Protein Interactions and Docking

Protein-protein association is essential for most of biological processes in living organisms. We want to understand the formation of specific complexes between proteins, and be able to predict structural details of such complexes at atomic level. For that reason, we are working on algorithmic solutions, based on physico-chemical principles, with the help of computational power. Our group is highly multidisciplinary and strongly motivated to contribute to this challenging scientific area. http://life.bsc.es/pid/pidweb

Objectives

Our research focuses on theoretical and computational approaches to protein-protein association. Two major goals of our research are: i) development of computational tools for protein docking and binding site prediction; and ii) understanding the mechanism of protein-protein association.

We aim to develop and optimise computational algorithms for characterising and understanding protein-protein interactions, which remains one of the most important challenges in Structural Biology. Among others, we have developed software for prediction of protein-protein complex structure by docking simulations, identification of binding sites on protein surfaces, prediction of hot-spot residues from energy calculations, and so on.

On the most practical side, we want to provide rationales for protein interactions of biological and therapeutic interest. With this aim, we have established collaborations with various experimental laboratories, and have thus provided atomistic models for protein-protein complexes involved in different biological processes, such as signal transduction, plant immune system, drug transport in bacteria, and
electron transfer during photosynthesis.

Our models are being continuously evaluated both by our in-house benchmarks, as well as externally through the CAPRI competition.

The ultimate goal of our research is to understand the subtle determinants of the specificity of protein-protein association, which in turn will help us to make more accurate predictions of complexes of biological and therapeutic interest.

All this knowledge will also help us to understand the interaction of small molecules with protein-protein interfaces, with the goal of designing compounds capable of inhibiting protein interactions of therapeutic interest.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación