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REVIEW ARTICLE

EFFICIENT WAY OF DRUG DESIGNING: A COMPREHENSIVE REVIEW ON COMPUTATIONAL TECHNIQUES

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As demand of novel drugs is increasing day by day, the need of efficient, inexpensive techniques arises which can help in drug design and discovery. In order to achieve the goal, computational techniques like docking, pharmacophore modeling, homology modeling are employed by researchers around the globe in search of novel potent drugs. In this review, relevant computational techniques are highlighted which will help new generations to carry out hassle free research in an efficient manner.

Key words: Computational, Docking, Methodology, Modeling, Drug design.

INTRODUCTION

The serendipitous part of drug discovery can now be overcome by rational designing of drugs with the help of computational techniques like molecular modeling, docking, virtual screening etc. that can identify promising candidates prior to synthesis. The structural aspects of active site (drug targets) composition and the orientation of different amino acids can be used in drug design and discovery. Nowadays, with the help of computational techniques, a specific potent lead molecule against a particular disease can be designed on the basis of nature of interactions like enzyme-substrate, drug-protein and drug-nucleic acid interactions that may provide a conceptual framework for designing the desired potency and specificity of potential drug leads for a given therapeutic target (Nantasenamat *et al* 2009; Aparoy *et al* 2012).

The active and time consuming process of drug discovery and development via traditional approaches like synthesis and evaluation of a potent medicinally active compound can be replaced by computational methods. The most important aspect of computer aided drug design is its crucial role in drug discovery that can save time and cost involved in drug development process. It can now easily be assessed from the literature survey that computational methods have become an interdisciplinary science with the involvement of different scientific fields like pharmacology, molecular biology, chemistry (Aparoy *et al* 2012).

In present review, it was attempted to describe all computational techniques with an idea to achieve wide circulation which in turn would be beneficial for new researchers where they can understand and design their research more efficiently. The literature study reveals the impact of computational approaches in drug designing and a wide number of publications are available on docking, mapping, homology modeling etc. (Teif, 2005; Todeschini and Consonni, 2008; Congreve and Marshall, 2010; Baron *et al* 2010; Yang, 2010; Kumar, 2011; Sharma *et al* 2011; Alberts *et al* 2013; **Figure 1**). **Table 1** enumerates different terms used in computational studies.