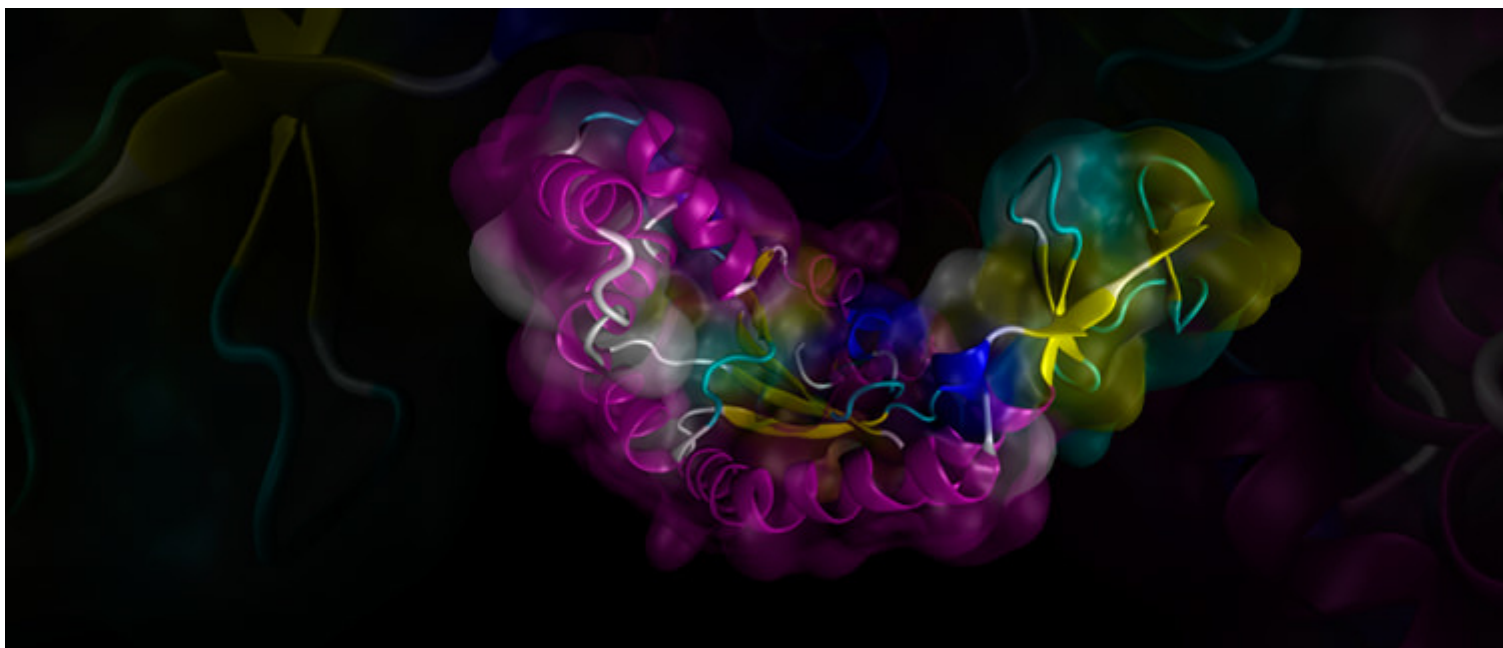# Advanced docking strategies

Molecular recognition is the basis of biological function. Docking is among a number of structural bioinformatics strategies trying to understand molecular recognition, both to understand structure to function relationships in macromolecules, and to derive tools useful in fields like drug design.

Summary

Molecular recognition is the basis of biological function. There are a number of structural bioinformatics strategies trying to understand molecular recognition, both to understand structure to function relationships in macromolecules, and to derive tools useful in fields like drug design. Our group is interested in contributing to some aspects of these strategies, in particular the introduction of specific effects of solvation (key water molecules, predicted hydration shells) in docking algorithms, and the use of coarse-grained and atomistic simulation to understand consequences of flexibility and dynamics of macromolecules in molecular recognition.

Objectives

- To catalogue and evaluate the effects of water molecules and ions, either from experiment, or calculation to improve docking.
- To evaluate the use of macromolecular flexibility parameters extracted from simulation on docking experiments.

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