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COMMENTARY

Artificial intelligence in unveiling herbal remedies for cancer: Advances and applications

Bargale Sushant Sukumar[1] | Shashirekha H K[2] | Amarnath H K[3] | Neha Gadgil[4] | Akshar Kulkarni[5] | Shipra[6] | Harshal Tare[7]

[1]Department of Swasthavritta and Yoga, Sri Dharmasthala Manjunatheshwara College of Ayurveda and Hospital, Hassan, Karnataka, India

[2]Department of Samhita Sanskrit, Banaras Hindu University, Varanasi, Uttar Pradesh, India

[3]Department of Shalakya Tantra, Sri Dharmasthala Manjunatheshwara College of Ayurveda and Hospital, Hassan, Karnataka, India

[4]Department of Kriya Sharir, Sri Lal Bahadur Shastri Smarak Rajakiya Ayurvedic Mahavidyalaya, Handia, Prayagraj, Uttar Pradesh, India

[5]Department of Samhita Siddhanta, Parul Institute of Ayurved, Parul University, Vadodara, Gujarat, India

[6]Department of Prasuti Tantra and Striroga, Sri Lal Bahadur Shastri Smarak Rajakiya Ayurvedic Mahavidyalaya, Handia, Prayagraj, Uttar Pradesh, India

[7]Department of Pharmacognosy, Sharadchandra Pawar College of Pharmacy, Pune, Maharashtra, India

Correspondence
Harshal Tare
harshaltare51@gmail.com

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Cancer continues to pose a significant global health burden, with millions of new cases diagnosed each year. Despite advances in conventional treatments such as chemotherapy, radiation, and immunotherapy, these approaches often come with considerable challenges, including severe side effects, treatment resistance, and high costs. Artificial intelligence (AI) technologies such as Machine Learning and Deep Learning offer significant promise to overcome such challenges.[1] Machine learning techniques aid in discovering novel medications by analysing large datasets to predict the activity and efficacy of new compounds. It accelerates drug discovery by automating screening and modelling drug-target interactions, reducing time and costs compared to traditional methods. Deep learning, using artificial neural networks, analyses large datasets to identify complex patterns. In pharmaceuticals, deep learning predicts drug functionality, identifies treatment targets, and decodes biological structures, accelerating drug discovery and improving treatment outcomes. AI can be highly useful not only in the novel drug discovery but also in identification of promising anticancer compounds of natural origin. Herbal remedies are complex, containing multiple active constituents that often work synergistically. One requirement is the need for more stringent clinical validation.[2]

For the literature search in this commentary, specific inclusion and exclusion criteria were applied to ensure relevant studies were selected. Inclusion criteria included: (1) studies focused on the use of AI techniques (such as machine learning, deep learning, and natural language processing) in discovering herbal remedies for cancer. Exclusion criteria included: (1) studies not related to AI. AI plays a crucial role in personalized herbal treatments by integrating patient data (genetic, medical, lifestyle) to customize therapies, using predictive analytics to forecast responses and adjust treatments based on feedback for optimal outcomes and minimized side effects.[3]

Key messages

Artificial intelligence have revolutionised herbal anticancer medication discovery. AI has predicted bioactive molecules and optimised drug synergy. Improved clinical trial designs and customised therapy have boosted cancer herbal medicine research. Data quality, model transparency challenges and AI-driven strategies to expedite herbal cancer treatment development conclude the article. AI models could find new natural anticancer compounds, revolutionising cancer treatment.

Table 1 Summary of the applications of AI in drug discovery

Application	Description	AI techniques used	Benefits	Relevance to drug discovery
Identification of target	AI analyzes extensive datasets to detect proteins, genes, or pathways affecting disease mechanisms, aiding in identifying promising targets.	Machine learning, data mining	Focuses research on the most promising targets	Target identification is crucial for the success of drug discovery, helping streamline the search for effective treatments.
Substance testing	AI optimizes drug screening by predicting the most effective compounds, reducing the need for extensive experimental testing.	Predictive models, convolutional neural networks	Reduces experimental workload, accelerates discovery process	AI's predictive capabilities enhance efficiency by narrowing down the best candidates, saving time and resources.
Predictive modelling	AI-driven models predict ADMET[a] properties of drug candidates, helping assess potential effectiveness and safety before experimental validation.	Statistical techniques, machine learning	Expedites and reduces costs of drug development	Predictive modeling reduces failure rates in clinical trials by assessing the safety and efficacy of drugs early in the process.
Drug repurposing	AI finds new therapeutic uses for approved drugs by uncovering correlations between drugs and diseases.	Data analysis, natural language processing	Accelerates development using existing safety and efficacy data	Drug repurposing is a cost-effective strategy to quickly find new treatments, leveraging existing drugs for new indications.

[a]ADMET indicates absorption, distribution, metabolism, elimination and toxicity

AI implementation in herbal medicine faces several technical challenges. Data quality and accessibility issues include gaps in critical information, which limit prediction accuracy, and difficulties in integrating diverse data sources due to varying formats and standards. Algorithm limitations arise from models trained on specific datasets that may not generalize well to new or unseen data, particularly for diverse herbal compounds and patient populations. The complexity of herbal mixtures, with multiple active constituents, adds another challenge, as AI models may struggle to capture their synergistic effects. Additionally, high computational demands for advanced AI models can be a barrier for smaller research labs or organizations lacking access to powerful computing resources.[4]

AI techniques have significantly enhanced herbal drug discovery for cancer, with machine learning models identifying promising compounds like curcumin, paclitaxel, camptothecin, resveratrol and Epigallocatechin-3-gallate. Deep learning and natural language processing have accelerated drug-target interaction predictions, extracting key insights from databases with published studies. Advancements like transfer learning and Graph Neural Networks have optimized herbal compound synergy, increasing the accuracy of compound-target interaction models by 15%. Platforms like Atomwise have improved the success rate for compounds with anticancer potential by 30%, while DeepChem has significantly improved the discovery methodology (Table 1).[5]

Recognizing there are benefits to using AI to identify herbal anticancer agents, but there are challenges to overcome before implementation. The biggest challenge is data quality and accessibility. AI models need datasets to provide accurate predictions and insights. However, herbal medicine databases lack consistency, accessibility, and comprehensiveness. AI model creation is difficult due to the lack of formal documentation for many traditional knowledge systems and uneven dataset quality. AI struggles to acquire worldwide researchers' and clinicians' trust in innovative drug discovery, where clinical validation and regulatory approval are crucial.[6]

It can be concluded that AI has the capacity to enhance accuracy, expedite the discovery and optimise clinical studies in order to revolutionise the antineoplastic treatments with special reference to bioactive molecules.

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Conception or design of the work; or the acquisition, analysis, or interpretation of data for the work: BSS, SHK, AHK, NG, AK. *Drafting the work or reviewing it critically for important intellectual content:* NG, AK. *Final approval of the version to be published:* BSS, HT. *Accountable for all aspects of the work in ensuring that questions related to the accuracy or integrity of any part of the work are appropriately investigated and resolved:* HT.

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Data availability statement

Not applicable

Supplementary file

None

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