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Software Used for New Drug Discovery and Development

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ABSTRACT: Exploration of model based tools and software used for the development and discovery of new drugs in pharmaceuticals industry, playing a vital role to expand the bioactive drugs. The proper use of software and modern based computers has reduced various hindrances in the drug discovery process. The software used in pharmaceutical industry are categorized as Pharmacokinetic Parameters which include DDDPlus (Dose Dissolution and Disintegration software) to study the dissolution and disintegration of drugs, GastroPlus for the study of In vitro and in vivo correlation for various formulations; Ligand interactions and molecular dynamic such as Schodinger for the study of ligand receptor docking, GOLD (Genetic Optimization for Ligand Docking) to study the protein –ligand docking; Molecular modeling and structural activity relationship, for the study of molecular modeling analysis, prediction of protein-ligand binding affinity, create and analysis of SAR models and molecular docking and calculations and molecular modeling package Maestro, Sanjeevini, PASS() and ArgusLab are used respectively; For the study of Behavioral parameters Ethowatcher for behavioral analysis and MARS (Multimodal Animal Rotation System) to check the enzyme activity, nanoparticle tracking and delivery study followed by Data Analysis QSARPro and REST 2009 Software are used to obtain the data of protein-protein interaction and In vivo imaging display and analysis. The above mentioned softwares provide valuable insights of experimental findings and mechanisms of action. These techniques help in reduction of cost of drug designing and development. In Pharmaceutical industry softwares areexhibiting imperative role in the different phases of drug discovery.

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