Homology Modelling: The Origin of Computational Modeling

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Abstract—*Homology modeling plays a key role in determining protein structure in the structural genomics projects. Homology modeling has been grabbing attention because of the large gap that exists between the overwhelming number of available protein sequences and experimentally solved protein structures, and also, more importantly, because of the increasing reliability and accuracy of the method. If the facts are seen then, a protein sequence with over 30% identity to a known structure can often be predicted with an accuracy equivalent to a low-resolution X-ray structure. The recent advances and modification in homology modeling, especially in detecting distant homologues, aligning sequences with template structures, modeling of loops and side chains, as well as detecting errors in a model, have contributed to reliable prediction of protein structure, which was not possible even several years ago. The ongoing efforts in solving protein structures, which can be time-consuming and often difficult, will continue to spur the development of a host of new computational methods that can fill in the gap and further contribute to understanding the relationship between protein structure and function. Homology modeling generally starts from selection of homologues with known structures from the PDB. If the query sequence has high sequence identity (>30%) to the structure, the homology detection is quite straightforward which is usually done by comparing the query sequence with all the sequences of the structures in the PDB. Homology models of proteins are of great interest for planning and analysing biological experiments when no experimental three-dimensional structures are available. Building homology models requires specialized programs and up-to-date sequence and structural databases. Integrating all required tools, programs and databases into a single web-based workspace facilitates access to homology modeling from a computer with web connection without the need of downloading and installing large program packages and databases.*