

# Ligand docking and virtual screening in structure-based drug discovery

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## **Abstract**

As the number of high-resolution three-dimensional protein and nucleic acid structures continues to grow, ligand docking-based virtual screening of chemical libraries to a receptor are playing a critical role in the drug discovery process by identifying new 'drug-candidates'. The capability to correctly predict ligand-protein interaction is fundamental to any accurate docking algorithm and the necessary starting point for any reliable virtual screening protocol. Furthermore, explicit consideration of receptor flexibility in computational ligand docking is emerging in many cases as crucial for an accurate prediction of the orientation and interactions of ligands within the binding pocket. The combination of ligand docking with a fast scoring algorithm that can account for the thermodynamics of binding, and discriminate between potential active/inactive compounds, can greatly reduced the number of compounds to be tested experimentally, while predicting a detailed structure of hits bound to the receptor useful enough to help the synthetic elaboration of leads.