Structural modeling of complexes of biomedical interest

We generate molecular models to understand how proteins interact to form specific complexes that are fundamental in biological processes. The structural and energetic characterization of such protein-protein complexes by computational approaches aim to complement experimental efforts.

Summary

We want to provide rationales for protein interactions of biological and therapeutic interest. With this aim, we have active collaborations with different 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. We have performed the structural and energetic characterization at molecular level of host/pathogen interactions in infectious diseases, in collaboration with Aitor Hierro (CIC-BioGUNE, Bilbao).

In collaboration with Manuel Palacín (IRB-Barcelona), we have studied the human xCT antiporter that is expressed in various cancers including malignant brain tumors (glioma). We are modeling this system at molecular level to identify potential inhibitors for future drugs against glioma. In collaboration with Bruno Villoutreix (Univ. Paris 7) and Samia Mourah (Hopital St Louis, Paris), we have also studied the role of EMMPRIN in VEGFR activation by homology-based modeling and computational docking. Based on our model, we have designed peptides that are capable of inhibiting such interaction and thus can be potentially useful for treatment of angiogenesis, an essential process in cancer. We are also studying the structural, dynamic and energetic determinants of known pathological mutations in proteins of the MAPK cascades causing RASopathies and cancer, in collaboration with Fabian Glaser (Technion Institute, Israel) and Rony Seger (Weizmann Institute, Israel).

Objectives
1. Structural characterization of specific complexes of biological and biomedical interest, in collaboration with experimental laboratories.


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