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Software based approaches for drug designing and development: A systematic review on commonly used software and its applications

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ABSTRACT

Drug discovery include drug designing and development, is a multifarious and expensive endeavor, where least number of drugs that pass the clinical trials makes it to market. Software based drug discovery and development methods have major role in the development of bioactive compounds for over last three decades. Novel software based methods such as molecular modeling, structure-based drug design, structure-based virtual screening, ligand interaction and molecular dynamics are considered to be powerful tool for investigation of pharmacokinetic and pharmacodynamic properties of drug, and structural activity relationship between ligand and its target. Computational approaches such as docking confer interaction of small molecules with structural macromolecules and thereby hit identification and lead optimization. These methods are faster, and accurately provide valuable insights of experimental findings and mechanisms of action. In addition, appropriate implementation of these techniques could lead to a reduction in cost of drug designing and development. Currently in biomedicine sciences these software are exhibiting imperative role in the different phases of drug discovery. The review discusses working principle and successful applications of most commonly used software for drug designing and development.

1. Introduction

Exploration of software and model based tools have become a key component of the drug discovery and development in pharmaceutical industry, playing a crucial role in expanding new bio-active drugs across a range of therapeutic areas. Proper use of software and computer based modern methods has reduced several hindrances in the process of drug discovery and hasten new drug development. Modern medicinal chemistry methods like molecular modeling, structure-based drug design, structure-based virtual screening, ligand based modeling and molecular dynamics are used as a powerful tool to know pharmacokinetic and pharmacodynamic properties, and structural activity relationship of ligands with its target (Table 1) [1,2]. Combine application of modeling such as ligand based computer aided drug designing (CADD) and simulations provide a powerful paradigm for modernizing clinical study design and analysis [3,4]. Implementation of these techniques can reduce the numbers of animals needed in the research and preclinical stages of drug discovery, help for trouble-free to handle huge data, and improve the accuracy of study results [5,6].

Successful drug discovery, development and launch of single new drug into the market costs about one billion dollar and it requires nearly 12 years for accomplishing. High cost, insufficient and lengthy time duration, high level of risk, uncertainty in the results, and highly complex procedures are the main challenges in the development of new drug. To overcome these problems, it is needed to employ new and more cost effective drug discovery and designing methods (Fig. 1) such as software and computer aided drug design and molecular docking [5,7]. The present review highlights commonly used software used for new drug development along with their potential uses.

2. Software for drug designing, discovery and development

The software are further categorized on the basis of task performing by the software and their working principle like software assessing pharmacokinetic parameters, ligand interactions and molecular dynamic, molecular modeling and structural activity relationship, image analysis and visualizers, data analyzer and behavior analysis software.

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Table 1
Software and computer based programs used during new drug discovery and development.

Sr. No.	Software name	Major use	References
1. Pharmacokinetic parameters			
1	DDDPlus	Dissolution and disintegration study	8,9
2	GastroPlus	In-vitro and in vivo correlation for various formulations	10,11
3	MapCheck	Compare dose or fluency measurement	12,13
2. Ligand interactions and molecular dynamic			
4	AutoDock	Evaluate the ligand-protein interaction	14,15
5	Schrodinger	Ligand-receptor docking	16,17
6	GOLD	Protein-ligand docking	18,19
7	BioSuite	Genome analyzing and sequence analyzing	20,21
3. Molecular modeling and structural activity relationship			
8	Maestro	Molecular modeling analysis	22,23
9	ArgusLab	Molecular docking calculations and molecular modeling package	24,25,26
10	GRAMM	Protein-protein docking and protein-ligand docking	27,28,29
11	SYBYL-X Suite	Molecular modeling and ligand based design	30,31,32
12	Sanjeevini	Predict protein-ligand binding affinity	33,34
13	PASS	Create and analysis of SAR models	35,36,37
4. Image analysis and Visualizers			
14	AMIDE (A Medical Image Data Examiner)	Medical image analysis in molecular imaging	38,39
15	Discovery Studio® Visualizer	Viewing and analyzing protein data	40,41
16	Imaging Software Scge-Pro	Cytogenetic and DNA damage analysis	42,43
17	Xenogen Living Image Software	In vivo imaging display and analysis	44,45
5. Data analysis			
18	GeneSpring	Identify variation across set of sample and for correction method in samples	46
19	QSARPro	Protein-protein interaction study	47,48
20	REST 2009 Software	Analysis of gene expression data	49,50
6. Behavioral study			
21	Ethowatcher	Behavior analysis	51
22	MARS (Multimodal Animal Rotation System)	Animal activity tracking, enzyme activity, nanoparticle tracking and delivery study	52

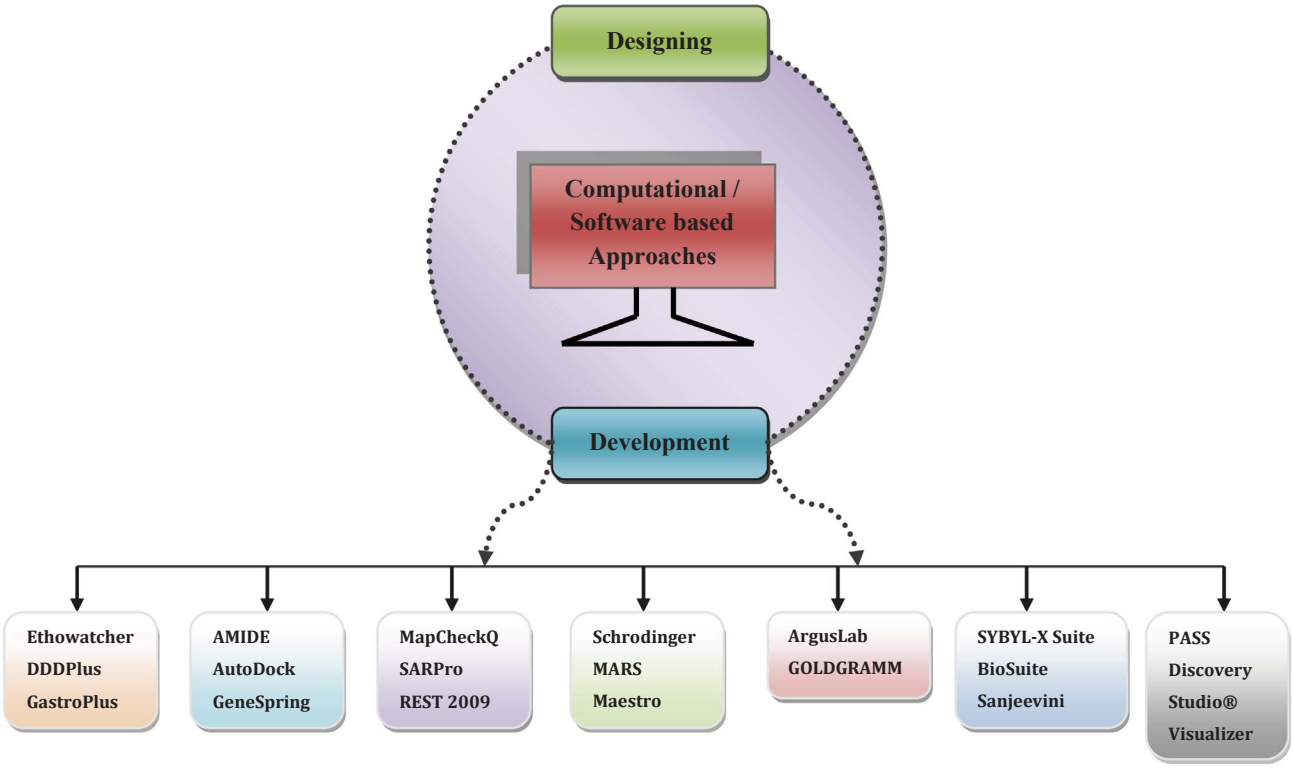

Fig. 1. Software based approaches for drug designing and development.

2.1. Pharmacokinetic parameters

2.1.1. DDDPlus (Dose Dissolution and Disintegration software)

DDDPlus (Dose Disintegration and Dissolution Plus) is used to study disintegration and dissolution pattern of dosage form and active ingredients. It is an advanced computer program employed by formulation scientists to simulate in vitro disintegration and dissolution of active pharmaceutical ingredients (API) and excipients under different