Chapter 11
Applications of Molecular Docking:
Its Impact and Importance outside the Purview of Drug Discovery

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ABSTRACT

Computational tools have extended their reach into different realms of scientific research. Often coupled with molecular dynamics simulation, docking provides comprehensive insight into molecular mechanisms of biological processes. Influence of molecular docking is highly experienced in the field of structure based drug discovery, wherein docking is vital in validating novel lead compounds. The significance of molecular docking is also understood in several environmental and industrial research, in order to untangle the interactions among macromolecules of non-medical interest. Various processes such as bioremediation (REMEDI Dock), nanomaterial interactions (NANO Dock), nutraceutical interactions (NUTRA Dock), fatty acid biosynthesis (FAD Dock), and antifoulers interactions (FOUL DOCK) find the application of molecular docking. This chapter emphasizes the involvement of computational techniques in the aforementioned fields to expand our knowledge on macromolecular interacting mechanisms.

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INTRODUCTION

Interactions between biomolecules are fundamental to all biological processes. Using these interactions, living organisms maintain complex regulatory and metabolic interaction networks that together constitute the processes of life (Cai, Li, Wang, & Chen, 2004). Understanding of the complexity of biological pathways and the interactions between the macromolecules involved has become imperative and molecular docking has catered to this need in a comprehensive manner. Molecular docking may be defined as a concept of computational chemistry which provides solutions to unravel the mechanism behind substrate-ligand interactions. It facilitates the interacting molecule to fit together based on their topography (Figure 1). The main objective of docking is to determine the best possible conformation of protein-ligand, protein-protein and/or other type of interactions with minimal energy. Docking is also seen as a vital technique in modelling the protein-ligand, protein-protein interactions and thereby involved in studies related to deciphering the molecular function of various complexes. Such studies pave way to explore novel products that could be very specific for a particular target (DesJarlais, Sheridan, Dixon, Kuntz, & Venkataraghavan, 1986; Goodford, 1984).

Molecular docking approach is a powerful mode to model the protein and small molecule interaction at the atomic level. It greatly helps in characterizing the behaviour of small molecules at their binding sites. The two major steps involved in docking are: (i) obtaining the stable ligand conformation and (ii) assessing its binding affinity, and in majority of cases, binding sites are predicted before performing docking. Binding sites are generally obtained by comparing the target of interest with the other proteins from same family bearing similar function (Meng, Zhang, Mezei, & Cui, 2011). The mechanism of molecular docking has evolved to a greater extent, starting from the “lock and key” model, which is the most primitive of all (Kuntz, Blaney, Oatley, Langridge, & Ferrin, 1982). “Induced-fit” model was seen as a logical extension of the basic lock and key model, where the active site changes its conformation based on the binding ligand (Koshland, 1963).

The applications are widespread, the information obtained are profound and docking has thrown the doors wide open to stride into new arena of research focussing on lead molecule designing, target discovery and analysing application potential of the compounds. Given the wide scope in studying the binding mode and affinities between various molecules, docking has become an indispensable approach that serves as a precursor to several wet lab researches. Concept of docking and its application has been

![Figure 1. Mechanism of molecular docking depicted through the interaction between the ligand, acetyl coA and the receptor, carboxyl transferase domain of acetyl coA carboxylase](image-url)