

Easymodel: Web-based Bioinformatics Software for Protein Modeling Based on Modeller

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Abstract : Presently, describing the function of a protein sequence is one of the most common problems in biology. Usually, this problem can be facilitated by studying the three-dimensional structure of proteins. In the absence of a protein structure, comparative modeling often provides a useful three-dimensional model of the protein that is dependent on at least one known protein structure. Comparative modeling predicts the three-dimensional structure of a given protein sequence (target) mainly based on its alignment with one or more proteins of known structure (templates). Comparative modeling consists of four main steps 1. Similarity between the target sequence and at least one known template structure 2. Alignment of target sequence and template(s) 3. Build a model based on alignment with the selected template(s). 4. Prediction of model errors 5. Optimization of the built model There are many computer programs and web servers that automate the comparative modeling process. One of the most important advantages of these servers is that it makes comparative modeling available to both experts and non-experts, and they can easily do their own modeling without the need for programming knowledge, but some other experts prefer using programming knowledge and do their modeling manually because by doing this they can maximize the accuracy of their modeling. In this study, a web-based tool has been designed to predict the tertiary structure of proteins using PHP and Python programming languages. This tool is called EasyModel. EasyModel can receive, according to the user's inputs, the desired unknown sequence (which we know as the target) in this study, the protein sequence file (template), etc., which also has a percentage of similarity with the primary sequence, and its third structure Predict the unknown sequence and present the results in the form of graphs and constructed protein files.

Keywords : structural bioinformatics, protein tertiary structure prediction, modeling, comparative modeling, modeller

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