REVIEW ARTICLE

Recent Prospects in Leveraging Artificial Intelligence for Phytochemical Research

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ABSTRACT
Traditional trial-and-error techniques are currently giving way to data-driven approaches by integrating artificial intelligence in herbal drug research. Although herbals have been recognized for centuries, for their potential in treatment of various health conditions but now confronting the difficulties with their identification, laborious extraction and inadequate bioavailability. Drug development, target recognition, quality assurance, precision medicines and poly or allo-herbal synergy assessment are among the many of the domains of the herbal research which are being transformed by Artificial intelligence strategies, such as machine learning, deep learning and natural language processing. Such techniques estimate the pharmacokinetics and toxicity profiles of bioactive components, enhance molecular screening and provide highly precise plant identification through these neural networks. Artificial intelligence's real time utility in quality control has been demonstrated by smartphone applications like 'Q-Check', 'Leaf-Snap' and 'Apleaf'. Artificial Intelligence additionally supports in synergy analysis, by forecasting advantageous combinations and avoiding harmful interactions, which results it easier for researchers to develop safer and more efficient allo-polyherbal formulations. Nonetheless constraints like universal accessibility, regulatory synchronization and data standardization persist for its continued existence. Irrespective of this, artificial intelligence continues to revolutionize herbal research and accelerating the production of next-generation phytomedicines by improving reliability, assurance and worldwide relevance.
Keywords: Artificial intelligence, Allo-poly herbal, Deep Learning, Drug Design, Drug Discovery, Herbal Drugs, Machine Learning, Pharmacovigilance, Polyherbal Synergy**.**
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INTRODUCTION

The utilization of artificial intelligence (AI) in drug discovery and research predicts an enormous shift away from traditional approaches to sophisticated algorithm-driven strategies, particularly in the context of herbals and natural products[1]. From decades, herbal medicines made from plants and occasionally animals have been used as curative agents. Prior the advancement of modern pharmaceuticals, they were frequently the primary means of illness. The world health organization affirms that the majority of individuals still utilize herbal medications or their derivatives, which still constitute an invaluable source for novel medication candidates[2]. However, barriers like complicated extraction procedures and inadequate bioavailability restricts them from being more widely used. Structural elucidation of herbal components is typically an exhaustive work and techniques like X-ray crystallography and mass spectroscopy are utilized in this process. Conventional techniques require time to produce results, maybe years. This scenario has been substantially altered by implementation of AI, which reinforces *de novo* drug design in herbal research and allows for efficient molecular screening[3]. Due to machine learning (ML) and sophisticated computational techniques, researches are able to more efficiently investigate the therapeutic potential of substances from nature while pushing beyond traditional barriers[4].

The clinical success rate in drug discovery is barely over 10%, and it still has an expensive and intricate process. A single approach that has shown promise for speeding up and conserving resources during this process is computer-aided drug design (CADD). By improving its ability for creativity, data analysis, and repurposed medicines, modern artificial intelligence improves CADD[5]. With strategies like 'Q-Check', 'Leaf Snap', 'Leaf Net', and 'Apleaf', which use deep neural networks (e.g. AlexNet, GoogLeNet, VGGNet) for image-based plant authentication and exhibit validation precision of up to 80% for pharmacovigilance (PV), quality control (QC), and quality assurance (QA), AI has also been utilized in these domains. Personalized medicine, natural language processing (NLP), product development, and herbal synergy analysis are further faces that are employing deep learning (DL) extensively[6,7].

AI Assisted Herbal Research: A New Synergy

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AI is revolutionizing drug discovery by enhancing predictive modelling, accelerating chemical synthesis, and identifying therapeutic candidates more efficiently[8]. In natural product development, AI especially via ML and DL reduces cost and timelines, overcoming challenges like complex molecular structures and isolation procedures, thereby advancing personalized medicine through patient-specific predictive models[9]. AI is transforming natural product research by enabling rapid identification, extraction, and prediction of bioactive compounds like flavonoids and alkaloids[10]. Drug development is strengthened by ML and DL, particularly through neural networks and bio-NLP, which predict bioactivity, refine methods for extraction, and conduct virtual screening. Target identification and gene prediction for secondary molecules are additionally facilitated by these techniques.

AI facilitates the development of herbal drugs by overcoming challenges with substrate specificity and molecular replication. AI minimizes toxicity while retaining efficacy by providing safer treatments using synergistic drug combinations at a smaller dose[11]. Cross-validation and grid search are two strategies used by ML and DL models in herbal QC and QA, that improves performance utilizing high-quality datasets. Through the usage of smartphone apps like Q-Check, Leaf Snap, Leaf Net, and Apleaf, AI models—including convolutional neural networks, (CNNs) have exhibited remarkable precision for determining adulterants and authenticating the legitimacy of plant species. Applications are created through architectures such as GoogLeNet and AlexNet are now extensively utilized worldwide[12]. AI positively impacts the understanding of structured as well as unstructured data in PV, enabling adverse drug reaction (ADR) monitoring as well as preliminary detection of diseases (e.g., HypoDetect for diabetes). Whereas

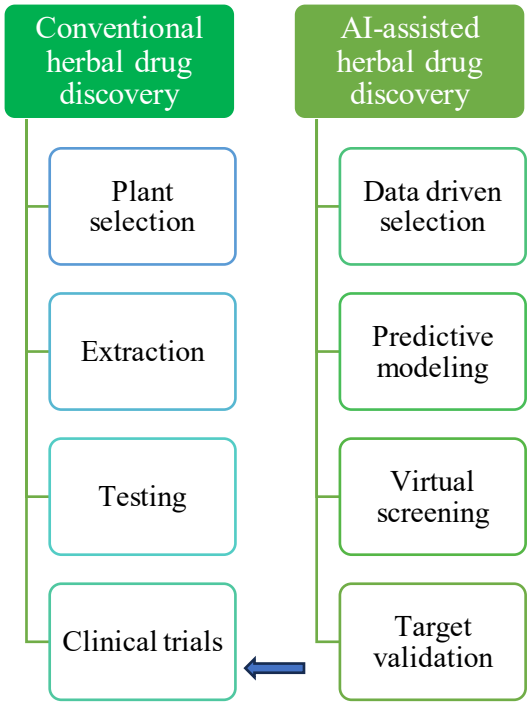

Figure 1: AI vs Traditional herbal drug discovery workflow

characterized terminology and procedures must be established for sustained development, firms like Novo Nordisk employ AI for managing data and quality assurance[13]. Personalized treatment relies on accurate diagnosis, which integrates genetic, phenotypic, and environmental data. By fusing contemporary pharmacogenomics with Ayurveda's "Prakriti" classification, Ayur Genomics reveals variation in genes (such CYP2C19 polymorphisms) which influence drug response. Strategies for treatment have been further refined by epigenomics and pharmacogenetics (e.g., by Polymerase chain reaction, Restriction Fragment Length Polymorphism). AI boosts data analysis in PV and herbal research, which strengthens both domains[14]. ADRs persist to be an overwhelming health burden, because many new medications ignore tropical conditions. In India, the population density and financial disparities rendered access to care immensely difficult. The primary objective of programs such as the Indian Genome Variation Consortium (2005) is to minimize these disparities and efficient therapies[15].

Herbal Drug Discovery- Current Status

Plants are outstanding resource for drug discovery due to their diversified chemical properties and therapeutic implications. Despite this, there have been over >75,000 exotic plant species reported in recent decades, very few of these are being used for traditional healthcare, and even a few were investigated via research, indicating tremendous unexplored potential[16]. Traditionally employed by ancient civilizations, herbal knowledge helps modern-day researchers opt for the species of plants to use, to provide further scientific assurance through botanical competence. The herbal pharmaceutical sector remains dependent heavily on phytochemistry to help decode the intricate structure of natural products and support the discovery of cost-effective, globally applicable treatments. Conventional research in medicines has been constrained by unreliable trial-and-error processes. Nowadays, this technique has been improved by shifting trend towards data-driven and AI-assisted approaches. Fig 1 highlights the procedural differences used in conventional and AI assisted herbal drug discovery.

AI is incorporated in medicinal chemistry and herbal drug development by simulating human cognitive processes, which is essential for analyzing comprehensive datasets and passing judgements based on them. The current methodology includes selection of valuable plants, extracting bioactive substances and investigation of results by in vivo and in vitro drug testing. The therapeutic potential of lead compounds is investigated through software tools and spectroscopic techniques are utilized to elucidate their molecular structure. Potential lead compounds are discovered and modified for enhanced therapeutic potential. This sequential process involves review of literature, data modelling, adequate safety and efficacy screening, economical extraction and biological investigation[17].

Artificial Intelligence Empowered Herbal Drug Discovery

In comparison to traditional techniques such as High Throughput Screening (HTS), AI has revolutionized each

step of drug development process by estimating biological activity, elucidating compound structures and boosting effectiveness. ML, a subfield of AI enables the algorithms to gather the information from enormous datasets without any explicit programming. It accomplishes this issue by employing techniques such as supervised, unsupervised and reinforcement learning for gradually improving prediction reliability and effectiveness. AI substantially decreases down both the duration and cost associated with drug development by integrating algorithm-driven models for primitive trial-and-error methods. AI offers novel opportunities in herbal drug research, which has previously hampered by laborious extraction processes, through investigating molecular interactions and recognizing significant patterns across extensive biological and chemical datasets[18]. Approaches such as virtual screening and structure- based drug synthesis enable rapid and affordable alternatives for conventional HTS[19]. Novel compounds have been made more conveniently using generative AI models like generative adversarial networks (GANs) and variational autoencoders (VAEs). Furthermore, they predict pharmacokinetic parameters i.e. absorption, distribution, metabolism, excretion and toxicity (ADMET) to determine how to avoid later stage failures while improving safety and efficiency of medications. ML methods such as random forests, decision trees and support vector machines aid in predicting toxic characteristics, distinguish compounds and assess binding affinities. DL methods like transformers, convolutional neural networks and artificial neural networks were particularly efficient in understanding complicated biological data, although reinforcement learning employs feedback loops to optimize drug design and chemical synthesis. AI approaches, have enhanced data visualization, predictability and efficiency in the workflow, modernizing the advancement of herbal drugs. Tools like GANs foster *de novo* drug design, NLP enables rapid data extraction and ML assists in bioactive assessment. Through the utilization of anticipatory data-driven techniques, merging of computer vision and multiomics streamlined the drug development[20]. Fig. 2 depicts the several steps utilized in AI method.

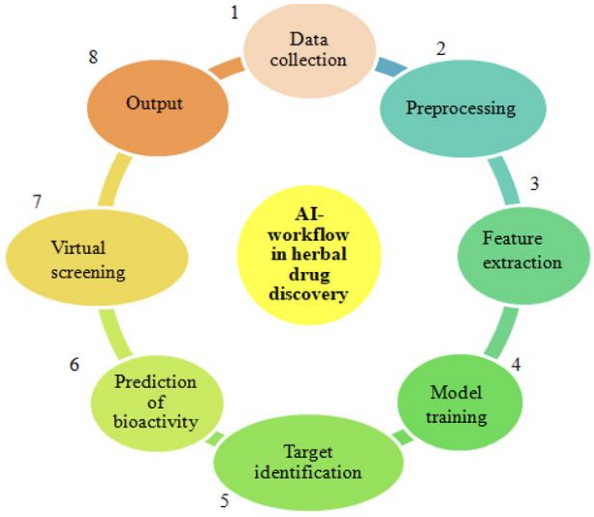

Figure 2: Steps involved in AI assisted herbal drug discovery

Applications of AI in Herbal Therapeutics

AI has completely modified the process of discovering herbal drugs due to the fact that it streamlines the critical steps such as target prediction, deorphanizing, metabolome mining, synthesis planning and virtual screening. Biosynthetic gene clusters and metabolic profiles are easily investigated with the incorporation of DL, while methods such as pharmacophore modelling, molecular docking and bioactivity fingerprinting enable precise molecular target identification[21,22]. By algorithmic forecasting of toxicity, bioactivity and pharmacokinetics, AI uncovers hidden patterns in large datasets to find potential bioactive compounds. Additionally, AI-particularly ML and DL, automatically identifies compounds and compare them with the known molecules in dereplication by accessibility to the spectroscopic data and CNNs[4,12]. It also expedites *de novo* drug design by utilizing *in silico* screening and reinforcement learning for multifaceted drug efficiency[23]. By establishing consistent quality control using ML pipelines, image-based authentication (e.g., CNN models like ResNet101, Inception V3) and real time adulterant detection, AI improves natural therapies[9,18,24,25]. Meanwhile, it makes much easier to analyze the synergy of polyherbal formulations (such as Diabet and Dihar are hypoglycaemic agents) and predict safer, more effective combinations utilizing DL models like Deep synergy, Synergy finder and network pharmacology[26]. PV is another domain in which AI is beneficial, it minimizes human error and strengthens safety surveillance by enabling real-time ADR detection, data synchronization and compliance automation through NLP and predictive analytics[27]. By refining the pharmacokinetic characteristics of potential bioactive compounds like quercetin, kaempferol and vancomycin, the merging of AI and natural product research by promoting precision medicine to offer customized, affordable treatments for numerous disease conditions[7].

Various Challenges Encountered during Herbal Research using AI are as Follows

- Trust among the researchers and regulators becomes compromised when AI estimations are not interpretable.
- Incorporation of AI into experiments is essential for the reliability of AI-generated drug candidates[28].
- Exploration of natural products has been constrained in terms of precision and utility due to the scarcity of high-quality datasets.
- The capability of AI to predict future outcomes is hindered by the complicated structure of the natural products.
- Multi-target interactions go unnoticed and model reliability declines when old data is used.
- Explainable AI techniques need to be developed for more widespread adoption because DL's 'black box' nature impedes transparency[29].

Future Prospects

AI integration in herbal medicine is projected to continue expanding, enhancing clinical application, research, and healthcare for society. To improve the accuracy of AI models, potential developments comprise herb-specific repositories and standardized image databases.

Multifaceted AI that incorporates evolutionary, genetic, phytochemical, along with image data will make authentication more effective. Transparency enhancements will facilitate regulatory approval with the help of explainable AI. Instantaneously, offline herbal identification in distant places will be supported by mobile and IoT-powered solutions. The alliance between AI and pharmacogenomics will enable tailored alternative therapies based on primordial concepts like Prakriti and genomic fingerprints. AI will additionally enhance *de novo* drug design and automated dereplication, which will accelerate up their search for novel bio-actives. These advances promise improved incorporation of traditional medicine into modernized treatment and safer, more effective herbal products[30].

CONCLUSION

AI has altered the development of herbal drugs by surpassing existing restrictions and enabling efficient bioactive ingredient discovery, plant authentication, formulation design, and toxicity prediction. It reduced expenditures, expedites up drug research, and builds dependability. Natural medicines are steadily reliable and efficient when AI is integrated into pharmacovigilance, quality control, and synergy imitation. Non-experts in quality assurance and adulteration detection have been enabled by instantaneous form technologies and deep learning smartphone apps. Additionally, AI statistically analyzes herbal combinations, reinforcing conventional systems. But there are still issues like worldwide approval, ethical concerns, and dataset standardization. Eventually, AI widens up the path to safer, economically feasible phytomedicines by automating and making more accessible the process of discovering.

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Abbreviations

ADR-Adverse Drug Reaction; **AI** – Artificial Intelligence; **CADD**- Computer-Aided Drug Design; **CNN**-Convolutional Neural Network; **DL**- Deep Learning; **HTS**-High Throughput Screening; **ML**- Machine Learning; **PV**-Pharmacovigilance; **QA**- Quality Assurance; **QC**- Quality Control.

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