novel enzymes. PSP is different from the problem of protein design -It is the rational design of new protein molecules to fold to a target protein structure, with the goal of designing novel function and/or behavior**.**

The PSP remains an extremely difficult and unsolved task. The two main difficulties are calculation of protein free energy and finding the global minimum of this energy.

Protein-structure-determination lab procedures carried out are used to define and determine the exact native structure of a given protein - such as X-ray Diffraction and NMR spectroscopy - are time-consuming, expensive, and could be subjected to retrials due to its complex nature. Those disadvantages forced the development of computationally driven prediction techniques.

My objective was to tackle the obstacles of finding a global minimum energy of any given peptide by building a hybrid model that could achieve this goal.

I compared a collection of PSP ab initio-based methods against the developed hybrid model 3dProFold in terms of their accuracy and time consumption. TM-Align tool was used to measure the quality of generated structures. Experimental results show that the model achieved better average accuracy than the other methods with comparable time.

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