

“Structural bioinformatics: Getting the most out of your protein structure”

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ABSTRACT

Proteins are the machinery of life and it is its three-dimensional structure that dictates its function and role inside cells. Therefore, the study and analysis of protein structures is central to many research questions in Biology. Structural bioinformatics, also known as computational structural biology, is a branch of bioinformatics that (broadly) relates to the analysis and prediction of the three-dimensional structure of biological macromolecules such as proteins, RNA and DNA. In this talk I am going to review ongoing research projects and part of the most recent work carried out in the lab in the field of structural bioinformatics. It will include the presentation of computational tools to predict the structure of proteins (M4T) and protein loops (ArchPRED), structure-based characterization of protein interfaces (PCRPI), rational design of bioactive peptides to modulate protein-protein interactions (RAS), and the discovery of novel agents to target highly relevant therapeutic proteins (Bcl6).