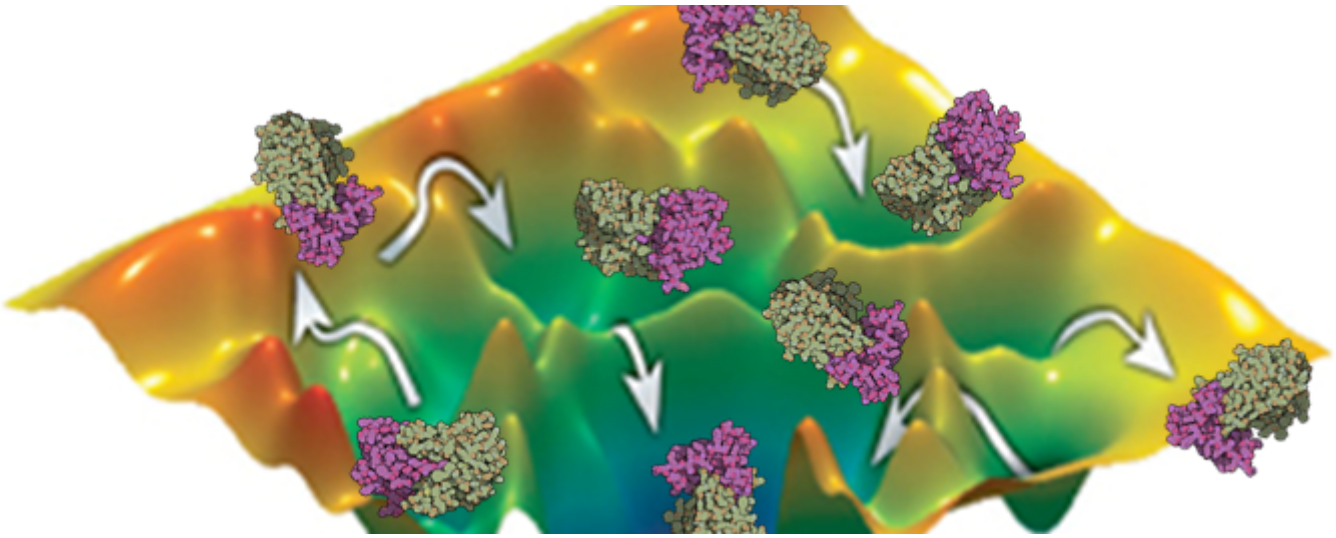
# Software development for protein-protein interactions



The main focus of our research is the development and optimization for High-Performing-Computing (HPC) of computational methodology for the structural and energetic characterization of protein interactions at molecular level.

## Summary

We aim to develop and optimize computational algorithms for characterizing 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, or prediction of hot-spot residues from energy calculations. The treatment of protein flexibility is currently a major bottleneck in protein docking. We are using the capabilities of MareNostrum to develop new algorithms based on molecular dynamics approaches. The use of unbound conformational ensembles prior to docking dramatically improve the predictive results in medium-flexible cases. We have also made available our software through different web servers, such as pyDockWeb for protein-protein docking, pyDockSAXS for the structural prediction of protein complexes using Small-Angle X-ray Scattering (SAXS) data in collaboration with Pau Bernadó (CBS, Montpellier), or OPRA for the identification of RNA-binding residues in proteins.

**Tools & Databases List** - Protein Interactions and Docking Group

We are continuously validating our docking methods in CAPRI, a world-wide community experiment that aims to evaluate the current state of protein-protein docking prediction. The results of our docking methods have been overall highly encouraging (within top 5 groups out of more than 60 participants in both the 5th and 6th CAPRI editions).

## Objectives

1. New efficient docking methods for HPC implementation.
2. More efficient identification of correct docking poses, especially in difficult cases such as weak interactions, multi-protein complexes or membrane proteins.
3. Inclusion of conformational flexibility by using conformational ensembles, interface refinement, and coarse-grained flexible docking.
4. Integration of low-resolution structural data from SAXS or EM.
5. New methods for protein-RNA and protein-DNA binding.
6. Multi-scale modeling of macro-complexes, such as transcriptional complexes, nucleosome or chromatin.

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