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# SOFTWARE APPLICATIONS IN DRUG DISCOVERY

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**Abstract**
*Artificial intelligence has significantly transformed the field of medicine, especially in drug discovery, by reducing time and costs. This study highlights key software tools that assist beginners in analyzing physicochemical properties, binding sites, protein interactions, and toxicity of potential drug molecules. These tools have simplified complex processes and sparked innovation within the pharmaceutical industry*

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## INTRODUCTION

Drug discovery is the process through which poent and new drug moieties are identified through the use of biology,chemistry, and pharmacology (1). New molecules with a strong therapeutic impact are produced by this process.Drug discovery is the most imperative activity that contributes to human health and comfort.However,the discovery of a new drugs either from synthetic or natural source like plant, animal and microbes etc. using wet laboratory testing,validations, and synthetic procedures is very complex, expensive, and lengthy processes(2).The financial burden is exacerbated by the low success rate and uncertainty of results in clinical trials. The discovery of a single new drug molecule,its characterization,and development costs approximately 2.6 billion USD and takes approximately 10-15 years on average (3). Todecrease costs and speed up the discovery of new drugs has became a demanding and critical issue in industry. The exercise to find ways to reduce expenses and expedite the process of discovering new drugs. Drug discovery can be usefully split into four components: drug design,polypharmacology, drug repurposing, and drug screening (4). Different strategies are used to tackle the cost burden of drugdiscovery. The use of software's is one of them and it revolutionized the drug discovery. Artificial intelligence software and databases have been successful used in compound identification,biological data analysis, and clinical trials,which brought attention to the pharmaceutical industry.It makes the search of new pharmaceuticals quicker, cheaper,easier, more effective, and reduces the uncertainty of results. Software's use can reduce the cost of preclinical drug development by 20-40% and can reduce the time span of drug screening upto 40-50% and accelerate design and validation of drug candidates by as much as 15times (5,6). Now a day's many pharmaceutical industries like GSK, Pfizer,Novartis, Roche,and Sanofi etc. used software's to predict the physicochemical properties, the 3D structure of proteins, drug protein interactions,

pharmacokinetic parameters, toxicity and bioavailability of drug molecule etc (7).

Drug screening involve physicochemical properties, bioactivity, and toxicity predictions of new drug molecules.For physicochemical parameters such as solubility, dissolution coefficient, log P, pka, number of rotatable bonds,and drug likeliness properties, software such as Mcule, Molinspiration, Chemicalize, Chemaxon,and pKCSM are used.For bioactivity and mechanism of action prediction, MANTRA, cMap dataset and MoAble tools, (9) are used,while LimTox, DeepTox, eToxPred, Lazar, ProTox, and Mcule toxicity calculator are used (5).

Drug designing includes the prediction of the 3D structure of a target protein, drug-protein binding interactions, drug activity, and de novo drug design. AlphaFold and MATLAB software's used for the prediction of protein structure (10,11),Autodock Vina,PyRx, Schrodinger, Mcule 1-click docking, molecule operating environment (MOE)and VDM software's are used for predicting drug-Protein binding interactions and for binding visualization UCSF Chimera,PyMOL and Discovery Studio software's are mostly used (12).For pharmacokinetic prediction like absorption, distribution, metabolism and excretion of drug molecules pkCSM, preADMET, SwissADME, PreMetabo, Molinspiration software's are used (8),for de novo drug design reinforcement learning based model ReLeaSE (13) the encoder-decoder-based model ChemVAE (14) the GAN-based model GraphINVENT (15) and the RNN-based model MolRNN (16) are used.

The self organizing map (SOM) and KinomeX softwares are employed to investigate the polypharmacology of molecules and create molecules that target at multiple sites (5). Drug repurposing involves identification of therapeutic targets and predicting new therapeutic uses of molecules. By assimilating the results in a unified and mechanized way, the **software** assists in evaluatinglearning, and solving pharmaceutical big data to expose new molecules.

## Conclusion

The conversion of new drug molecule into the medicine takes many years,but by using software's we can not only compare the new drug moiety with the pre-existing ones but also modify them before introducing into the market in less time and expenses.

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