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Modeling and Simulations of Protein Structures

Protein complexes
Protein structure prediction
Simulations
Molecular docking

Dr. Márcio Dorn
Dr. Bruno César Feltes

A protein of interest does not always have its structure available. Moreover, even when available, that structure does not explain how that molecule behaves when in a cellular environment or bound to other molecules, such as proteins or chemical compounds. Our group has a journey in the application and creation of new tools to predict protein structures efficiently. Likewise, we have experience modeling and simulating proteins, protein complexes, and understanding the behavior of proteins bound to chemical compounds. The simulation of proteins bound to drugs or other compounds is directly linked to an effective reduction in the costs of choosing new drugs of interest. Similarly, they can be used to understand different molecules' behavior in solution and optimize biotechnology processes.

Prof. Dr. Márcio Dorn
mdorn@inf.ufrgs.br
(51) 3308 - 6824

Instituto de Informática
UFRGS
Av. Bento Goncalves 9500
Prédio 43427 - CxP. 15064
Porto Alegre - RS - Brasil

Centro de Biotecnologia
UFRGS
Av. Bento Goncalves 9500
Prédio 43421 - CxP. 15005
Porto Alegre - RS - Brasil

SBCB
Structural Bioinformatics and Computational Biology Lab