Chapter 2
Implications of Molecular Docking Assay for Bioremediation

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ABSTRACT

Bioremediation utilizes microbes to control environmental pollution, primarily through diverse enzymatic processes. With the incorporation of computation in biological experimentation, bioremediation has also been influenced by computational techniques. Molecular docking assay is one such pedestal of computational assisted bioremediation, which has been elaborated in this chapter. It helps in inferring whether the active site accommodate the pollutant molecules or not, depending on the stearic hindrance of the residues and nature of the active site pocket. The spotting of consequential active site residues and binding characteristics of compounds under study can conceivably be employed for site-directed mutagenic testing. From a vantage point, no one had expected such a remarkable usefulness of molecular docking assay for environmental research. Positive shades of low cost and efficiency, combined with eco-friendliness have made it a valuable method for analyzing biodegradative properties of enzymes responsible for pollution remediation.

INTRODUCTION

The world is facing an ever increasing menace of pollution due to industrialization and other anthropogenic activities. It is, therefore, at the foremost agenda of environmental scientists to find better, fast and eco-friendly solutions to mitigate pollution. Bioremediation is one such endeavor that exploits microbes

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to detoxify or degrade harmful contaminants in the environment. Bacterial enzymes are pollutant degradation workhorses that act to decontaminate environment. Molecular docking accelerates the procedure of choosing and improving enzymatic properties for a particular pollutant by quick computational scrutiny. The technique shows inordinate potential in its ability to predict enzyme adhesion and functionality in degrading or adsorbing the pollutant and presents a lucid picture of the relation and communication between pollutant and enzyme molecule. It helps in inferring whether the active site of certain enzymes accommodate the dye molecules or not, depending on the stearic hindrance of the residues and nature of the active site pocket. Protein-pollutant association is checked by assessing thousands of potential docking conformation poses. Picking poses that are reliable is an arduous task and one with lowest energy score is usually seen as the best match. Blind docking is attempted for proteins with unknown active site by entire protein surface scanning (Schnecke & Kuhn, 2000; Verdonk et al., 2005). Docking also provides information on mediator accommodation in the active site pocket to surmise about productive or non-favoured binding. The spotting of consequential active site residues and binding characteristics of compounds under study can conceivably be employed for site-directed mutagenic testing. These results then need to be tested in the lab experimentally and a critical evaluation of docking tools which gives better results might help define a set of rules and define a benchmark for such studies.

Molecular docking in remediation experienced a lag phase but now transitioned to alog phase in its-frequency of application and attention of environmental scientists. It is now a noticeable area of research methodology assisting bioremediation studies. Bioinformatics boasts of numerous successful techniques developed for protein-ligand docking but shape complementarity and simulation approaches are most popular. In shape complementarity approach a matching procedure portrays the protein and the ligand as complementary surfaces (Meng, Shoichet, & Kuntz, 1992). In the simulative approach, interaction energies of ligand and protein are calculated (Feig, Onufriev, Lee, Im, Case, & Brooks, 2004). Knowledge derived information from docking assays for bioremediation is critical for a reliable evaluation of the state of the enzymatic micro-environment besides the transformations taking place inside enzyme, as well as for crafting strategies for sozotechnical measures aimed at environment clean up. This chapter discusses foundation of eco-analytical information for bioremediation, gained from molecular docking assay and provides information on some studies conducted until now. Finally the challenges and barriers to the molecular docking based bioremediation studies have also been analyzed and future perspective of such studies is also provided. The predictions are valuable for environmental chemists perusing metabolic intermediates, supervisory bodies/controllers endeavoring probable toxic products, microbiologists seeking to perceive microbial biodegradation, besides others having wide array of fascinations.

OVERVIEW

Molecular docking is a technique which calculates the preferred binding positioning of one molecule relative to the other, at a minimum energy conformation during complex formation (Lengauer & Rarey, 1996; Brooijmans & Kuntz, 2003). Docking can be carried out among protein and a small molecule, protein-protein, Protein-DNA, protein-RNA, protein-lipid, protein-sugar, polymer-ligand etc. where larger moiety is treated as a substrate and smaller one as the ligand. In case of protein-ligand interaction, which is the focus of this chapter, ligand generally fits inside cavity of the protein, which is usually predicted by a search algorithm (Westhead, Clark, & Murray, 1997; Gohlke, Hendlich, & Klebe, 2000; Brooijmans & Kuntz, 2003). This protein cavity turns active as a result of contact with substrates. It is formed of