REVIEW ARTICLE

The Role of Artificial Intelligence in Modern Pharmacognosy: Advances and Applications

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Abstract

A new era of natural product research has been brought about by the application of computational intelligence (also known as AI) into pharmacognosy, which has greatly improved the identification, examination, and creation of therapeutic chemicals originating from natural sources. This review comprehensively examines the role of AI in modern pharmacognosy, highlighting recent advances and diverse applications. Key areas of focus include AI-driven methods for natural product identification, compound isolation, bioactivity prediction, and structure elucidation. Machine learning algorithms and neural networks are increasingly utilized to analyze complex biological data, predict pharmacological properties, and streamline the drug discovery process. Furthermore, AI technologies facilitate the optimization of extraction processes and the development of novel formulations, contributing to improved efficacy and safety profiles of natural products. Case studies illustrate successful implementations of AI in pharmacognosy, demonstrating its potential to overcome traditional challenges and accelerate research timelines. This review also highlights some biological activities predicted with the help of AI. It also discusses the ethical considerations, potential limitations, and future directions of AI applications in this field. Overall, AI stands as a transformative tool in modern pharmacognosy, offering unprecedented opportunities for advancing natural product research and development.

Keywords: Drug discovery, Natural compounds, Pharmaceutical sciences, AI applications, Computational biology.

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Introduction

Natural compounds offer a wide range of bioactive chemicals with different chemical structures and powerful therapeutic effects, making them a fundamental component of drug discovery efforts. Derived from plants, microorganisms, and marine organisms, these natural compounds continue to inspire and drive the development of novel pharmaceuticals, addressing various contemporary health challenges.[1] Over the past 15 years, research in the pharmaceutical industry on natural products has waned, partly due to a focus on high-throughput screening of synthetic libraries. This has contributed to a significant drop in new drug approvals and the looming expiration of patents on key medications. However, untapped biological resources, advanced "smart screening" techniques, robotic separation with structural analysis, metabolic engineering, and synthetic biology present promising opportunities for the discovery of new natural product-based drugs.[2] In the 21st century, natural products have re-emerged as vital sources for drug discovery, bolstered by advancements in high-throughput screening, genomics, and artificial intelligence. These innovations enhance the identification and development of novel bioactive compounds, reaffirming the significance of natural products in creating new therapeutic agents.[3] Significant drug discoveries derived from natural ingredients have been made possible by the invaluable information on therapeutic effects that traditional and ethnic remedies have contributed. The distinct properties of therapeutic plants—including their adverse effects—have motivated researchers to create brand-new tiny compounds. Endogenous active compounds found in people and animals, as well as microorganisms, have emerged as significant resources for drug discovery. New approaches to natural product drug discovery have been made possible by tremendous technological advancement, with bioinformatics and artificial intelligence greatly aiding research and development in this area.[4] In drug discovery and development, artificial intelligence (AI) has become a disruptive force. AI uses computing power to evaluate enormous volumes of data and produce insights that are impossible for human researchers to obtain on their own. AI includes a wide range of approaches and technologies, such as natural language processing (NLP), deep learning (DL), and machine learning (ML), each of which has a distinct impact on the pharmaceutical industry.[5]

Drug discovery has been known for being a costly, time-consuming, and unsuccessful procedure. A new drug's development can take over ten years and costs over 2.6 billion US dollars on average. Furthermore, less than 10% of drugs successfully make it from Phase I clinical trials to the market. But over the last ten years, the field of drug discovery has seen

profound changes brought about by the quick development of AI. Virtual screening, de novo drug design, retrosynthesis and reaction prediction, and de novo protein design are just a few of the potent uses of AI in drug development. Predictive and generative tasks are the two primary categories into which these applications fall. Predictive tasks involve forecasting the properties or behaviors of molecules, such as bioactivity or toxicity, while generative tasks involve creating new molecular structures or predicting reaction pathways.[6] Natural products are considered privileged structures for interacting with therapeutically relevant protein targets, which has inspired the development of both small molecules and macrocyclic drugs. Approximately two-thirds of novel human therapeutics in development originated from natural products between the 1980s and 2010s. Unaltered NPs (5%) are directly isolated from natural sources without modification. NP Analogues (28%) are derivatives or semi-synthetic compounds based on natural product structures. NP Pharmacophores (35%) contain key structural motifs derived from natural products, even if synthetically produced.[7] Scientific research shows that health can be maintained, delayed, or treated with health-promoting functional food ingredients (FFIs). As consumer demand for information on food and nutrients rises, the nutrition industry is growing, driven by consumer choices. AI has the potential to expand the range of characterized and annotated FFIs by systematically discovering and characterizing effective bioactive ingredients. Despite this, FFI-producing companies have been slow to adopt AI, resulting in inefficient ingredient development. The integration of AI can revolutionize the characterization of FFI molecules, increasing the availability of bioactives tailored to specific health needs.[8]

Machine Learning in Natural Compound Screening

Machine learning (ML) is a branch of AI that empowers computers to learn from data and make predictions or decisions. In natural drug discovery, ML algorithms analyze vast datasets of natural compounds to identify potential drug candidates. Using machine learning models trained on pharmacological target similarity, bioactivity assessment of natural chemicals leverages the similarity between biological targets to predict compound efficacy. By analyzing known drug-target interactions, these models can forecast the potential biological activities of natural compounds. Supervised learning methods like random forests and neural networks, along with similarity metrics such as Tanimoto coefficients, are used to pinpoint promising compounds. This approach accelerates drug discovery by efficiently screening vast compound libraries, reducing experimental costs, and enhancing predictive accuracy. Integrating diverse data types and improving model interpretability are ongoing challenges that promise to further advance this innovative methodology.[9] Unsupervised learning in drug design progresses from self-organization techniques such as clustering and dimensionality reduction to advanced deep chemistry approaches. Self-organization identifies patterns and structures in molecular data without labeled outcomes, aiding in the discovery of novel compounds. Deep chemistry utilizes deep learning techniques to model complex molecular interactions and generate new drug candidates. By uncovering hidden relationships in chemical space, these methods enhance our ability to design effective drugs, streamline the discovery process, and address challenges such as predicting molecular properties and optimizing lead compounds, ultimately revolutionizing the landscape of drug development.[10] AI algorithms can analyze comprehensive patient data, including genomic, lifestyle, and environmental factors, to improve diagnostic accuracy. This holistic approach aids in the precise determination of an individual's Prakriti (constitution) and health imbalances. AI can digitize traditional Ayurvedic diagnostic tools, such as pulse and tongue examination. This transformation ensures standardized measurements and consistent diagnostic results, enhancing the reliability and reproducibility of assessments.[11] The molecular docking approach investigates how potential phytochemicals interact with target active sites to reveal their interactions and therapeutic properties. Molecular dynamics (MD) simulations provide a detailed view of biomolecules' dynamic behavior at the atomic level, offering high-quality representations. Recent advances in computer science have greatly enhanced these tools, improving speed, system configuration, and software capabilities. These developments offer deeper insights into biological mechanisms and facilitate the structural optimization of biomolecules for disease treatment.[12] The use of AI in natural product drug discovery offers several advantages over traditional methods of identification, analysis, and formulation of herbal drugs such as AI algorithms can analyze vast datasets from various sources, such as chemical libraries, genomics, and phytochemical databases, to identify potential bioactive compounds more efficiently than manual methods and Machine learning models can detect complex patterns and relationships within large datasets that might be missed by traditional methods, leading to the discovery of novel compounds with therapeutic potential.[13]

Data Collection and Preprocessing

Drug-Target Interaction Data

Collect comprehensive datasets of known drug-target interactions from databases like ChEMBL, DrugBank, and PubChem. These datasets include information on drug structures, target proteins, and interaction strengths shown in Table 1.

Natural Compound Libraries

Access to a curated database containing information on plants, their associated natural products, and their chemical structures can greatly facilitate *in-silico* drug discovery.[29] In this direction, there has been substantial recent progress in

Table 1: Natural products data collection and preprocessing

S. No.	Database	Website	Description	References
1.	COCONUT	https://coconut.naturalproducts.net	The Collection of Open Natural products (COCONUT) online database is a comprehensive repository of natural products available for public access. It aggregates data on the structures and properties of natural compounds from diverse sources, facilitating drug discovery and chemical research. Researchers can use COCONUT to search for compounds based on various criteria such as structure, source, and biological activity.	14-16
2.	INPUT	http://cbcb.cdutcm.edu.cn/INPUT	INPUT is a sophisticated network pharmacology platform tailored for traditional Chinese medicine (TCM), emphasizing advanced intelligence and comprehensive functionality. It integrates TCM knowledge with modern pharmacology, enabling the analysis of complex herbal interactions and therapeutic mechanisms. INPUT facilitates drug discovery and development by providing insights into the multi-component, multi-target nature of TCM formulations.	17, 18
3.	ChEMBL	https://www.ebi.ac.uk/chembl	ChEMBL is a comprehensive bioactivity database containing detailed information on drug-like molecules and their interactions with biological targets. It aggregates data from scientific literature, providing a valuable resource for drug discovery and development. Researchers use ChEMBL for pharmacological insights, compound activity predictions, and identifying potential therapeutic agents.	19, 20
4.	DGIdb	http://www.dgidb.org	The Drug-Gene Interaction Database (DGIdb) is a resource that curates and organizes information on drug-gene interactions and the potential drug's ability of genes. It integrates data from various sources, enabling researchers to explore and identify interactions relevant to drug discovery, precision medicine, and the development of new therapeutic strategies.	21-23
5.	PDTD	http://www.dddc.ac.cn/tarfisdock	The Potential Drug Target Database is a specialized repository that catalogs information on potential drug targets. It includes data on protein structures, ligand binding sites, and related pharmacological interactions, aiding in drug discovery efforts. Researchers use PDTD to explore and analyze target-specific information crucial for designing and developing new therapeutic agents.	24
6.	Drug Bank	http://www.drugbank.ca	The DrugBank database is a comprehensive resource that provides detailed information on drugs, drug targets, and drug interactions. It includes data on chemical structures, pharmacological properties, mechanisms of action, and therapeutic uses of drugs approved for clinical use. Drug Bank is widely used by researchers, clinicians, and drug developers to explore drug information, predict drug-drug interactions, and facilitate drug discovery and development processes.	25-27
7.	PubChem	https://pubchem.ncbi.nlm.nih.gov	PubChem, maintained by the NCBI at the NLM, is a freely accessible database serving as a repository for small molecule biological activities. It aggregates chemical, biological, and screening data from diverse sources like literature, patents, and vendors. Researchers globally utilize PubChem to explore compound structures, properties, and biological activities, supporting drug discovery and biomedical research.	28

developing databases on natural products with a focus on the phytochemistry of edible and herbaceous plants shown in Table 2.

In-silico techniques for DTI forecasting

Predicting Drug-Target Interactions (DTIs) is pivotal in drug discovery and development, particularly for natural compounds sourced from plants, microorganisms, and marine organisms, historically abundant in therapeutic agents. Anticipating these interactions can expedite the discovery of novel drugs and therapeutic applications.[42,43]

- *Ligand based approaches for DTI prediction*

Ligand-based approaches for predicting drug-target interactions in natural products rely on the chemical properties and structures of known compounds. Techniques like quantitative structure-activity relationship (QSAR) models, similarity-based methods, and pharmacophore modeling are frequently utilized. QSAR models assess the correlation between chemical structure and biological activity through statistical analysis, while similarity-based methods predict potential interactions by comparing new compounds with known ligands. Pharmacophore modeling identifies the essential features required for interaction with a specific protein target. These methods help in identifying potential protein targets for natural products by leveraging existing chemical and biological data.[43,44]

- *Target based approaches for DTI Prediction*

Target-ligand-based approaches for predicting drug-target interactions in natural products focus on the structural and binding properties of both the target protein and the ligand. Techniques such as molecular docking simulate the interaction between the ligand and the target, predicting preferred orientations and binding affinities.[45] Molecular dynamics simulations offer insights into the stability and

Table 2: Details of natural compound libraries

S. No.	Database	Website	Description	References
1.	NPASS	http://bidd2.nus.edu.sg/NPASS/	The Natural Product Activity and Species Source Database is a comprehensive resource that centers on the bioactivity of natural products and their species sources. It offers detailed information on the chemical structures and biological activities of natural compounds from diverse species, supporting researchers in drug discovery and development efforts.	30, 31
2.	NANPDB	http://african-compounds.org/nanpdb/	The Northern African Natural Products Database (NANPDB) is a curated repository of natural compounds derived from Northern African flora. It provides detailed information on chemical structures and biological activities, supporting drug discovery and research. NANPDB aids in exploring the pharmacological potential of the region's unique botanical resources.	32
3.	Super Natural	http://bioinf-applied.charite.de/supernatural3 http://bioinformatics.charite.de/supernatural	The Supernatural Database is an extensive digital repository containing information on paranormal phenomena, mythical creatures, and supernatural events. It serves as a comprehensive resource for researchers, enthusiasts, and writers, offering detailed records, historical accounts, and cross-referenced data to explore the mysteries of the supernatural world.	33, 34
4.	CVDHD	http://pkuxxj.pku.edu.cn/CVDHD	The CVDHD Herbal Database is a specialized repository that catalogs herbs and natural remedies used in managing cardiovascular and heart diseases. It includes detailed information on efficacy, traditional uses, active compounds, and potential interactions, serving as a valuable resource for researchers and practitioners in integrative medicine.	35
5.	KNApSAcK-3D	http://kanaya.naist.jp/KNApSAcK_Family/ http://kanaya.naist.jp/knapsack3d/	The KNApSAcK-3D Database is an extensive resource for 3D structures of natural products. It provides detailed information on molecular geometry, biological activity, and chemical properties, aiding researchers in drug discovery, bioinformatics, and cheminformatics by offering a comprehensive collection of structurally annotated natural compounds.	36
6.	NutriChem	http://cbs.dtu.dk/services/NutriChem-1.0	The NutriChem Database is a comprehensive resource detailing the chemical composition and nutritional properties of various foods. It includes data on vitamins, minerals, bioactive compounds, and their health effects, aiding researchers, nutritionists, and healthcare professionals in studying and promoting optimal dietary practices and nutrition-based interventions.	37
7.	Phytochemica	http://home.iitj.ac.in/bagler/webservers/phytochemica	The Phytochemica Database is a detailed repository of phytochemicals found in plants. It provides information on chemical structures, biological activities, and therapeutic uses. This resource supports research in pharmacognosy, herbal medicine, and nutraceuticals, aiding in the discovery and application of plant-derived compounds for health and wellness.	38
8.	TCMID	http://www.megabionet.org/tcmid/	The TCMID (Traditional Chinese Medicine Integrated Database) is a comprehensive resource that compiles information on herbs, compounds, formulas, and their interactions used in Traditional Chinese Medicine. It supports research by offering detailed data on molecular mechanisms, pharmacology, and therapeutic applications, facilitating the integration of TCM with modern medicine.	39
9.	TCM-Mesh	http://mesh.tcm.microbioinformatics.org/	The TCM-Mesh database integrates Traditional Chinese Medicine (TCM) knowledge with biomedical concepts from MeSH (Medical Subject Headings). It provides a structured ontology linking TCM terms to MeSH terms, aiding in the interpretation and integration of TCM practices in biomedical research and healthcare, promoting cross-disciplinary understanding and collaboration.	40
10.	MEDDB	http://www.ladydoakcollege.edu.in/meddb/home.html	MEDDB is a medicinal plant database compiled from knowledge shared by tribal communities near Madurai, Tamil Nadu. It catalogs traditional uses, chemical constituents, and pharmacological properties of local plants. MEDDB serves as a valuable resource for ethnobotanical research and drug discovery, preserving indigenous knowledge and biodiversity.	41

conformational changes of the protein-ligand complex over time. Machine learning models analyze large datasets of known interactions to predict new ones, while network-based approaches study protein interaction networks to understand the broader effects of ligand binding. Integrating these methods provides a comprehensive understanding of natural product interactions with protein targets, aiding drug discovery and development.[46]

- *Target ligand-based approaches for DTI Prediction*

Target ligand-based approaches for drug-target interaction (DTI) prediction utilize the characteristics of both drugs

Table 3: List of Biological activities of medicinal plants predicted with the help of artificial intelligence

S. No.	Purpose	Source of drug	Extract	Chemical Constituent	Methodology Used	Reference
1.	Anticancer	*Saponaria vaccaria* L. seeds	Aqueous methanol	Saponins	An artificial neural network (ANN) was employed to predict the extraction kinetics and yields, using MeOH concentration, temperature, and extraction time as inputs. The ANN model achieved predictions with an error margin of less than approximately 12%. It slightly outperformed a numerical diffusional model and simplified the prediction process by avoiding the need for partition coefficient and effective diffusivity calculations. This demonstrates that the ANN model is a viable and efficient approach for predicting saponin yields and similar extraction processes.	[49]
2.	Antimicrobial	*Lindera triloba* Leaf, branch	Aqueous extract by hydro distillation	A-cardinol, epi-α-muurolol, camphor, limonene, bornyl acetate, δ-cadinene, α-muurolene, alloaromadendrene, β-bisabolene	The methodology employed in this strategy led to the identification of antimicrobial activity in essential oils from *Lindera triloba* and *Cinnamomum sieboldii* against *Staphylococcus aureus*. The study highlights that using machine-learning classification within semantic space proves to be a highly effective approach for discovering and exploring bioactive plant extracts	[50]
3.	Antimicrobial	*Cinnamomum sieboldii* Leaf, branch, stem, bark	Aqueous extract by hydrodistillation	Linalool, cinnamaldehyde, geranial, 1,8-cineole	The methodology employed in this strategy led to the identification of antimicrobial activity in essential oils from *Lindera triloba* and *Cinnamomum sieboldii* against *Staphylococcus aureus*. The study highlights that using machine-learning classification within semantic space proves to be a highly effective approach for discovering and exploring bioactive plant extracts	[50]
4.	Antioxidant	*Glycyrrhiza glabra*	Methanol/ aqueous/ phosphoric acid	Liquiritin apioside, liquiritin, liquiritigenin, glycyrrhizic acid, Isoliquiritoside, Isoliquirigenin	The strategy involves identifying and quantifying the chemical components of Glycyrrhiza extract using techniques like HPLC and MS to create a chemical fingerprint. Fingerprint-activity relationship modeling then correlates these profiles with biological activities to discover potential biomarkers linked to the extract's therapeutic effects. This approach enhances understanding of the extract's efficacy and ensures consistent quality.	[51]
5.	Antioxidant	*Chamomilla recutita* Ligulate flowers	Ethanol extract by microwave assisted extraction	Gallic acid, protocatechuic acid, p-hydroxynenzoic acid	Optimization of process parameters was conducted using an artificial neural network (ANN) model with the solid-to-solvent ratio, microwave power, and extraction time as inputs, and the yield of total phenolic compounds (TPC) as the output. The optimized conditions were a solid-to-solvent ratio of 1:80, microwave power of 400 W, and an extraction time of 30 minutes. The ANN predicted the TPC content, which was experimentally confirmed. The extract obtained under these optimal conditions exhibited a rich composition and high biological activity. Additionally, chamomile extract demonstrated promising potential as a growth medium for probiotics.	[52]
6.	Anti-inflammatory activity	*Lonicera species*	Ethanolic extract	Luteolin, Quercetin, Apigenin, Caffeic acid, p-coumaric acid	The methodology involves extracting compounds from Honeysuckle (Lonicera sp.) and analyzing them using ATR-FTIR spectroscopy to obtain spectral data. Artificial intelligence is employed to process and interpret the spectra, identifying key bioactive compounds and correlating them with anti-inflammatory properties through advanced data analysis and pattern recognition techniques.	[53]

7.	Antioxidant	*Neptuna oleracea* Leaf and stem	Ethanolic extract	Vitexin-2-O-rhamnoside, Quercetin, Kaempferol, Myricetin, Catechin, Caffeic acid, Gallic acid, 3,4-O-dimethyl gallic acid	It facilitates the integration of metabolomics data with biological activity data, enabling the discovery of correlations and insights into the mechanisms underlying the antioxidant and α-glucosidase inhibitory effects.	[54]
8.	Anti-inflammatory	Lauraceae plant species (*Cinnamomum* and *Persea americana*)	Ethanolic extract	Laurotetanine, Quercetin, Kaempferol, Rutin	Metabolomics data is analyzed using statistical and machine learning approaches (e.g., PLS-DA, Random Forest) to correlate metabolite profiles with anti-inflammatory activity. Predictive models are built to classify and predict anti-inflammatory effects based on the metabolite composition of plant extracts.	[55]
9.	Anti-inflammatory	Dried hops of *Humulus lupulus*	Acetone / Methanol	Xanthohumol, 4-deoxyposthumulone, posthumulone, cohumulone	The study used machine learning techniques, Elastic Net and Random Forests, to identify bioactive compounds in hop (*Humulus lupulus*) extracts. By analyzing 40 fractions with anti-inflammatory assays and mass spectrometry, the top predictors of bioactivity, including xanthohumol and prenylated flavonoids, were identified, demonstrating that machine learning can expedite the discovery of bioactive natural products without extensive fractionation.	[56]
10.	Anti-inflammatory	*Sesamum indicum* (seeds), *Rosa damascene* flower	Methanol Extract of *S. indicum* Petroleum ether extract of *R. damascene*	Sesamin and Sesamolin isolated from *S. indicum* Farnesol, Limonene, Citronellol isolated from *R. damascene*	The study investigated the efficacy of *Sesamum indicum* (sesame) seeds combined with *Rosa damascena* (rose) oil for treating uncomplicated pelvic inflammatory disease (PID). Using machine learning classifiers AdaBoost (AB), Naive Bayes (NB), and Decision Tree (DT), the study analyzed experimental data to predict treatment outcomes. The classifiers helped accurately classify patient responses, demonstrating the therapeutic potential of the herbal combination in managing PID.	[57]
11.	Antioxidant	*Rosa sterilis* mature fruits	Ethanolic extract	Quercetin, Kaempferol, Catechin	The study optimized the extraction of flavonoids from *Rosa sterilis* using ultrasonic methods, with modeling by response surface methodology and an ANN-GA algorithm. The results showed a high extraction rate, confirming the model's accuracy, and identified material-to-liquid ratio as the most influential factor. Additionally, the flavonoids demonstrated strong antioxidant activity, and the extraction process followed Fick's first law.	[58]
12.	Antioxidant	*Juglans mandushurica* bark	Ethanolic extract by ultrasonic assisted extraction technique	Rutin, Quercetin, Kaempferol, myricetin	The study explores the ultrasonic-assisted extraction (UAE) of flavonoids from *Juglans mandshurica Maxim*. and utilizes artificial intelligence for optimizing extraction conditions. The research focuses on determining optimal parameters for maximizing flavonoid yield through machine learning techniques. Kinetics of the extraction process are analyzed to better understand the rate and efficiency. Additionally, the antioxidant potential of the extracted flavonoids is evaluated, highlighting their potential health benefits. The integration of AI optimization and UAE offers a novel, efficient approach for extracting bioactive compounds with high antioxidant properties.	[59]
13.	Antioxidant	*Amaranthus viridis*	Methanolic extract	Quercetin, Rutin, β-sitosterol	It predicted the antioxidant activities of *Amaranthus viridis* seed extract using four machine learning models: ANN, SVM, k-NN, and DT. The Decision Tree (DT) outperformed the others with high accuracy and precision, exhibiting a correlation coefficient of 0.9878 and an AUC of 0.979. The results confirmed DT's effectiveness in predicting the antioxidant properties of *Amaranthus viridis*.	[59]

14.	Anticancer	*Albizia lebbeck* stem bark	Methanolic extract	Hexadecanoic acid, quercetin, tetradecylester, 9,12,15-octadecatrienoic acid	The study investigated the cytotoxic, anti-proliferative, and anti-migratory effects of *Albizia lebbeck* methanolic extract on MDA-MB 231 and MCF-7 cancer cells. Artificial neural networks (ANN), adaptive neuro-fuzzy inference systems (ANFIS), and multilinear regression (MLR) models were used to predict cell migration and detect early metastasis. The models were applied to analyze experimental data from treated cancer cells.	[60]
15.	Wound healing/ skin protective	*Hypericum perforatum* aerial parts	Chloroform extract	Hypericin	The study aimed to predict the hypericin content in *Hypericum perforatum* under different ecological and phenological conditions using artificial neural network techniques, specifically Multi-Layer Perceptron (MLP), Radial Basis Function (RBF), and Support Vector Machine (SVM).	[61]
16.	Antidiabetic/ Antioxidant	*Parkia biglobosa* stem bark	Hydro-methanol extract	Gallic acid, protocatechuic acid, caffeic acid, vanillic acid, p-coumaric acid, trans-ferulic acid	The study evaluated the antidiabetic and antioxidant effects of hydromethanol extract from *Parkia biglobosa* stem bark (PBSBHM) in type 2 diabetic rats. After 28 days of oral administration, PBSBHM showed significant antioxidant activity and improved glucose tolerance, reducing serum glucose levels and glycosylated hemoglobin. The extract was rich in phenolic compounds, particularly protocatechuic acid, and contained high levels of minerals. Molecular docking suggested moderate affinity of protocatechuic acid for key enzymes.	[62]
17.	Anti-oxidant/ Antidiabetic/ Neuroprotective	*Hibiscus cannabinus* seed	Acetone extract	p-hydroxybenzoic acid, gallic acid, ϒ-tocopherol, caffeic acid, β-sitosterol, catechin, vanillic acid, syringic acid, kaempferol, ferulic acid, linalool	The study evaluated the antioxidant properties and predicted drug-like potential of polyphenolic-rich extracts from *Hibiscus cannabinus* L. seeds. The research focused on assessing the extract's antidiabetic and neuroprotective effects through both *in-vitro* experiments and *in-silico* computational modeling. The findings aim to identify promising compounds for drug development targeting diabetes and neuroprotection.	[63]
18.	Antioxidant	*Saragassum fusiforme*	Aqueous ethanol extract	Phloroglucinol, fucophlorethol-A, bifuhalol, Iso-propyl-3-(3,4-dihydroxyphenyl)-2-hydroxy propanoate, 3'-O-methylcatechin	The study optimized conditions for extracting high antioxidant activity from *Sargassum fusiforme* (SF) using advanced models and high-resolution mass spectrometry. The four-factor central composite design achieved optimal results for DPPH, ABTS, TPC, and TFC antioxidant assays. Over 79 secondary metabolites were identified, including 12 novel compounds. These findings suggest that the identified compounds may enhance the antioxidant potential of SF, and the optimized models could help discover and commercialize new bioactive compounds.	[64]

(ligands) and targets (usually proteins) to forecast potential interactions. These methods combine various computational techniques and data sources to achieve accurate predictions.[47] There are two main approaches: structure-based methods, such as molecular docking, predict the preferred orientation of a ligand bound to a target protein and estimate binding affinity. Tools like AutoDock and DOCK are commonly used, requiring 3D structures of both ligands and target proteins. Another method, molecular dynamics (MD) simulations, studies the physical movements of atoms and molecules over time, providing insights into the stability and dynamics of the ligand-target complex. Tools such as GROMACS and AMBER are used, requiring detailed force fields and initial structures.[48]

Recent Progress in Computational Techniques for Predicting Compound Biological Activity of herbal extract

Artificial intelligence (AI) is transforming the prediction of biological activities in herbal extracts by analyzing vast datasets and identifying bioactive compounds with high accuracy. Machine learning algorithms and computational models can predict therapeutic potential, toxicity, and interactions of plant-based compounds, accelerating the discovery of new natural remedies. This approach enhances

efficiency, reducing the need for extensive *in-vitro* or *in-vivo* experiments. Some biological activities of medicinal plants are predicted with the help of artificial intelligence cited in Table 3.

Applications of DTI Prediction

Predicting bioactivity of natural compounds

Machine learning approaches can identify active molecules derived from natural products (NPs), improving human health across various areas of interest through diverse methodologies. Machine learning facilitates the discovery of NP or NP-like chemical compounds for cardiovascular and metabolic diseases by predicting bioactivity, identifying novel therapeutic targets, and optimizing compound structures. These approaches accelerate drug discovery, enhance treatment efficacy, and contribute to the development of innovative therapies for these prevalent conditions.[65] Assessing drug bioactivity has become a primary focus in drug discovery. While *in-vitro* and *in-vivo* experiments replicate molecular functions, they are time-consuming and expensive. AI techniques have proven cost-effective and efficient in predicting drug bioactivities, encompassing anticancer, antiviral, and antibacterial activities.[66] A network-based strategy identifies candidate flavonoids for non-alcoholic fatty liver disease (NAFLD) by analyzing interactions between flavonoids and biological targets. This approach integrates data from molecular networks and disease pathways, highlighting potential therapeutic compounds that modulate key proteins and pathways involved in NAFLD.[67] Quantitative and systems pharmacology uses *in-silico* methods to predict drug-target interactions of natural products, enhancing targeted cancer therapy. This approach analyzes molecular interactions and biological networks to pinpoint natural compounds that selectively bind to cancer-specific targets, paving the way for personalized medicine in oncology with novel therapeutic opportunities.[68] Virtual screening of Indonesian herbal compounds for COVID-19 supportive therapy utilizes machine learning and pharmacophore modeling. This method forecasts potential interactions between herbal compounds and viral proteins, facilitating the discovery of effective treatments. It integrates computational techniques to expedite the identification of promising candidates for combating the virus.[69] InflamNat is a web-based database and predictor designed to identify and evaluate anti-inflammatory natural products. It offers a comprehensive repository of natural compounds with known or predicted anti-inflammatory properties, facilitating research and discovery. You can You can access it at InflamNat. (http://www.inflamnat. com/ or http://39.104.56.4/).[70] The study aimed to identify novel phytochemicals targeting the S100B protein, a key player in epileptogenesis, using machine learning-enabled virtual screening. Multiple algorithms, including Random Forest (RF), SVM, kNN, and Naive Bayes, were applied for feature extraction and compound selection, with RF achieving 93.43% accuracy. Screening a library of 9,000 phytochemicals, 180 potential S100B inhibitors were identified, and docking studies highlighted compounds like rhinacanthin K and maslinic acid as promising S100B antagonists. This demonstrates the potential of machine learning in discovering novel epilepsy therapeutics.[71] Using data from molecular docking studies, a machine learning model was developed to identify potential breast cancer-fighting compounds from ginger. The model predicted chemicals that inhibit KIT and MAPK2 proteins, key factors in breast cancer progression. Compounds like beta-carotene, curcumin, and Shogaol were found to outperform a reference ligand in targeting MAPK2. Lycopene, Shogaol and Paradol demonstrated low toxicity and met Lipinski's drug-likeness criteria, though beta-carotene showed toxicity. All three substances were predicted to possess anticancer properties.[72]

Drug Repurposing

Computational methods in drug design primarily utilize molecular docking and network pharmacology. Numerous studies have focused on developing these methods, particularly using traditional Chinese medicine (TCM), to combat COVID-19. Findings suggest TCM compounds can potentially exert therapeutic effects against the virus directly or through anti-inflammatory and immune regulatory mechanisms.[73] Compared with traditional de novo drug discovery, drug repurposing has become an attractive strategy due to its low cost and high efficiency. Compared to traditional de novo drug discovery, drug repurposing has emerged as an appealing strategy due to its cost-effectiveness and efficiency. Extensive analysis of candidates identified for drug repositioning reveals that certain drugs, initially ineffective for their original indications, may exhibit significant effects in other diseases. Moreover, some drugs demonstrate synergistic effects, enhancing clinical efficacy when combined. Drug repositioning has proven beneficial during current public health crises, such as the COVID-19 pandemic, underscoring its substantial potential.[74] The bioactive compounds in garlic, including organosulfur compounds (allicin and alliin) and flavonoids (quercetin), which have shown immunomodulatory effects and inhibited the attachment of SARS-CoV-2 to the ACE2 receptor. GC/MS analysis detected 18 active chemicals, predominantly organosulfur compounds, with allyl disulfide and allyl trisulfide exhibiting the strongest activity. Molecular docking revealed these compounds' inhibitory effects on the ACE2 protein, while artificial intelligence technology was employed to further analyze allicin's interaction with SARS-CoV-2 receptors, demonstrating its potential efficacy in reducing viral load.[75]

Multi-target approach for natural products

The concept of multi-target drugs explores strategies to harness the extensive pharmacological knowledge of natural products with privileged structures (e.g., curcumin, epigallocatechin-3-gallate, resveratrol, salicylate, and quercetin) for developing anti-inflammatory therapies.

This approach involves selecting crucial molecular targets, evaluating their significance, and addressing safety considerations. The goal is to optimize natural products' affinity for specific but multiple molecular targets, aligning with current understanding of inflammation pathways, while preserving their broad and beneficial target profile.[76] Advances in target identification technologies for marine natural product research include high-throughput screening, genomics, transcriptomics, proteomics, bioinformatics tools, and CRISPR/Cas9 gene editing. These innovations enhance the discovery of novel drug targets and therapeutic compounds from marine organisms, accelerating the development of new treatments.[77] Combination screening of synthetic drugs and plant-derived natural products offers potential for enhanced therapeutic efficacy and reduced resistance. However, challenges include complex interactions, variability in natural product composition, and regulatory hurdles. Addressing these issues can unlock new avenues for innovative drug development and optimized treatment strategies.[78]

Ayurnano

Ayurnano represents a cutting-edge convergence of ancient Ayurvedic principles and modern scientific advancements, particularly in the fields of nanotechnology and artificial intelligence (AI). This innovative approach aims to enhance the efficacy, precision, and personalization of herbal therapeutics, paving the way for more effective and targeted treatments.[79]

Conclusion

The integration of AI in pharmacognosy represents a transformative advancement in the discovery, analysis, and development of natural products. By leveraging machine learning algorithms, AI enhances the efficiency and accuracy of identifying bioactive compounds from diverse natural sources. It facilitates the prediction of pharmacological activities, optimizes the extraction processes, and supports the synthesis of novel therapeutic agents. Furthermore, AI-driven data analysis aids in the understanding of complex biological interactions and accelerates the drug discovery pipeline. As AI technologies continue to evolve, their application in pharmacognosy promises to unlock new potentials in natural product research, ultimately contributing to the development of innovative and effective healthcare solutions. Artificial intelligence has revolutionized the prediction of biological activities in medicinal plants, enabling accurate identification of bioactive compounds and their therapeutic potential. By employing machine learning algorithms and computational models, AI streamlines the discovery of natural remedies, reducing reliance on traditional experimental methods. This technology holds great promise in advancing the understanding and utilization of herbal extracts in modern medicine.

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Conflict of Interest

The authors declare that there is no conflict of interest.

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