DOI: 10.53660/CLM-4175-24T09

Bioinformatics approaches to explore the discovery of new plant-derived drugs: a brief review

Received: 15-08-2024 | Accepted: 15-09-2024 | Published: 20-09-2024

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ABSTRACT

This article reviews the role of bioinformatics approaches in drug discovery from medicinal plants, with an emphasis on the use of computational tools for the analysis of genomic, proteomic, and metabolomic data. These techniques facilitate the screening of bioactive compounds with therapeutic potential, optimizing the identification of new drug candidates. Methods such as molecular docking and molecular modeling are fundamental for predicting interactions between ligands and target proteins, supporting the rational development of new drugs. The article also discusses the importance of metabolic pathway analyses and molecular interaction networks in the selection of promising plant species. The combination of bioinformatics and phytochemistry emerges as a crucial strategy to accelerate the drug discovery process, reducing both costs and development time, with great potential to enhance medical therapies.

Keywords: Computational analyses; Virtual screening; Molecular docking; Phytochemistry; New drugs.

INTRODUCTION

The discovery of new drugs is a complex and time-consuming process, especially when it involves exploring the vast chemical diversity of medicinal plants. For millennia, people have relied on the medicinal properties of plants to treat various diseases. According to a report from the World Health Organization (WHO), around 80% of the global population uses traditional medicine as part of their healthcare (Michelle, Rani, Husain, 2020). Many of these therapies involve the use of extracts and active compounds derived from medicinal plants (Craig, 1999).

The oldest written evidence of plant use for health purposes was found on a Sumerian clay tablet from Nagpur, approximately 5,000 years old. Other historical written records have been found in Mesopotamia, Egypt, and Greek and Islamic civilizations (Petrovska, 2012). Plants play a fundamental role due to their metabolites, present in about 250,000 species.

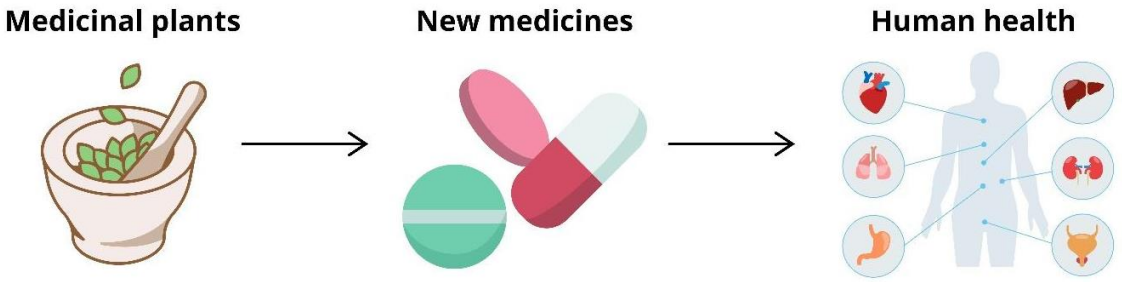
These plants not only share primary metabolites, essential for basic cellular functions, but also produce a wide range of phytochemicals, known as secondary metabolites, which play roles in interactions between organisms, as highlighted by Verpoorte (1998).

In this context, the objective of this review is to discuss the application of bioinformatics approaches in the discovery of new drugs derived from medicinal plants, highlighting how these techniques can accelerate and optimize the identification and development of bioactive compounds with therapeutic potential, contributing to innovation in modern medicine.

MEDICINAL PLANTS AND THE NEED FOR NEW DRUGS

Natural compounds are chemical substances produced by living organisms through primary and/or secondary metabolic pathways, often exhibiting useful pharmacological activities for treating various diseases (Kerwin, 2012; Woldeyes et al., 2012). These natural compounds can be obtained through chemical synthesis or semi-synthesis and frequently serve as starting points in drug discovery, where analogs are synthesized to achieve greater purity, efficacy, potency, and safety (Li, Yeung, 2013; Raafat, 2013; Oliveira, Piva, Lung, 2015), ultimately benefiting human health (Figure 1).

Figure 1 – Schematic representation of the use of medicinal plants in drug development and their application in human health through secondary metabolites.



Source: The authors (2024).

During the 19th century, the discovery and isolation of compounds, particularly alkaloids, which could be separated relatively easily from other organic compounds, represented a significant milestone in the history of medicine. This advance enabled the use of pure substances in Western medicines, resulting in safer and more effective dosages, marking a notable improvement over herbal medicine prescriptions. With advancements in chemistry, the ability to produce semi-synthetic and synthetic compounds emerged as a significant advantage in the early 20th century. This advantage comes from the ability to produce the necessary compounds in sufficient quantities through the development of synthetic procedures (Suntar, 2020).

The use of plants for therapeutic treatments is preferable in many cases, as plant materials are more accessible and economical compared to synthetic drugs, especially in certain countries. Approximately one-third of the population in the United States and European countries also rely on herbal remedies for healthcare. It is estimated that around 70,000 plant species are used to treat diseases, yet only about 15% of these species have been investigated for potential medical uses. Despite this low percentage, approximately 25% of conventional medicines currently used in modern medicine are plant-derived (Fabricant, Farnsworth, 2001; Yuan et al., 2016). This suggests there are still opportunities for further research into natural sources that could be explored for medical purposes.

Considering the existence of several diseases for which there is still no effective medication available, it becomes imperative to conduct drug discovery studies. Research and development are essential to driving the investigation of new drugs by pharmaceutical industries (Toole, 2012).

Before a new drug can be registered, many compounds require detailed investigation. Screening methods used in the search for effective plant compounds may include the random selection of plant materials or the identification of potential candidates through specialized databases for this purpose (Vuorela et al., 2004). However, these methods are expensive, time-consuming, and have low productivity, often resulting in a low success rate. To promote therapeutic innovation, high-throughput screening methods, genomics, and combinatorial chemistry technologies are utilized (Suntar, 2020).

However, the growing interest in alternative and complementary medicine is becoming increasingly prominent, especially in cultures where traditional healing practices are highly revered and valued (Agbor; Naidoo, 2016). This phenomenon is driving significant expansion in research and development of plant-derived medicines, with the goal of complementing conventional healthcare approaches.

The research and development of plant-based medicines are being driven by several factors, including the growing recognition of biodiversity's importance in medicine, advances in extraction and bioactive compound analysis techniques, genomic analyses, and market demand for more natural and less invasive therapeutic options (Bilal; Iqbal, 2020). These plant-derived medicines are not only considered alternatives to conventional therapies but also as complements that can enhance the efficacy of existing treatments, reduce adverse side effects, and provide additional therapeutic options for a variety of health conditions.

Thus, with the rise in interest in alternative medicine, there is a growing demand for new treatments derived from medicinal plants, highlighting the importance of research and development of drugs based on natural sources. By integrating knowledge of medicinal plants with the capabilities of bioinformatics, a promising horizon opens for the identification and development of new nature-based drugs, thereby expanding the therapeutic options available to modern medicine.

BIOINFORMATICS: CONCEPTS AND SOFTWARE

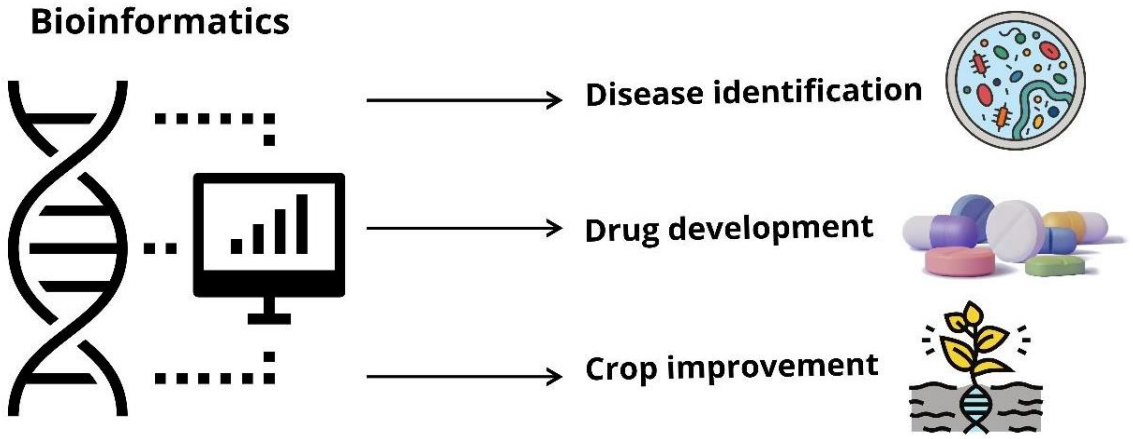
Bioinformatics is an interdisciplinary field that combines biology with informatics, using computational techniques to analyze and interpret complex biological data (López-López, Bajorath, Medina-Franco, 2020). It involves the development and application of computational methods to collect, organize, store, analyze, and visualize biological information such as DNA sequences, proteins, molecular structures, and gene

expression. Bioinformatics is crucial in the era of genomics, proteomics, and other "omics" fields, enabling the understanding of biological processes at both molecular and systemic levels (Tolani et al., 2021).

The role of bioinformatics in biological data analysis is multifaceted and comprehensive. It offers tools and algorithms to compare genomic and proteomic sequences, identify genes and regulatory elements, predict protein structures, and model molecular interactions (Tolani et al., 2021). Additionally, bioinformatics is essential for the analysis of gene expression data, metagenomics, phylogenetics, and epidemiology, providing valuable insights into biological diversity, evolution, the functioning of biological systems, and relationships between organisms (Diniz, Canduri, 2017).

In a broader context, bioinformatics supports drug discovery, agricultural biotechnology, biodiversity conservation, and much more. Its application is fundamental for understanding the genetic basis of diseases, identifying therapeutic targets, developing vaccines, improving crop varieties, and conserving endangered species (Diniz, Canduri, 2017) (Figure 2). Therefore, bioinformatics not only drives scientific research but also has a direct impact on human health, sustainable agriculture, and environmental conservation.

Figure 2 – Examples of bioinformatics applications.



Source: The authors (2024).

With the emergence of genetic sequencing techniques, particularly the growing use of Next-Generation Sequencing (NGS), it has become possible to explore and interpret biological data through bioinformatics. One of the most significant areas is genomic sequence analysis, which involves identifying and comparing DNA and RNA sequences to understand the genetic structure, evolution, and function of genes (Ogbe, Ochalefu, Olaniru, 2016). Methods such as sequence alignment, genome assembly, and

genomic annotation are fundamental to this analysis, providing insights into genetic diversity and gene regulation mechanisms (Hawkins, Hon, Ren, 2010).

Another key tool in bioinformatics is molecular modeling, which uses computational techniques to predict the three-dimensional structure of proteins and other biological molecules (Dorn et al., 2014). Molecular modeling allows researchers to understand how proteins interact with other molecules, such as ligands or substrates, and provides essential information for drug design and protein engineering with specific functions. Methods like molecular docking and molecular dynamics are widely used to simulate and investigate complex molecular interactions (Naqvi et al., 2018).

Furthermore, the prediction of biological activity is an important area of bioinformatics, aimed at forecasting the functional properties and biological effects of molecules, such as chemical compounds or proteins. This involves the use of machine learning algorithms and statistical modeling techniques to analyze large datasets and identify patterns that may be correlated with specific biological activities (Walker, Clardy, 2021). Predicting biological activity is crucial for drug development, computational toxicology, and the discovery of biomarkers for disease diagnosis. These computational approaches are essential for managing the increasing complexity of biological data and accelerating scientific and technological progress in various fields of biology and medicine.

Thus, bioinformatics provides the computational foundation for analyzing large genomic, proteomic, and metabolomic datasets, enabling the identification of genes, proteins, and metabolic pathways related to bioactive compounds in plants. This analysis allows for a more targeted approach in selecting plant species with therapeutic potential, maximizing efficiency in identifying active compounds. By using bioinformatics tools to understand the molecular interactions and mechanisms of action of compounds found in plants, researchers can expedite the discovery of new therapeutic agents.

SELECTION OF PLANT SPECIES AND IDENTIFICATION OF ACTIVE COMPOUNDS

Bioinformatics can be applied to the selection of promising plant species based on their genomes, metabolites, and traditional medicinal properties (Ma et al., 2020). Comparative genomic analysis helps identify genes associated with the production of bioactive compounds in various plant species, aiding in the selection of candidates with

therapeutic potential (Semenzato et al., 2022). Furthermore, bioinformatics facilitates the analysis of metabolites present in plants, revealing their chemical composition and pharmacological potential.

By integrating genomic, metabolomic, and traditional medicinal data, bioinformatics offers a holistic approach to selecting plant species with therapeutic potential (Mawalagedera et al., 2019). This approach enables researchers to identify patterns and correlations between genetic and metabolic characteristics, allowing them to prioritize species with a higher likelihood of producing desirable bioactive compounds. Moreover, bioinformatics enables the development of predictive models to estimate the biological activity of plant compounds based on their chemical structure and molecular interactions (Sharma, Sarkar, 2013). Various tools can be applied to discover the biological activity of sequences for different purposes, including identifying antimicrobial, antiviral, and antifungal activities (Calderone et al., 2014).

Through computational simulations, it is possible to analyze the three-dimensional conformation of compounds and predict their biological activity, contributing to the understanding of their mechanisms of action. Additionally, the analysis of genomic and metabolomic databases helps identify genes and metabolic pathways related to the synthesis of bioactive compounds, as well as map metabolic pathways to understand the biosynthetic processes involved in their production. These computational approaches allow for a more efficient screening of plant species and the identification of potential targets for experimental studies (Fitzgerald, Heinrich, Booker, 2022).

It is worth noting that the development of new drugs is a complex, time-consuming, and expensive process. The time from the discovery of a new drug to its clinical application is approximately 12 years, involving investments of over 1 billion dollars (Katiyar et al., 2012). Therefore, methods that accelerate this process can bring benefits not only in economic terms but also in reducing the time required for products to reach the market. In this context, bioinformatics has emerged as a powerful ally in the drug discovery and development process. Another critical point is the urgency of developing a vaccine for SARS-CoV due to the rapid spread of the pandemic (Waman et al., 2021). Bioinformatics played a fundamental role in the rapid sequencing of the virus, the identification of therapeutic regions, and vaccine development, significantly reducing the time between research and its availability to the public.

ANALYSIS OF METABOLIC PATHWAYS AND INTERACTION NETWORKS

Plants have the ability to produce a wide array of chemical compounds, significantly greater than that of other living organisms, such as mammals. Medicinal plants, in particular, are a rich source of organic compounds that hold great promise for various biotechnological applications (Saito & Matsuda, 2010).

Some of these compounds include alkaloids, anthocyanins, and flavonoids, which are used for a variety of purposes. These range from drug production (Zhao, Ge, & Miao, 2024), analysis of key metabolites associated with oxidative damage for therapeutic applications (Yang et al., 2024), to potential drugs for controlling depression, cancer, and diabetes (Veeramohan et al., 2023).

These advancements in medicinal plants for drug production have been made possible due to progress in genomics and transcriptomics, which have revolutionized research on plants and important crop species (Chen et al., 2024). However, metabolomics has been the most transformative tool for analyzing the chemical compounds produced by plants. This robust analytical technique focuses on the diversity of metabolites plants produce (Rai et al., 2017; Sharma & Yadav, 2022).

One of the primary goals of metabolomics is to link a plant's chemical constituents with its therapeutic value. Understanding the regulatory cascades related to plant metabolism is considered the first step toward generating genetically edited plants that can produce compounds beneficial to humanity (Babar et al., 2017; Ma et al., 2020).

A variety of laboratory and computational tools are available for elucidating these metabolic compounds, including chromatographic techniques (McCullagh & Probert, 2024) and spectrometry techniques (Deschamps et al., 2024). These include Gas Chromatography-Mass Spectrometry (GC-MS), Liquid Chromatography-Mass Spectrometry (LC-MS), Nuclear Magnetic Resonance (NMR), Fourier Transform Infrared Spectroscopy (FT-IR), and more, along with bioinformatics and chemoinformatics tools (Santamaria & Pinto, 2024; Kumar et al., 2024).

Currently, there are numerous tools available for metabolite analysis aimed at understanding the structural and functional aspects of these compounds in medicinal plants. Data mining and interpretation is one of the most interesting fields of bioinformatics (Babar et al., 2017). These computational techniques are growing rapidly and contributing to drug discovery by evaluating genes and their behavior in relation to

the expression of bioactive compounds linked to the pathophysiology of medical interest diseases (Sharma & Yadav, 2022).

While there are several databases like Ensembl (Aken et al., 2017), GOLD (Mukherjee et al., 2016), TAIR (Poole, 2007), RGI (Kwatra, 2021), Phytozome (Goodstein et al., 2012), and GDR (Jung et al., 2007), all of which are considered valuable resources for the biosynthesis and functional studies of these plant-produced metabolites, other tools are also available to further our understanding of these compounds (Table 1).

Table 1 – List of tools used in metabolomics analysis.

Tool Name	Database	Reference
BioCyc	https://biocyc.org/	Karp et al., 2015.
Diagramas de Venn	https://www.nia.nih.gov/research/labs/vennplex	Cai et al., 2013
Galaxy-M	https://github.com/Viant-Metabolomics/Galaxy-M	Davidson et al., 2016.
GenePattern	https://www.genepattern.org/#gsc.tab=0	Reich et al., 2006.
GNPS	https://gnps.ucsd.edu/ProteoSAFe/static/gnps-splash.jsp	Schmid et al., 2021.
HumanCyc	https://humancyc.org/	Romero, 2012.
IMPaLA	http://impala.molgen.mpg.de/	Kamburov et al., 2011
KEGG	https://www.kegg.jp/	Kanehisa, 2026
MAVEN2	https://github.com/eugenemel/maven/releases/latest	Seitzer; Bennett; Melamud, 2022.
MetAssign	https://mzmatch.sourceforge.net/MetAssign.php	Gardinassi et al., 2017.
MetaCyc	https://metacyc.org/	Shrestha et al., 2022.
Metscape3	https://metscape.med.umich.edu/calculator.html	Basu et al., 2017.
MetPA	https://metabolomicscentre.ca/software-databases/software-data-analysis/	Xia and Wishart, 2010a.
MetExplore	https://metexplore.toulouse.inrae.fr/metexplore-portal/	Cottret et al., 2010.
MetaboAnalyst	https://www.metaboanalyst.ca/	Xia; Wishart, 2016.
Metabox	https://metsysbio.com/tools_protocols/metabox-2-0/	Wanichthanarak et al., 2024.
MSEA	https://github.com/bsml320/MSEA?tab=readme-ov-file	Xia; Wishart, 2010b.
MS-DIAL	https://systemsomicslab.github.io/compms/msdial/main.html	Tsugawa et al., 2015
mzMine	https://sourceforge.net/projects/mzmine/	Du et al., 2020.
OpenMS	https://openms.de/	Alka et al., 2019.
RECON2	https://github.com/mcisb/mcisb-recon	Swainston et al., 2016.
Reactome	https://reactome.org/	Bohler et al., 2016.
Workflow4Metabolomics	https://workflow4metabolomics.org/	Giacomoni et al., 2015.
XCMS	https://xcmsonline.scripps.edu/landing_page.php?pgcontent=mainPage	(Mahieu; Genenbacher; Patti, 2016)

Source: The authors (2024).

Metabolomics is the leading field in omics sciences that has been contributing to the understanding of the diversity and function of metabolites and bioactive compounds in various medicinal plants (Rai, Saito, Yamazaki, 2017). In this context, new tools are being developed with the primary aim of providing new insights into the mode of action

and activity of these medicinal plants, as demonstrated in Table 1 (Gonulalan, Nemutlu, Demirezer, 2019).

VIRTUAL SCREENING AND DRUG DEVELOPMENT

In the quest for new medications, increasingly accurate computational tools have been developed. Without the need to dissect animals, computational simulations are used to calculate the numerous biological consequences and potential toxicity of a prospective drug (Sharma and Yadav, 2022). These simulations allow only the most promising compounds discovered through virtual screening to proceed to in vivo testing (Mensa et al., 2023; Sharma and Yadav, 2022). For in vivo tests, for example, it is necessary to determine the receptor binding site of the drug to be tested, and this determination can be predicted using software such as Computer-Aided Drug Design (CADD) (Hussain et al., 2021; Sharma and Yadav, 2022). By identifying potential binding sites, CADD allows for the selection of compounds with the highest biological activity (Sharma and Yadav, 2022).

Virtual screening strategies play an essential role in identifying plant compounds with potential pharmacological activity. Several studies have demonstrated the applicability of methods such as molecular docking, bioinformatics, and in silico drug design to select natural phytocompounds for therapeutic purposes (En-nahli et al., 2023; Erlina et al., 2022; Shreya et al., 2023; Sultana et al., 2023). For instance, in silico methods were used to select possible phytochemical compounds from medicinal plants with potential inhibitory action against COVID-19 (Firouzi and Ashouri, 2023). Therefore, computational approaches not only speed up the drug discovery process but also provide more cost-effective and efficient means of identifying bioactive plant compounds for pharmacological applications (Kotadiya, 2023; Sultana et al., 2023).

In molecular docking studies, for example, pharmaceutical and toxicity assessments are conducted using tools such as SwisDock and SwissADME, which can analyze the therapeutic potential of plant-derived compounds such as Durva, Bael, Custard apple, Moringa, and Kokum (Gupta et al., 2023). Moreover, computational tools enable the discovery of small antiviral molecules from plants to combat infectious diseases like COVID-19 through molecular docking and molecular dynamics simulations targeting specific viral proteins (Halder et al., 2023).

Among the most widely used tools are GOLD (Nurisso et al., 2012) and AutoDock Vina (Trott and Olson, 2010), applied in molecular docking to predict

interactions between proteins and ligands. Schrödinger Suite offers an integrated interface combining various functionalities, facilitating large-scale virtual screening (Bhachoo and Beuming, 2017). MOE (Molecular Operating Environment) is a robust platform that supports both docking and molecular modeling and dynamics, essential for refining potential drugs (Vilar et al., 2008). Databases like ZINC (Irwin et al., 2012) and ChEMBL (Willighagen et al., 2013) provide compounds ready for virtual screening. SwissDock (Bitencourt-Ferreira and de Azevedo, 2019) and GLIDE (Repasky et al., 2007) assist in pharmacophore identification and molecular docking, while software such as GROMACS (Lindahl et al., 2001) and RDKit (Bento et al., 2020) complement the process with molecular dynamics simulations and cheminformatics analyses, supporting the rational design of new drugs (Table 2).

Table 2 – Principais ferramentas utilizadas para triagem virtual e desenvolvimento de fármacos.

Software	Description	Applications	Reference
AutoDock Vina	Molecular docking software that predicts the binding of small molecules to macromolecules.	Virtual screening of ligands, drug design, molecular docking.	Trott and Olson, 2010
Schrödinger Suite	Set of tools for molecular modeling and drug development.	Virtual screening, docking, molecular dynamics, protein modeling.	Bhachoo and Beuming, 2017
GOLD	Molecular docking tool that uses genetic algorithms to predict protein-ligand binding.	Virtual screening, drug design, molecular docking.	Nurisso et al., 2012
MOE (Molecular Operating Environment)	Integrated platform for molecular modeling and drug development.	Molecular modeling, docking, virtual screening, molecular dynamics.	Vilar et al., 2008
GLIDE	Molecular docking software known for its high accuracy in predicting protein-ligand interactions.	Virtual screening, drug design, molecular docking.	Repasky et al., 2007
ZINC Database	Database of chemical compounds prepared for molecular docking.	Virtual screening, drug design, molecular docking.	Irwin et al., 2012
ChEMBL	Database of bioactive compounds with known activities.	Virtual screening, drug discovery, bioactivity analysis.	Willighagen et al., 2013
SwissDock	Online platform for molecular docking that uses the EADock DSS software.	Virtual screening, molecular docking, drug design.	Bitencourt-Ferreira and de Azevedo, 2019
RDKit	Set of tools for cheminformatics, molecular modeling, and virtual screening.	Molecular modeling, virtual screening, drug design.	Bento et al., 2020
GROMACS	Software package for molecular dynamics simulations of biomolecules.	Molecular dynamics, protein stability and flexibility studies.	Lindahl et al., 2001

Source: The authors (2024).

Virtual screening accelerates the identification of potential drug candidates by offering a cost-effective and efficient pathway for new therapeutic discoveries. Studies have used these techniques to identify potential therapeutic targets for diabetes mellitus (Abdullah et al., 2023), cancer treatment (Rodosy et al., 2024), allosteric modulators (Jiang et al., 2023), involvement in apoptosis (Vong et al., 2022), and the development of antiviral drugs against SARS-CoV-2 (Parihar et al., 2022).

By analyzing phytochemical compounds through molecular docking, evaluating pharmacokinetic behavior, and conducting molecular dynamics simulations, it is possible to predict the affinity of ligands for target proteins, understand protein-ligand interactions, and estimate the stability and efficacy of potential drug candidates. These computational methodologies provide valuable insights into the mechanisms of action of compounds, aiding in the identification and development of new drugs with therapeutic potential.

Molecular modeling and simulation of ligand-receptor interactions allow for the prediction of interactions between plants and drugs, as well as refining drug design and detecting potential therapeutic targets. Several studies have already used pharmacokinetic analysis, molecular docking, and molecular dynamics simulations to estimate the binding affinity of compounds to target proteins, such as EGFR in cancer treatment (Rodosy et al., 2024), apoptosis-related proteins in studies with piperine (Vong et al., 2022), and the insulin receptor in the discovery of antidiabetic drugs (Abdullah et al., 2023). In these studies, molecular dynamics simulations have proven to be an excellent tool for refining receptor-ligand complexes, increasing the precision of drug binding modes and assisting in the development of potential drugs from plant sources (Kapla et al., 2021). Therefore, these tools are fundamental in accelerating drug discovery and enhancing its efficiency.

CHALLENGES AND FUTURE PERSPECTIVES

The main challenges in the discovery of plant-derived drugs include the complexity of natural product structures, as well as the slow screening methods and the limited identification of efficient phytocompounds due to the reliance on in vitro and in vivo tests (Rallabandi et al., 2020; Sultana et al., 2023). In this context, bioinformatics facilitates this discovery with methods such as pharmacophore modeling, molecular

docking, and molecular dynamics simulations for initial screening and characterization of anticancer phytocompounds (Iwaloye et al., 2023; Satpathy, 2001).

The isolation of bioactive phytochemicals from plants has been a promising strategy in the development of therapies against infectious diseases and metabolic disorders, and computational tools enhance the efficiency of this process (Khan et al., 2022). Ethnopharmacological approaches introduce polypharmacology, allowing natural products to target multiple human physiological pathways for enhanced efficacy (Nasim et al., 2022). The future of drug discovery lies in the integration of multi-omics data and the development of new computational tools. Advanced multi-omics technologies allow for a comprehensive understanding of disease mechanisms and the identification of therapeutic targets (Bouhaddani et al., 2023; Rakshit et al., 2023). The integration of omics data, such as genomics, transcriptomics, and proteomics, enables the exploration of new treatment options (Rakshit et al., 2023).

Innovative in silico methods assist in predicting drug-induced proteomic profiles and phenotypes, favoring compound screening and systems pharmacology (Wu et al., 2023). Integrated computational tools improve the analysis of multi-omics data, enabling personalized medicine strategies and accelerating drug discovery (Cominetti et al., 2023; Rao et al., 2022). These advances facilitate drug development and also create opportunities for repurposing existing compounds for new therapeutic uses.

CONCLUSION

Virtual screening tools and computational simulations play a crucial role in accelerating the drug discovery process, offering an efficient and cost-effective approach. By integrating techniques such as molecular docking, molecular dynamics, and pharmacokinetic modeling, it is possible to predict protein-ligand interactions, optimize drug candidates, and identify new therapeutic targets. The use of multi-omics data and advanced bioinformatics tools expands the possibilities for developing more effective and personalized treatments. These technological advances have the potential to transform drug development, opening new opportunities for innovative therapies, especially from natural compounds.

ACKNOWLEDGMENTS

We thank ChatGPT, a language model developed by OpenAI, for its assistance in translating this article into English.

DECLARATION OF COMPETING INTEREST

The authors have no ethical, legal and financial conflicts related to the article. All authors read and approved the manuscript to publish.

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