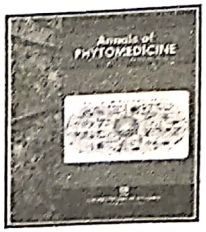
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Invited Commentary

Artificial intelligence-driven molecular target identification for precision phytotherapy

Sevgi Gezici

Gaziantep University, Faculty of Medicine, Department of Medical Biology and Genetics, 27310, Gaziantep Turkiye

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Abstract

Artificial intelligence (AI) has emerged as a powerful tool in biomedical research, offering new opportunities for molecular target identification and the development of precision phytotherapy. AI enables the systematic identification of bioactive plant compounds by integrating machine learning (ML) and deep learning (DL) approaches with phytochemical and multi-omics datasets, including genomic, transcriptomic, and metabolomic data. It also facilitates the prediction of their pharmacological activities and the elucidation of their molecular mechanisms of action. Advanced computational models such as neural networks, support vector machines, and generative algorithms are increasingly applied in virtual screening, QSAR modeling, and ADMET prediction, accelerating the discovery and optimization of plant-derived therapeutic candidates. Furthermore, AI-driven platforms facilitate the design of novel phytochemical analogues and support drug repurposing strategies, thereby enhancing the efficiency and scalability of natural product-based drug discovery. Despite existing challenges such as data heterogeneity, model interpretability, and the need for clinical validation, the integration of AI with phytochemistry and precision medicine provides a promising framework for translating complex biological data into personalized therapeutic strategies.

1. Introduction

as fundamental components of computer-aided drug discovery (Sheridan *et al.*, 2000; Willett, 2006; Solimeo *et al.*, 2012; Sprague *et al.*, 2014; Ashiwaju *et al.*, 2023).

The emergence of large-scale biological datasets and improvements in computational infrastructure have significantly increased the importance of deep learning approaches in drug discovery since the 2010s. Advances such as GPU-accelerated computing and cloud-based platforms enabled the training of complex deep neural networks capable of capturing nonlinear relationships between chemical structures and biological activities. These models have demonstrated strong predictive performance in tasks such as toxicity prediction, drug-target interaction analysis, and multi-task learning from large pharmacological datasets (Wen *et al.*, 2017; Workman *et al.*, 2019). At the same time, the growing recognition of variability in individual drug responses has strengthened the concept of precision medicine, which aims to tailor therapeutic strategies according to patient-specific biological characteristics. Medicinal plants and natural products represent valuable resources due to their remarkable structural diversity and multi-target biological activities, making them particularly relevant for the development of precision phytotherapeutic approaches (Zhu *et al.*, 2020; Asharif, 2024; Ajabali *et al.*, 2025). Accordingly, this review provides an overview of current AI-driven strategies for molecular target identification in

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