Modelling – Structure Prediction

Aim

To predict the three- dimensional structure of our gained proteins, we conducted modeling process using SWISS-MODEL. SWISS-MODEL, the Molecular Modeling Server developed by the Geneva Biomedical Research Institute, is the most widely used server in predicting the three-dimensional structure of unknown proteins. Its principle is to extract the simulated structure information of the known protein similar to the query protein from the classical database Brookhaven PDB with the aid of sequence alignment, and to establish the structure of the unknown protein based on the similarity of the protein.

Procedure

We submitted the amino acid sequence of the proteins to the database to gain the three dimensional structures and the analysis results.

1. We submitted our sequence to the SWISS MODEL server and click the 'Build Model' icon.

2. The server matches the template for the submitted amino acid sequence and works out the model.

3. From the summary page, we can get general quality of the model built. The template chosen for the building are presented on the page.

4. The one with the best QMEAN score is chosen to view its full result.

5. Ramachandran Plots , 3D-view of the structure and the alignment view are shown in the full result page. Since these three demonstrations are correlated, we can click on the spots on the Ramachandran Plots to view the represented residue's location in the 3D structure. Similarly, by clicking specific area of the 3D structure, the residues can be highlighted on the residue quality result part.

6. We can the information we want by clicking the icon and choose the suitable modes.

7. We shot 4 pictures from different angles of each model we choose under 'QMEAN' mode, in order to present the 3D structure here while show its residue quality on the pictures.

8. Ramachandran Plots are downloaded from the wed.

9. We use screen shots of either the report page download from the web or the result web page to document the QMEAN and the alignment results.

Evaluations:

The server takes about five steps to get the returned results.

1. BLASTP2 program was used to search the ExNRL3D database for proteins with known tertiary structure as modeling templates.

2. SIM program was used to select all sequences whose similarity with the query sequence is greater than 25% and sequence length was greater than 20 amino acids

3. Generate the input file of Generate ProModII format

4. according to the tertiary structure of the template, the ProModII program and ExPDB database were used to generate the three-dimensional structure model of the target protein.

5. minimize the energy of the model with Gromos96