

Molecular Docking

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The goal of molecular docking approaches is to anticipate a ligands optimum binding mode to a macromolecular partner (here, just proteins are considered). It entails creating various potential ligand conformations/orientations, or poses, within the protein binding site. As a result, accessibility to the molecule targets three-dimensional structure is a must; it can be an empirically solved structure (such as through X-ray crystallography) or a structure generated by computational techniques.

The two significant steps of molecular docking are an engine for sampling conformations and orientations and assigning a score to each expected positions scoring function.

The sampling procedure should examine the conformational space given by the free energy landscape, where the scoring process in docking approximates energy. The scoring function should be able to correlate the native bound-conformation to the energy hyper surfaces global minimum.

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