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Anjali A
Department of Pharmaceutics,
AKRG College of Pharmacy,
Nallajerla, E.G, Andhra Pradesh,
India

SS Prasanna Kumar P
Department of Pharmaceutics,
AKRG College of Pharmacy,
Nallajerla, E.G, Andhra Pradesh,
India

N Sai Krishna
Department of Pharmacology,
AKRG College of Pharmacy,
Nallajerla, Andhra Pradesh,
India

Devisri R
Department of Pharmaceutics,
AKRG College of Pharmacy,
Nallajerla, E.G, Andhra Pradesh,
India

Hema Sri Sai Sravya R
Department of Pharmaceutics,
AKRG College of Pharmacy,
Nallajerla, E.G, Andhra Pradesh,
India

Sakhina Manisha SK
Department of Pharmaceutics,
AKRG College of Pharmacy,
Nallajerla, E.G, Andhra Pradesh,
India

Balu CH
Department of Pharmaceutics,
AKRG College of Pharmacy,
Nallajerla, E.G, Andhra Pradesh,
India

Jyothika Eswari S
Department of Pharmaceutics,
AKRG College of Pharmacy,
Nallajerla, E.G, Andhra Pradesh,
India

Corresponding Author:
Anjali A
Department of Pharmaceutics,
AKRG College of Pharmacy,
Nallajerla, E.G, Andhra Pradesh,
India

In silico drug discovery in traditional medicinal plants- a review

Anjali A, SS Prasanna Kumar P, N Sai Krishna, Devisri R, Hema Sri Sai Sravya R, Sakhina Manisha SK, Balu CH and Jyothika Eswari S

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Abstract

Medicinal plants have been a rich source of therapeutic traders for centuries. They have offered many bioactive compounds with gigantic pharmacological potential. Nevertheless, classical drug discovery from plants is often slow, time-consuming, and expensive. In recent years, in-silico protocols have been found to be useful tools to speed up and systematize this process. Computational strategies coupled with molecular docking, pharmacophore modeling, virtual screening, and ADMET prediction allow scientists to quickly identify and analyze plant-derived molecules with strong interactions against novel organic targets. This approach unites traditional know-how with current technology, offering novel perspectives for herbal product research and opening gates to the development of safe, efficient, and affordable plant-based altogether therapeutics. This review highlights various insilico studies including databases, computational tools & techniques, softwares used to identifying, designing, and optimising the drug molecule and predict the protein binding of drug, suitability of drug to specific diseases.

Keywords: *In-silico* drug discovery, Traditional medicine, Molecular docking, Phytochemicals, computational pharmacology

Introduction

In the past, drug discovery began with traditional knowledge people observed how certain plants or natural substances helped treat illnesses and passed this wisdom down through generations. Over time, scientists began isolating the active compounds from these plants to understand and use them more effectively. Researchers often start by using computer simulations to predict which molecules might work as drugs. Once they find a promising molecule, they look for its source in nature. This method is faster and more precise, the potential drugs still need to be tested in the lab and in living organisms to confirm that they are safe and effective. (Pirintsos. S *et al*.,2022) [12].

Moving from Traditional Drug Testing to Modern Safety Monitoring in Medicine- Pharmaceutical evaluation makes sure that medicines are safe and work as expected. However, traditional testing methods sometimes struggle to keep up with today's more complex drug formulations.

To address this, advanced techniques like GC-NMR (Gas Chromatography-Nuclear Magnetic Resonance) and HPLC-MS (High-Performance Liquid Chromatography-Mass Spectrometry) have been developed. (Dharma Moorthy G 2025) [3].

Some examples of in silico tools relevant in drug design are:

1. QSAR [Quantitative Structure-Activity Relationship]
2. Homology modelling
3. Molecular dynamics

These methods help increase the chances of discovering new and powerful drugs that will work well in real life (Wankhede YS *et al*.,2024) [16]. However, these computer predictions still need to be confirmed through lab tests or animal studies before the drugs can be trusted. (Aarón R-H *et al*., 2025) [1].

In Silico Methods: A Modern Way of Drug Discovery- helps how these modern approaches help in finding new medicines from natural sources. With advanced software, scientists can now quickly check thousands of natural compounds to see which ones might work as safe and effective drugs, making the whole search process much faster. (Monisha D et al., 2025) [8].

Evaluation of Natural Compounds Using Docking and Transcriptome Technologies- used computer tools like molecular docking, RNA sequencing (RNA-seq), and shape analysis to compare similar natural compounds.

The results suggest that compounds working through similar mechanisms tend to have similar effects. This helps us better understand how natural mixtures work inside the body. (Park M *et al*.,2023) [11].

Natural SIRT2 Inhibitors for Cancer Found In-Silico- focuses on targeting the cancer-related enzyme SIRT2 using an in-silico approach. Researchers identified three natural compounds NPA009578, NPA006805, and NPA001884 that showed stronger docking interactions than existing known inhibitors, along with promising in-silico drug-likeness profiles. (Khanfar MA *et al*., 2021) [6].

Advanced modelling techniques- developing new medicines is a very slow and expensive process, and many potential drugs fail because they are either not absorbed properly in the body or turn out to be toxic. To avoid such failures, researchers now use ADMET tools, which predict how a drug will behave inside the body how it is absorbed, distributed, metabolized, excreted, and whether it could be harmful.

This looks at how advanced computer-based techniques like QSAR (Quantitative Structure-Activity Relationship), machine learning, molecular docking, and PBPK (Physiologically Based Pharmacokinetic) modelling are used to check a compound's safety and "drug-like" properties before moving further.

By combining these in-silico predictions with real-world lab tests and animal studies, scientists can greatly reduce costs, speed up the drug discovery process, and improve the chances of finding a successful medicine.

The study of In-Silico Gilroy Against COVID-19- Gilroy, a well-known Indian medicinal herb, was studied using computer-based (in-silico) methods to see if it could fight SARS-CoV-2, the virus that causes COVID-19. Out of five compounds tested, berberine showed the strongest ability to attach to the virus's main protease and had good drug-like properties. This makes berberine a promising herbal antiviral and shows how traditional medicine can work together with modern drug discovery, especially during global health emergencies.

Objectives

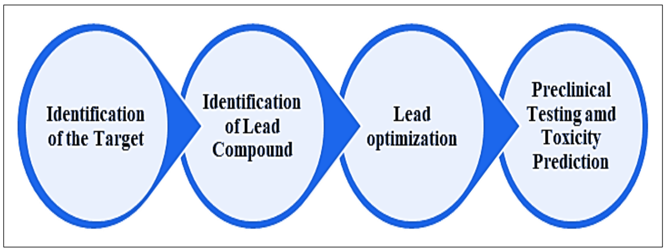
- Select and identify traditional medicinal herbs with proven or reported therapeutic potential, using knowledge from ethnopharmacology and published literature.
- Use molecular docking to study how plant-based compounds (phytochemicals) interact with specific protein targets, predicting their binding strength and possible interactions.
- Gather or extract details of bioactive compounds from selected plants using online phytochemical databases such as IMPPAT, PubChem, and ChEMBL.
- Carry out molecular docking experiments to confirm predicted binding affinities and interaction patterns between phytochemicals and target proteins.
- Evaluate the drug-likeness and ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) profiles of selected phytochemicals using in-silico tools like SwissADME and pkCSM.

Previous Studies

Munir Ibrahim *et al*. [2025] [4] reported that Tuberculosis (TB), caused by *Mycobacterium tuberculosis*, remains a significant global health challenge, particularly in developing nations. Side effects and increasing drug resistance often limit conventional pharmaceutical treatments for TB. This has highlighted the urgent need for novel therapeutic agents. Traditional medicine offers a promising avenue for discovering effective and safer alternatives. *In silico* approaches play a crucial role in pharmaceutical research by facilitating the identification of novel therapeutic compounds. These techniques are widely employed to explore potential treatments for diverse diseases. This study aims to identify lead molecules with anti-tuberculosis potential that could be further studied for their inhibitory potential and possible optimization for the treatment of tuberculosis. *Chlorophytum borivilianum* and *Asparagus racemosus* were selected for their diverse phytochemical profiles and proven pharmacological activities, including significant antimicrobial properties that make them promising candidates for in silico exploration of anti-tuberculosis therapeutics. The drug-likeness and pharmacokinetics of phytochemicals from the plants were evaluated using Lipinski's rule of five, and ADMET predictions. Phytochemicals meeting these criteria were subjected to molecular docking against *Mycobacterium tuberculosis* targets: CYP51, InhA, and EthR, using Vina (PyRx)platform to calculate binding affinities and assess interaction stability. Molecular dynamics simulations (100 ns) were performed to validate the stability of the docked complexes, focusing on key parameters such as RMSD, RMSF, and Rg. This approach identified hecogenin, sarsasapogenin, and isoflavone as potential inhibitors of CYP51 with high binding affinities and stable interactions, suggesting their promise as lead compounds for tuberculosis treatment. (Ibrahim M *et al*., 2025) [4].

Nawaz A *et al*. [2024] [10] and his team explained that In silico drug design uses computing techniques and algorithms to simplify the process of identifying, improving, and assessing prospective candidates for drugs. CADD (Computer-Aided Drug Design,) allows experts to effectively investigate extensive chemical spaces, anticipate interactions among drugs and targets, and evaluate the pharmacokinetics and cytotoxic features of drug molecules. This is achieved by merging many fields of study, such as molecular modelling, computational biology, and cheminformatics. The use of CADD methods, such as virtual screening, structure-based drug design, and ligand-based drug design, has culminated in significant progress in the discovery of prospective lead compounds, the enhancement of current therapies, and the reutilization of authorized pharmaceuticals. In addition, artificial intelligence and machine learning have played a significant role in decreasing the duration and expenses related to the pharmaceutical manufacturing procedure, thereby becoming an essential element in decision-making for improved and safer therapeutic agents. This chapter emphasizes the crucial importance of CADD in speeding up the process of discovering new drugs. (Nawaz A *et al*., 2024) [10].

Stages of drug development and in silico integration



Target identification is the initial stage of drug discovery, where researchers search for chemicals associated with disease by browsing databases and in-silico tools. Following virtual screening and molecular docking for lead compound identification, QSAR, ADMET, and molecular simulations are employed to develop the lead as a safe, effective, and bioavailable drug. Finally, only the most secure candidates reach clinical trials due to preclinical screening and toxicity prediction with software such as pkCSM and Toxtree, which is cost-effective, time-saving, and avoids lab labor. (Zhang X *et al*., 2022) [17].

Computational Tools and Techniques in Drug Discovery

Molecular docking

Molecular docking used to check how well a drug candidate (small molecule) can fit into a protein's active site (the disease-related target). It works like trying to see if a key (drug) fits into a lock (protein). The computer tests many possible positions of the drug in the protein and chooses the best fit. It also gives a score that shows how strongly the drug might bind to the protein. This helps scientists quickly find promising drug candidates before doing lab or animal tests.
Common tools: AutoDock, PyRx, SwissDock, Schrödinger Glide.

Molecular dynamics simulations

Molecular dynamics is a computer method that shows how a drug and its target protein move and interact over time. Unlike docking, which gives just a static snapshot, MD is like watching a movie of the interaction at the atomic level. It helps check if the drug stays stable in the protein's binding site. It also shows how flexible or strong the interaction is under conditions similar to the human body.
Common tools: GROMACS, AMBER, NAMD.

Quantitative Structure - Activity Relationship [QSAR]

QSAR is a computer method that helps us predict how a drug will act in the body based on its chemical structure. It looks at features like the molecule's shape, water-liking (hydrophobicity), and electrical properties.
The computer learns from known compounds:
"Molecules with these features worked well", "Molecules with these features were toxic". Then it can guess the effects of new compounds before we test them in the lab.
Common tools: PaDEL-Descriptor, MOE, and KNIME.

Pharmacophore modelling

Pharmacophore modelling is a computer-based method that shows the 3D arrangement of important chemical features that are responsible for a drug's activity. It is especially useful when the target protein structure is unknown. The model acts like a template or pattern to search for other molecules in databases that have a similar arrangement of features. This helps scientists find new molecules that might work as drugs and understand how changes in structure affect activity (Structure-Activity Relationship, SAR).
Common tools: Ligand Scout, Phase, Catalyst.

Virtual screening

Virtual screening is a computer method used to find promising drug candidates from huge libraries of chemicals.
It works in two ways:

1. Structure-based: Looks at how molecules fit into the target protein.
2. Ligand-based: Finds molecules that are similar to known active compounds.

Tools like machine learning, pharmacophore models, or molecular docking are often used to improve the predictions. The main goal is to filter thousands of compounds down to a smaller number that are most likely to work in experiments.
Common tools: ZINC, DrugBank, PubChem, PyRx, DOCK.

ADMET prediction

In the early stages of drug development, ADMET prediction helps scientists check how a compound behaves in the body and whether it is safe. ADMET stands for:

- Absorption - how well the drug is absorbed
- Distribution - how it spreads in the body
- Metabolism - how the body breaks it down
- Excretion - how it is removed from the body
- Toxicity - whether it causes harmful effects

Common tools: pkCSM, SwissADME, and admetSAR.
They can predict drug-likeness (how likely it is to be a good drug), Solubility in water or body fluids, Stability during metabolism, Ability to cross the blood-brain barrier, Potential harmful or toxic effects. (Kitchen DB *et al*., 2004) [7].

1. Database and software used

Public Databases

Scientists rely on these databases to quickly find and use data instead of starting from scratch. Some well-known free databases include PubChem (by NIH), ChEMBL (by the European Bioinformatics Institute), DrugBank, PDB (Protein Data Bank), and BindingDB. These are widely used in academic research and early drug screening, there are commercial databases such as GVK BIO, SciFinder, and Reaxys. These are paid and more detailed.

Proprietary database

Some databases are public free Examples include PubChem, ChEMBL, DrugBank, PDB, and BindingDB. Other databases are commercial (paid), like GVK BIO, SciFinder, and Reaxys. These are mainly used by pharmaceutical companies for complex research and drug development.

Commonly used software

Auto Dock, a free program that shows how small molecules might fit into proteins and how strong their attachment could be. MOE (Molecular Operating Environment), which is very popular because it can do many things at once like docking, visualizing molecules, studying drug properties, and modelling drug-target interactions. (Surya Ulhas R, *et al*., 2023) [13].

Applications in Specific Therapeutic Areas

Oncology

(Cancer Treatment) is used to find anti-cancer compounds from medicinal plants like withaferin A (from *Withania somniferous*) and curcumin (from *Curcuma longa***).** Example- Docking studies have shown that withaferin A can bind to HER2, a protein involved in breast cancer, suggesting its potential as an anti-cancer agent. (Vadapalli J *et al*., 2018)

Infectious Diseases

Traditional medicinal plants have many natural compounds like azadirachtin (from *Azedarach indica*, neem) and allicin (from garlic) that can fight infections. Example- Docking studies have shown how neem compounds interact with proteins of the malaria parasite. Plasmodium falciparum, indicating their potential as anti-malarial agents. (Morenikeji OR *et al*., 2022) [9].

Neurological Disorders

Medicinal plants used in traditional medicine, like bacosides from *Bacopa Monnier* have been studied for their ability to bind with acetylcholinesterase, an enzyme linked to memory loss. Example: Docking studies have tested plant alkaloids against amyloid-beta aggregation, a key factor in Alzheimer's disease, to find potential therapeutic compounds. (Zhavoronkov A, *et al*., 2019) [19].

AI and machine learning in in silico drug design

Deep learning (DL) is a type of artificial intelligence that can automatically find useful patterns in large amounts of data using multi-layered neural networks. In drug discovery, DL algorithms like Convolutional Neural Networks (CNNs) and Graph Neural Networks (GNNs) can screen chemical formulas, molecular structures, and 3D shapes to identify potential new drugs.properties AI doesn't just help us spot existing drugs it can help design completely new ones. (Ton a.T *et al*., 2020) [14].

Case Studies and Success Stories

HIV Protease Inhibitors: 1990s: Scientists used computer models to look closely at the shape of this enzyme. Once they understood this shape, they were able to design medicines that could stop the enzyme from working, which meant the virus could no longer multiply as easily. This led to the discovery of drugs like saquinavir and indinavir.

Discovery of Antivirals Against COVID-19 (2020): Computer method called High-throughput virtual screening was used to study existing drugs. This helped researchers identify remdesivir, an already known drug, as a possible treatment for COVID-19 by showing how it could attach to and block important viral enzymes.

Oseltamivir (Tamiflu) for Influenza: Scientists at Roche used in-silico structure-based design with crystal data of the influenza neuraminidase protein to develop oseltamivir. Using computational modelling, they were able to improve how strongly the drug binds to the target and its behaviour in the body, resulting in one of the most widely used antiviral drugs during flu outbreaks.

Matinib: Gleevec - Targeted Cancer Therapy: Scientists used computer modelling to study a protein called BCR-ABL tyrosine kinase, which plays a major role in chronic myeloid leukaemia (CML). By looking closely at the protein's structure, they were able to design a drug called imatinib.

Regulatory considerations

Big drug regulators like the EMA in Europe and the FDA in the U.S. are beginning to trust computer models as part of drug development.Big drug regulators like the EMA in Europe and the FDA in the U.S. are beginning to trust computer models as part of drug development.

For these models to be accepted, they must be reliable. That means if another scientist runs the same model with similar data, they should get the same result. The methods also need to be explained clearly how the model was built, what assumptions were made, and where its limits are. If this information is missing, regulators won't trust the model, and the drug approval process will be delayed.

So, the best practice is to test the model inside the lab, compare it with outside data, and share every detail openly. When this is done, regulators feel more confident, and computer models can truly speed up the path to safe, effective medicines.

Challenges and limitations

Data Quality and Availability: The computer can only work with the information we give it so if that information is incomplete, old, or has mistakes, the results won't be accurate.

Computational Cost and Complexity: Some advanced computer simulations, such as quantum mechanical calculations require a lot of memory, processing power, and storage, which many research labs do not have. This makes it difficult to study large or complex systems or to run simulations for long periods of time. (Uzundurukan A *et al*., 2025) [15].

Future Perspectives and Emerging Trends

Digital Twins and Pharmacology: Digital twins in pharmacology are like a virtual copy of a patient on a computer. These sophisticated computer models will show a person's response to a certain medicine. Rather than exposing people to risk during clinical trials, scientists can conduct these fictitious experiments to test efficacy on different treatment regimens to identify the lowest effective dose or discover side effects at an early developmental stage.

Integration with Experimental Approaches: What makes digital twins so powerful is their ability to combine a wide range of personal health data from genetic makeup (genomics) and protein activity (proteomics) to metabolism (metabolomics), medical scans, and clinical history. Bringing all these layers together creates a detailed picture of how a specific body works and reacts. This means treatments can be designed to match an individual's unique biology, turning the idea of truly personalized medicine into reality. (Björnsson B *et al*., 2019) [2].

Conclusion

In silico drug discovery is changing how new medicines are developed. Traditionally, researchers had to depend mostly on long, expensive, and risky laboratory experiments. Now, with the help of computers, things are much faster and smarter. Using tools like molecular modelling, computer simulations, and AI-based predictions, scientists can identify possible drug candidates and adjust their properties before even testing them in the lab. This reduces the number of failures, saves time, lowers costs, and allows researchers to study millions of possible compounds something that would be impossible to do one by one using only traditional methods. So, in silico drug discovery does not completely replace traditional research, but instead works hand-in-hand with it. By connecting theory with real-world experiments, it speeds up the discovery process and helps deliver safer, more effective medicines to patients much faster.

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