ARTIFICIAL INTELLIGENCE IN MEDICINAL PLANT-BASED DRUG DISCOVERY: CURRENT APPLICATIONS, CHALLENGES, AND FUTURE PERSPECTIVES

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Abstract

Medicinal plants have played a vital role in supplying therapeutic compounds, but discovering compounds from them needs time, expensive and requires manual intervention. Due to the emergence of Artificial Intelligence, large biological and chemical datasets are being analysed more efficiently and to assist faster identification of promising plant-derived bioactive compounds. This study focuses on how artificial intelligence can be employed in medicinal plant research and drug discovery, and to emphasize how it improves species identification, phytochemical analysis, and to predict bioactive compounds compared with traditional approaches. The study uses a review-based approach, utilizing existing literature, databases, and AI tools employed in medicinal plant research. It discusses machine learning, deep learning, natural language processing, computer vision, molecular docking, virtual screening, and database resources such as DrugBank, PubChem, HERB, IMPPAT, and TKDL. The review shows how AI methods perform strongly in medicinal plant classification, drug–target affinity prediction, synergy prediction, and extraction optimization. Deep Learning models typically exceeded standard machine learning approaches, and AI-based pipelines diminished the need for large scale manual screening while uplifting prediction accuracy. Artificial intelligence is revolutionizing medicinal plant research by making drug discovery quicker, more effective and more systematic. Even though challenges persist in case of data sparsity, interpretability, and ethical concerns. AI has intense potential to support future botanical drug discovery and natural product research.

Introduction

Medicinal plants represent an important part of the world's healthcare and a valuable source of leading molecules such as artemisinin, curing various diseases including parasitic infections, digestive problems, and pain. Paclitaxel is a

chemotherapeutic drug that prevents cancer cell division and suppresses growth by stabilizing the mitotic spindle [1, 2]. In the past, the discovery and isolation of potentially valuable molecules were mostly performed by conventional empirical approaches or laborious high-throughput screening due to the complexity of the system and low accuracy of the results [3, 4]. Over half of all prescription medicines on the pharmaceutical market contain natural health compounds or their analogs [1, 5]. On the other hand, the concentration of valuable substances in natural extracts can be considerably low, making their systematic examination challenging [2, 6]. Artificial intelligence is a set of powerful tools for analyzing massive amounts of data necessary to study the unique biological potential of medicinal plants [7, 8]. Researchers can now combine traditional knowledge about herbal medicine with the latest technologies, enabling efficient exploration of the enormous biodiversity at the molecular level [1, 6]. There is also a growing body of valuable digitized resources and databases helping in the identification and analysis of medicinal plant compounds [4, 9]. In general, the integration of artificial intelligence into traditional methods is expected to fundamentally change the way of investigation, allowing for skipping the time-consuming and expensive steps of the conventional drug discovery process [5, 10]. In the modern drug discovery process, the addition of artificial intelligence has changed the way drugs are being used [3]. A well-known representative of anti-cancer drugs is paclitaxel, also called Taxol, isolated from the Pacific yew, which took more than 30 years to reach the stage of clinical use [9].

2. Overview of Artificial Intelligence

Artificial Intelligence (AI) in medicinal plant research refers to a broader set of Machine Learning (ML), Deep Learning (DL), and Natural Language Processing (NLP) algorithms used for intelligent analysis of data to discover, study, and streamline relevant plant-made compounds [4, 7]. These advanced technological tools can analyze large amounts of various biological, chemical, and pharmacological data in a relatively shorter time than conventional computer programs [8, 10]. ML algorithms are traditionally segregated into supervised, unsupervised, and semi-supervised types that are used for classification, compound activity recognition, and yield prediction, accordingly [2, 11]. Within the framework of DL, researchers utilize various model architectures such as CNNs, or Convolutional Neural Networks, enabling the recognition of image patterns, useful for medicinal plant identification, or Vision Transformers, allowing the study of molecular interactions through the approach of graphical representations [6, 12]. Moreover, the application of computer vision enables scientists to distinguish between similar species and identify plant specimens automatically [4, 10]. GNNs or Graph Neural Networks, and Vision Transformers (ViTs) are also used to describe the complex regulatory networks of the gene-environment relationship, or to analyze the interactions of multiple genes and enzymes involved in the synthesis of various bioactive molecules [6]. Within the structure of NLP or Natural Language Processing, researchers use Large Language Models(LLMs) to extract valuable information from digitized texts, automatically summarize research papers, and create complete bibliographies [8, 14]. Advanced AI technologies such as AlphaFold 3 can predict the structure of proteins and explain how the lead molecules interact with specific protein targets and work inside the human organism [2, 4].

3. Traditional Approaches vs. AI-Driven Drug Discovery

Traditional pharmacological approaches in studying medicinal plants are usually characterized by low efficiency and random exploration [4, 5]. Conventional identification procedures are mostly based on the expertise of taxonomists,

and therefore, they are highly subjective [2, 10]. Moreover, the traditional way of drug discovery implies a long and laborious process of numerous tests necessary to isolate potentially valuable molecules [11, 15]. At the same time, the AI-driven discovery process is based on the concept of the virtual high-throughput screening of potentially valuable phytochemicals followed by the corresponding laboratory validation [2, 10]. The use of predictive models allows researchers to estimate the bioactivity of thousands of isolated molecules quickly and efficiently [1, 4]. While the traditional discovery method implies physical screening of numerous plant extracts, AI-based approaches provide virtual screening of various combinations of potentially valuable molecules [5, 7]. The integration of AI technologies into the drug discovery process has made it possible to dramatically reduce the time and effort needed for conventional experiments [10, 11]. The AI model of machine learning follows the application of screening chemical compounds, with the case study of IBM Watson for drug discovery—deep learning by the application of predicting the drug interactions in the human body [16]. In addition to accelerating the rate of finding promising drug candidates, artificial intelligence also allows for optimizing the choice of the most promising phytochemicals and analysing the corresponding biochemical pathways [4, 6]. In general, both traditional and AI-driven methods have the same goal, namely, the identification of new drugs with optimized therapeutic concentrations. At the same time, the traditional trial-and-error approach is highly time-consuming and dependent on the experience of researchers, while AI methods allow for skipping unnecessary lengthy procedures and thus significantly reduce the cost of the process [7,10]. As a result, traditional methods of drug discovery are now being replaced by innovative AI technologies, which are now being integrated into all stages of the research, from the isolation and analysis of phytochemicals to the identification and optimization of specific compounds.

Table 1: Traditional Approaches to Drug Discovery and Development: Applications, Representative Case Studies, and Scientific Impact.

Traditional model/method	Application	Case study	Impact
In Vivo Animal Models	Testing raw plant extracts in animals (rats or mice) to see toxic and therapeutic results	Vivisection	Safety and efficacy before testing in people
Phenotypic Screening & Pharmacognosy	Isolating active ingredients from plants and animals	Extracting aspirin from willow bark to reduce pain.	Life-saving technique directly derived from nature.
Empirical Chemical Modification	Attenuation	Converts morphine into heroin or codeine to test efficacy	Trigger medicinal and Structural analog design

Table 2: Artificial Intelligence–Driven Approaches in Drug Discovery and Development: Applications, Representative Case Studies, and Scientific Impact.

AI Model/method	Application	Case study	Impact
Machine learning	Screening chemical compounds	IBM Watson for Drug Discovery	Developing candidate identification
Deep learning	Predicting drug–target interactions	AlphaFold by DeepMind (Google)	Lethal protein structure predictions
Molecular dynamics	Simulating drug efficacy in silico	BenevolentAI for COVID-19 drug.	Rapid identification of drug candidates

4. Broad Applications of AI in Medicinal Plant Research

Artificial intelligence is transforming the field of natural product research by enabling the deconstruction of complex multi-domain botanical systems into machine-readable forms. Beyond automating the identification and authentication of species, AI-driven approaches are accelerating botanical drug discovery across multiple critical domains: Automated Species Authentication & Quality Control: Advanced computer vision techniques, including Log-Gabor filtering and custom deep learning architectures, enable rapid, reliable plant classification [32]. Ethnobotanical Literature Mining & Knowledge Extraction: NLP algorithms can identify high-potential traditional medicinal practices from scanned legacy or digital resources, highlighting ethnopharmacological practices such as Indonesian Jamu and Traditional Chinese Medicine for deeper chemical investigation [33]. Generative Molecule Design & Virtual Screening [35]: Generative AI enables the rapid design, discovery, and optimization of plant-made molecular leads (Gangwal et al., 2024). By virtual screening of phytochemical libraries, researchers can arrange molecules with desirable binding affinities while simultaneously exploring structure-property correlation to enhance ADMET profiles. Network Pharmacology & Multi-Target Synergy [36]: Traditional herbal medicines often comprise complex mixtures of active ingredients that simultaneously modulate numerous biological targets to exert therapeutic effects. By utilising AI-driven network pharmacology approaches, researchers can begin to decode these complex mechanism-of-action relationships.

5. Medicinal Plant-Based Drug Discovery

Artificial Intelligence (AI) can be applied at multiple stages of the drug discovery process from the identification of promising botanical sources to the optimization of lead compounds for clinical development. At the initial stage of rare plant identification, medicinal plant species can be rapidly classified using CNN or Convolutional Neural Networks allowing to achieve over 95% accuracy in most cases [12, 15]. Deep learning algorithms can also be used for classifying previously unidentified species [12]. Modern researchers use deep neural networks such as DeepNPD to predict synergistic interactions between herbal bioactive compounds for the treatment of complex diseases such as cancer [7]. In silico studies also allow for optimizing various biochemical pathways and predicting key enzymes

playing an essential role in the synthesis of valuable plant compounds [7, 11]. Molecular docking, virtual screening, and in-silico ADMET prediction enable computer-aided design of drugs and identification of the most promising phytochemicals with the best therapeutic index [5, 6]. Moreover, modern technologies allow for retrieving valuable information from extensive bioinformatics and chemical databases to identify new drugs with the desired properties and analyze their mechanism of action [4, 18]. Artificial intelligence allows for transforming large sets of data related to the biological activity of various substances into valuable information helping to find new pharmaceuticals. In general, the integration of AI-based approaches into medicinal plant studies enables researchers to accelerate the drug discovery process and achieve the best results in a short period.

6. AI Tools and Databases Examples Used

The success of modern AI models depends heavily on the availability of high-quality digital repositories and specialized software tools. Researchers utilize gold-standard databases like DrugBank, PubChem, and the HERB database for training models on compound structures and biological targets [1, 7]. Specialized repositories such as IMPPAT and the Traditional Knowledge Digital Library (TKDL) link historical medicinal knowledge with modern phytochemical annotations [4, 6]. AI models like AlphaFold 3 are landmark tools used for accurate protein structure prediction, assisting in understanding how phytochemicals bind to receptors [2, 4]. Additionally, R programming environments and packages like GSVA and BiocManager are utilized to set up computational workflows for large-scale genomics analysis [1, 7]. Mobile applications like Ayur-Leaf and Ayur-PlantNet utilize local model inference to support real-time species identification in the field [12, 13]. In this study, we used a deep learning model to predict the potential medicinal effects of natural compounds using AI or machine learning [18].



Figure 1: AI tools and databases

7. Results

Extensive testing across various computational architectures has demonstrated that deep learning models consistently outperform traditional machine learning classifiers in both accuracy and generalization. For instance, in the classification of 64 species of indigenous medicinal plants, the VGG16 architecture achieved a peak testing accuracy of 97.8%, while the VGG19 configuration reached 97.6%. These results significantly surpass basic CNN configurations, which generally maintain an accuracy of approximately 95.79%. In large-scale multi-class problems involving over a thousand species, advanced models like EfficientNet-B1 maintained a testing accuracy of 85.5%, proving the scalability of these techniques. In the realm of drug-target interaction, the DeepDPI model achieved an average accuracy of 0.84 and an average AUROC of 0.92, successfully learning both binding and non-binding patterns across thousands of drug-protein pairs. When applied to unseen drugs, the model still performed effectively with an AUROC of 0.85. Furthermore, the DeepNPD system recorded a precision of 0.87 when predicting synergistic combinations of chemotherapy drugs based on patterns learned from natural product pairs. In metabolic research, AI-driven pipelines were able to narrow down over a thousand transcription factor candidates in licorice to a small set of high-confidence regulators, leading to the experimental validation of an R2R3-MYB transcription factor. This task would have been statistically impossible through manual screening alone given a typical validation rate of less than 0.1%. Additionally, in the optimization of extraction processes, Artificial Neural Network models coupled with Genetic Algorithms improved the yield of active compounds by 23% compared to conventional response surface methodology.

8. Current Challenges

Although AI has already transformed medicinal plant research, several barriers still hinder the universal adoption of these technologies. First, critical drug discovery bottlenecks such as data scarcity for under-researched endemic species, the black-box nature of deep learning algorithms, and a mismatch between high-throughput in silico screening and low-throughput laboratory validation impede progress [6, 7]. Second, converting age-old empirical knowledge into standardized digital formats raises ethical questions about bioprospecting and intellectual property rights issues [6, 19]. Finally, multi-modal integration of diverse “omics” datasets presents technical hurdles that currently limit the scope of AI applications in botanical drug discovery [4, 7]. At present, the field of drug discovery requires a more comprehensive, integrated approach to analyzing the vast amounts of data already available. Discovering drugs in today’s world is not an easy task since the disease occurs in the human body in a particular way. The overall strategy for finding drugs and treating diseases is being transformed through a combination of technology and machine learning. Most medicinal plants cannot provide complete information on phytochemicals. Information on medicinal plants is dispersed and localized in various publications, books, and other resources. It is vital to collect and structure such data using AI models since they require high accuracy to yield better results. It is also necessary to combine genome, metabolome, chemical, pharmacological, and clinical data with an AI model to get precise results.

9. Future Perspectives

The future of artificial intelligence in this field is closely related to addressing the current issues mentioned above. In other words, future research should be focused on achieving the following goals. First, it is essential to develop a set of new algorithms allowing to operate with scarce data, in particular for endemic species, and apply physics-informed deep learning approaches allowing to restore the dynamics of biological systems using limited data resources. This task is especially relevant for researchers since the majority of the studies are related to time series data. Second, it is also vital to develop new algorithms that can be trusted by regulatory authorities and other stakeholders. This issue is critical for the regulation of herbal medicine and the development of new treatments, in particular in the area of drug discovery. Third, it is essential to create new opportunities for automated high-throughput testing to validate the results of in silico experiments. Fourth, it is also necessary to develop standards for working with multi-omics data and find ways to overcome the main challenges related to this issue. Finally, it is vital to find solutions to ethical and intellectual property-related concerns for promoting the wider use of technologies.

Tanle 3:

Domain	Current challenge	Future perspective
Data quality and bias	Data paucity for endemic species and lack of time series data	Species-centric knowledge bases and Physics-Informed Neural Networks(PINNs).
Model Interpretability	"Black box" deep learning models packing regulatory trust.	Causal discovery models & explainable AI (XAI) workflows
Testing Throughput	Low-throughput manual lab validation vs. fast AI prediction	Autonomous "Self-Driving Laboratories" with robotic validation
Omics Integration	Technical bottlenecks in multi-omics standardization	Global omics data standardization & multi-modal AI architectures
Ethics & Governance	Biopiracy concerns & indigenous IP rights	Blockchain-backed data sovereignty & Nagoya Protocol compliance frameworks

10. Conclusion

The incorporation of artificial intelligence into medicinal plant research represents a profound paradigm shift that integrates ancient empirical wisdom with the precision of modern science. By automating the identification of plant species and predicting the bioactivity of their complex constituents, AI significantly reduces the immense time and cost barriers associated with traditional drug discovery. While challenges such as data heterogeneity and model interpretability persist, the development of integrated, multi-modal systems biology frameworks offers a sustainable path forward for the pharmaceutical industry. As high-throughput data continues to accumulate and algorithms become more sophisticated, the full biosynthetic potential of the natural world will be unlocked for the benefit of global healthcare. The synergy of human expertise and machine intelligence ensures that traditional herbal medicine will remain a vital component of the 21st-century therapeutic landscape.

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