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Building Bridges in Structural Biology: The Power of Comparative Protein Modelling

Juan Kim*

Department of Biochemistry, Sejong University, South Korea

INTRODUCTION

Comparative protein modelling, also known as homology modelling, is a computational technique used to predict the three-dimensional structure of a protein based on its sequence similarity to known protein structures. This method leverages the fact that protein structures are more conserved than their sequences, allowing researchers to construct reliable models even when experimental structures are unavailable. Comparative protein modelling has become an indispensable tool in structural biology, enabling insights into protein function, drug design, and molecular interactions. The foundation of comparative protein modelling lies in the principle that proteins with similar sequences often adopt similar structures. The process begins with identifying a homologous protein with a known structure, called the template, that shares significant sequence similarity with the target protein. This sequence alignment is crucial, as it determines the correspondence between residues in the target and the template, guiding the subsequent modelling steps.

DESCRIPTION

Once a suitable template is selected, the next step is to build the model. This involves transferring the backbone coordinates of the aligned regions from the template to the target protein. Regions of the target protein that do not align well with the template, such as loops or insertions, are modelled using ab initio methods or loop modelling techniques. The side chains of the target protein are then placed, often based on the template's side-chain conformations or through rotamer libraries, which provide the most likely conformations for side chains. Comparative protein modelling has numerous applications in biological research and biotechnology. One of the most significant applications is in drug discovery. By predicting the structure of a protein target, researchers can identify potential binding sites for small molecules, facilitating the design of novel drugs. Structure-based drug design relies heavily on accurate protein models to perform virtual screening, docking studies, and optimization of lead compounds. For instance, the discovery of inhibitors for the HIV protease and other critical enzymes has been accelerated by comparative modelling.

In functional genomics, comparative protein modelling helps elucidate the functions of newly discovered genes. The structure of a protein often provides critical insights into its function, mechanisms of action, and interactions with other biomolecules. By modelling the structure of a newly identified protein, researchers can infer its potential biological roles and identify conserved active sites or functional motifs. This approach has been instrumental in characterizing enzymes, receptors, and other proteins involved in vital cellular processes. Comparative protein modelling also plays a crucial role in understanding disease mechanisms and developing therapeutic strategies. Many diseases, including cancer, neurodegenerative disorders, and infectious diseases, are linked to alterations in protein structure and function. Modelling the structures of disease-related proteins helps identify mutations that disrupt normal function and provides a basis for designing targeted therapies.

CONCLUSION

In conclusion, comparative protein modelling is a powerful and versatile technique in structural biology that enables the prediction of protein structures based on sequence similarity. By leveraging known protein structures, researchers can construct models that provide valuable insights into protein function, facilitate drug discovery, and aid in understanding disease mechanisms. While challenges remain, ongoing advancements in computational methods and the integration of experimental data are continually improving the accuracy and applicability of comparative protein modelling. As the field progresses, this technique will undoubtedly play an increasingly important role in unravelling the complexities of protein structure and function, ultimately advancing our understanding of biology and medicine.

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Corresponding author Juan Kim, Department of Biochemistry, Sejong University, South Korea, E-mail: kimj@la.re.kr

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