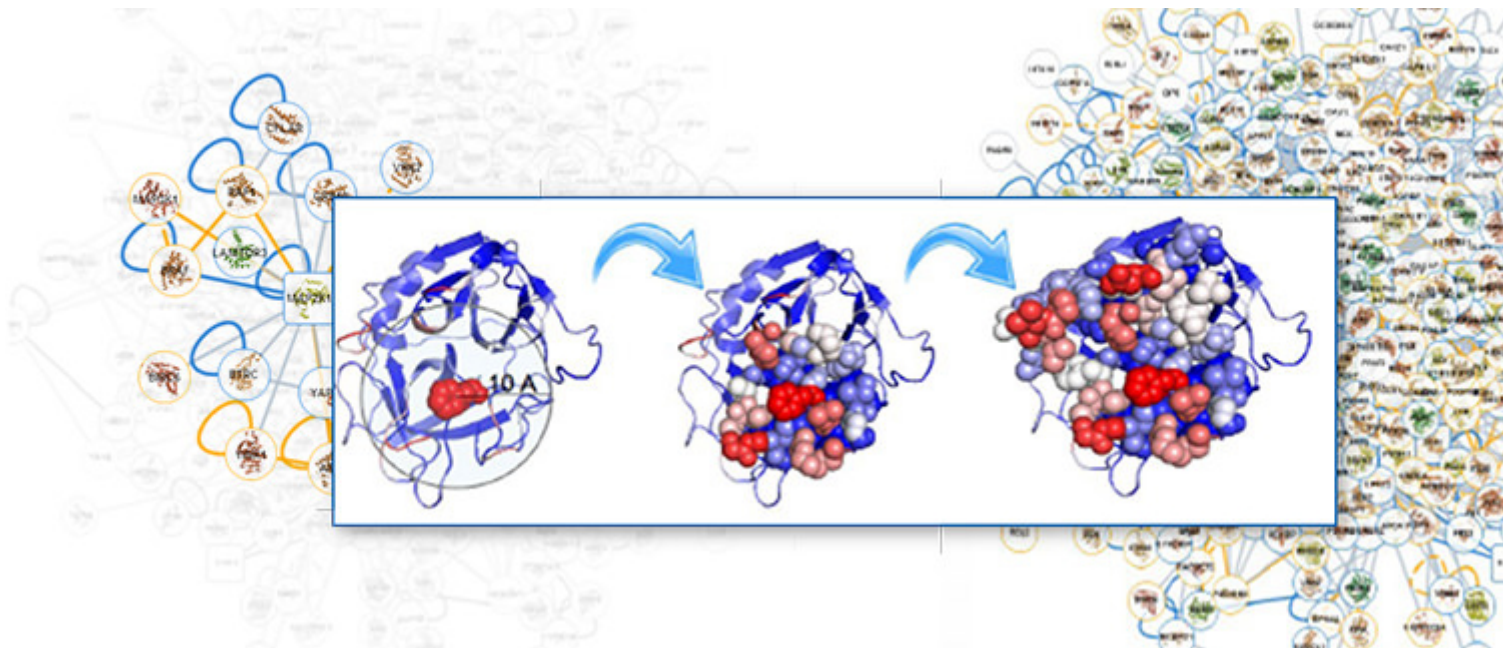


Docking for interactomics and personalized medicine



The ultimate goal of our protein-protein docking tools and their application to the characterization of protein interactions of therapeutic interest is to contribute towards personalized medicine and drug discovery targeting protein-protein interactions.

Summary

One of the goals of our research is to describe at molecular level the effect of disease-related SNPs and other genomic variations involving protein-protein interactions. For this, on the one hand we have compiled the largest data set of experimental data of binding affinity changes upon mutation in [SKEMPI server](#). On the other hand, we have implemented in the [CCharPPI webservice](#) over a hundred structure-based functions for the characterization of protein-protein complexes.

Using our computational tools for protein-protein docking and interface prediction, we aim to characterize pathological mutations that could be involved in protein interactions. This can be used to help to characterize annotated pathological SNPs as well as to improve multi-parametric predictors of pathogenicity in order to improve diagnosis from genetic data.

All this knowledge will also help to understand the interaction of small molecules with protein-protein interfaces, with the goal of designing compounds capable of inhibit protein interactions of therapeutic interest. Our aim is to integrate protein-protein docking, interface and hot-spot predictions, together with molecular dynamics for the identification of transient cavities within protein-protein interfaces, which could be used to host small compounds capable of specifically modulating protein-protein interactions.

Objectives

1. Application of homology modelling, docking and binding site prediction tools to provide structural models for human protein interactome.
2. Map pathological mutations on protein-protein structural models to understand better the effect of sequence variants in disease development (prevention, diagnosis) and/or drug response (treatment).

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