



USE OF SOFTWARE'S IN DRUG DISCOVERY

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DOI: <https://doi.org/10.5281/zenodo.15193687>**Keywords**drug discovery, software's,
Polypharmacology**Article History**

Received on 02 March, 2025

Accepted on 02 April, 2025

Published on 11 April, 2025

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Abstract

The use of artificial intelligence is very common now a days and has a great influence on our lives. It changes the style of thinking in the entire field of medicine. The use of software's in drug discovery brings a tremendous change in terms of time, and expenses. The aim of the study is to point out some basic software's which make drug discovery easier for the beginners to study physicochemical properties, binding sites, protein interactions and toxicity parameters of new drug molecules. pharmaceutical industry has engaged in an arduous and compelling brainstorming.

**INTRODUCTION**

Drug discovery is the process through which potent 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 drug 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). To decrease costs and speed up the discovery of new drugs has become 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 drug discovery. The use of software's is one of them and it revolutionized the drug discovery. Artificial intelligence software and databases have been successfully 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 up to 40-50% and accelerate design and validation of drug candidates by as much as 15 times (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 involves 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-likeness properties, software such as Mucle, 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 Mucle 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 are used for the prediction of protein structure (10,11), Autodock Vina, PyRx, Schrodinger, Mucle 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 evaluating learning, 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.

Authors' contributions

All the authors have contributed equally and have approved the final manuscript.

Funding

Not applicable.

Acknowledgments

Not applicable.

DECLARATIONS Ethics approval

Not applicable.

Competing interests

The authors declare that they have no competing interests.

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