Protein Structure Prediction by Homology Modeling

By Gulseher Sarah Sirin

Homology modeling is a method to predict the 3D structure of a given protein sequence based primarily on its alignment to one or more proteins of known structure. Using homology modeling to predict unknown protein structure is possible because proteins with high sequence identity have similar structure. Proteins activated by a given ligand have the similar regional structures as well. The protein prediction process consists of: fold assignment, target-template alignment, model building and model evaluation. Using the program MODELLER, I have predicted the structure of the binding domain of cyclic nucleotide gated (CNG) channels using the experimentally determined structure of hyperpolarization-activated, cyclic nucleotide modulated (HCN) ion channel protein as a template. Furthermore, I also predicted the amino acid residues important in ligand binding of CNG channel.