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Molecular Docking
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Chapter

Molecular Docking in the Study of Ligand-Protein Recognition: An Overview

Iqbal Azad

Abstract

Molecular docking is a bioinformatics-based theoretical simulation strategy. It is employed to study ligand-protein interaction profiles and predict their binding conformers and affinity through computational tools. Since the 1980s, computational tools have been used in the drug discovery process. The initial molecular modeling approaches available at the time focused on a rigid view of the ligand-protein interaction due to the limited computational capabilities. The advancement of hardware technology has made it possible to simulate the dynamic character of the ligand-protein interactions throughout time. The current chapter deals with an outline of the progression of structure-based drug discovery methodologies in the investigation of the ligand-protein interaction profiles from static to improved molecular docking strategies.

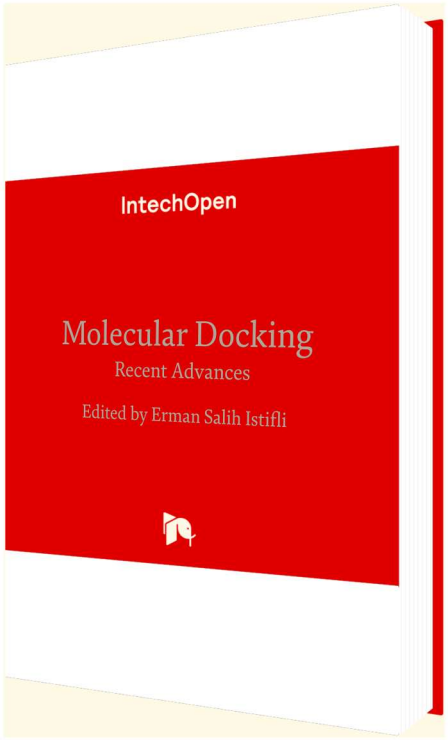
Keywords: Molecular docking, AutoDock, Vina, AutoDockFR, iGEMDOCK, Drug discovery process, Virtual screening

1. Introduction

Docking tools have simplified the study of interactions between drug molecules and receptor proteins, DNA, or biological molecules [1]. These interactions take place covalently. Furthermore, critical molecular mechanisms, ligand binding approaches, and factors influencing the ligand-protein interaction profile can be estimated with the help of the docking results [2, 3]. Docking suites can be used to calculate the binding energies associated with the most stable conformation of drug-receptor interactions (**Figure 1**) [4, 5].

2. Types of docking

In 1982, Kuntz et al. developed the first molecular docking algorithm through the estimation of the released binding energy [6, 7]. Docking evaluations are performed to regulate the interaction profile between the ligand and target and to search for the most suitable conformation of the ligand in the complex. Empirical scoring functions are also explored, which transform binding energy into the docking score [8]. There are numerous free online tools available to generate 3D ligand and target interaction



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Molecular docking is a widely used bioinformatics method in biology, medicine, and biochemistry. This method, which can model interactions between different receptors and their various ligands at the molecular level, can represent intermolecular interactions at an unprecedented resolution that may not be achieved by classical experimental approaches. This book describes different aspects of this m...

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