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REVIEW ARTICLE

Computational Docking Technique for Drug Discovery: A Review

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ABSTRACT:

Computational and experimental techniques are two complimentary approaches that have important roles in drug discovery and development. Earlier time and cost of bringing a new drug in market bears a question as it takes seven to twelve years and $ 1.2 billion are often cited. Furthermore, five out of forty thousand compounds tested in animals reach human testing and only one of five compounds reaching clinical studies is approved. This accounts for a large input in terms of time, money and human and other resources. Therefore, new approaches are needed to facilitate, expedite and streamline drug discovery and development, save time, money and resources. Among many computational tools, molecular docking is one of the important means that can be used in drug discovery. It provides the information regarding the binding affinities between small molecules (ligands) and macromolecular receptor targets (proteins). Various approaches, methodology are cited in various literatures for describing the cost, time effect with success of drug discovery task. In this review, introduction of the available molecular docking methods, with simple methodology of docking and examples of drug design and discovery through computational docking methods is discussed and emphasis is made on various examples of sampling algorithms, scoring functions with their relevant characterstics with summary on type of ligand binding with receptors.

KEYWORDS: Modelling, Docking, ligand, algorithm, scoring.

INTRODUCTION:

In today's scenario there is increasing demand of genetics and molecular biology science which result in the identification of increase number of potential molecular targets for new drug discovery and development. These potential targets can be achieved through exploitation of emerging structural biology, "rational" drug design, screening of chemical libraries, or a combination of these methods.

In the past 5-10 years the processes used by academic and industrial scientists to discover new drugs has recently experienced a true renaissance with many new and exciting techniques being develop. For discovery of compounds exhibiting high specificity and efficacy structure-based drug design is perhaps the most elegant approach [1]. Nowadays, structure-based research approach results in a number of recent successful drugs. These advances in structure-based drug design are likely to have impact on the economics of drug discovery. Thus for lead discovery docking technique is widely accepted as by implementation of this technique the structures of more and more proteins and nucleic acids become available [2]. Hit-rate enhancement of docking screens and the accuracy of docking structure predictions are considered in recent studies. In this review article, various methods of docking technique are considered by summarizing about algorithms used,

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