



# The transformative potential of artificial intelligence in enhancing the safety and efficacy of herbal medicines

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## Dear Editor,

Artificial intelligence (AI) represents a transformative opportunity to significantly enhance the safety and efficacy of herbal medicines derived from medicinal plants and natural products. Current methodologies for phytochemical profiling and toxicity assessment are often time-consuming, costly, and limited in scope, thereby hindering the efficient development and safe utilization of these increasingly popular remedies. AI-powered tools, which leverage deep learning and machine learning algorithms, offer a robust solution to these challenges. These tools can automate the identification and quantification of phytochemicals, thereby improving the speed and accuracy of analyses substantially. Furthermore, AI's predictive capabilities facilitate the assessment of individual compound toxicity and the complex interactions among multiple phytochemicals, enabling earlier detection of potential safety concerns and guiding the development of safer formulations. Beyond the analysis of individual compounds, AI can integrate diverse datasets—including genomic, metabolomic, and ethnobotanical information—thereby accelerating the discovery and development of novel therapeutics from natural sources. However, to realize the full potential of AI in this domain, it is imperative to prioritize the establishment of high-quality datasets, foster robust interdisciplinary collaboration, and carefully address issues related to data bias and model interpretability. Investment in AI research within the field of phytochemistry is crucial for the development of safer and more effective herbal medicines, which ultimately contributes to improved global health outcomes. In light of these considerations, this paper aims to highlight the transformative potential of AI in advancing the safety and efficacy of herbal medicines derived from medicinal plants and natural products. The increasing global utilization of these products necessitates the development of robust and efficient methods for phytochemical profiling and toxicity assessment, areas in which AI offers significant advantages over traditional

approaches (1).

Common biases in AI models encompass data bias, sampling bias, and label bias. These biases can be effectively mitigated by ensuring that training data is diverse and representative of the population it seeks to model. Additionally, implementing rigorous validation techniques is essential to assess the performance of AI systems accurately. Continuous monitoring and updating of these systems are also critical to address and reduce biases over time.

Current methodologies for analyzing the complex chemical composition of medicinal plants are frequently time-consuming, costly, and constrained in their scope (2). AI-powered tools, including deep learning algorithms and machine learning models, can automate the identification and quantification of phytochemicals, thereby significantly accelerating the analytical process and enhancing accuracy (3). Furthermore, AI possesses the capability to predict the potential toxicity of individual compounds and their interactions, enabling earlier identification of safety concerns and guiding the development of safer formulations. This predictive ability is particularly valuable due to the complex interplay among phytochemicals and their potential for both synergistic and antagonistic effects (4).

Researchers have successfully utilized AI to automate the identification and quantification of phytochemicals in herbal medicines. For instance, AI models have been employed to analyze the complex chemical composition of medicinal plants, resulting in quicker and more accurate profiling. This advancement has contributed to the development of safer formulations and the earlier identification of potential safety concerns. A notable example is the development of JAMU, a traditional Indonesian medicine, which was enhanced by scientists using AI (5).

The application of AI in this field extends well beyond simple compound identification. AI can analyze complex datasets from various sources, including genomic data,

metabolomics profiles, and ethnobotanical information, to identify potential drug candidates and predict their efficacy and safety (6). This integrated, multi-omics approach can expedite the discovery and development of novel therapeutics derived from natural sources, potentially addressing unmet medical needs.

However, the successful implementation of AI in this field necessitates careful consideration of several factors. High-quality, well-annotated datasets are crucial for training robust and reliable AI models. Additionally, interdisciplinary collaboration among AI specialists, phytochemists, toxicologists, and regulatory agencies is essential to ensure the responsible and ethical development and application of these technologies. Addressing issues of data bias and model interpretability is also vital for building trust and ensuring the acceptance of AI-driven approaches within the regulatory landscape.

It is worth mentioning that advancements in AI and technology are poised to transform the landscape of herbal medicine by enabling personalized treatment regimens, expediting research and development processes, and enhancing safety and quality control measures. These innovations will lead to more effective and tailored therapies, making herbal medicine increasingly accessible and reliable.

## Conclusion

The integration of AI into phytochemistry and natural products research promises to revolutionize the field, resulting in safer, more effective herbal medicines and a deeper understanding of the therapeutic potential of medicinal plants. Continued research and investment in this area are essential to fully realize the benefits of AI in improving global health and ensuring the safe and effective use of herbal medicines worldwide. We invite you to engage in further research and interdisciplinary

collaboration to explore the transformative potential of AI and technology in herbal medicine. By combining expertise from diverse fields, we can unlock new insights, innovate more effective therapies, and ultimately improve health outcomes for all. Join us on this exciting journey towards a future where tradition meets cutting-edge science.

## Competing Interests

None.

## Ethical Approval

Not applicable.

## Funding

Nil.

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