

AI and natural medicines

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Editorial

AI and natural medicines

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Natural products (NPs) derived from plants, microbes, and marine organisms have historically been a cornerstone of pharmacotherapy, accounting for approximately 35% of FDA-approved small-molecule drugs since 1981¹. These compounds have been instrumental in drug discovery, particularly for cancer and infectious diseases, as well as in other therapeutic areas such as cardiovascular diseases (e.g., statins) and multiple sclerosis (e.g., fingolimod). NPs possess unique features compared to conventional synthetic molecules, offering significant advantages in the drug discovery process. Characterized by remarkable scaffold diversity and structural complexity, NPs exhibit greater rigidity, which can be beneficial in addressing challenging protein–protein interactions. Additionally, evolution has optimized NPs to perform crucial biological functions, such as regulating endogenous defense mechanisms and interacting—often competitively—with other organisms. This evolutionary refinement underscores their relevance in combating infectious diseases and cancer, as well as providing valuable insights into efficacy and safety through traditional medicinal use². However, the traditional NP drug discovery pipeline, which includes bioactivity-guided isolation, structural elucidation, and mechanistic validation, faces several inefficiencies. These include high rates of rediscovery due to challenges with dereplication and resource-intensive workflows. Recently, artificial intelligence (AI) has emerged as a transformative force in this field, offering computational frameworks that can address these bottlenecks and unlock novel therapeutic opportunities for NPs³.

Herein, we guest-edit this special issue of CJNM with the theme of “AI and Natural Medicines” to summarize the advancements in the field. First, Chen et al. comprehensively reviewed the applications in the research of molecular pharmacokinetic and pharmacological mechanisms of traditional Chinese medicine (TCM) formulas⁴. Yuan et al. explored the implementation of AI technology in virtual screening, compound optimization, and synthetic pathway design in natural products research⁵. Subsequently, recent advancements of AI-based molecular representations and their applications were discussed for natural medicines. For instance, Liu et al. present a comprehensive review of small molecular representations and AI-driven drug–target interaction prediction, drug–target affinity prediction, drug property prediction, and drug generation, utilizing these representations⁶. Tang et al. proposed a deep learning model called DeepGCCR to identify glucagon receptor (GCCR)-targeting compounds for the development of Type 2 Diabetes Mellitus therapeutics⁷. Li et al.

proposed molecular properties prediction with parallel-view and collaborative learning (MolP-PC), an AI framework that integrates 1D molecular fingerprints, 2D molecular graphs, and 3D geometric representations⁸. Yue et al. proposed KG-CNNNTI, a novel knowledge graph-enhanced framework for DTI prediction, which integrates heterogeneous biological information to improve model generalizability and predictive performance⁹. Notably, the new paradigm of TCM network pharmacology driven by AI and high-throughput multi-omics technologies were reviewed. For example, Wang et al. introduced the progress of network target methods combined with AI in predicting disease molecular mechanisms and drug–target relationships in analyzing TCM formulae, syndromes, and toxicity¹⁰. Shao et al. focused on the key strategies for constructing various networks and analyzing constructed networks using AI methods, highlighting the cell–cell communication-based TCM network pharmacology for the mechanism elucidation and drug discovery¹¹. Lastly, AI-based predictions of synergistic effects for TCM were summarized. For instance, Wang et al. reviewed the application progress of AI in the synergistic prediction of TCM active compounds and explored the challenges and prospects of its application in modeling combination relationships¹². Niu et al. comprehensively examined recent advances in AI-driven natural product-based drug combination prediction, presented relevant data resources and algorithmic frameworks, and evaluated current limitations and prospects¹³. Yan et al. identifies major challenges and opportunities that constrain the development of robust research capabilities—particularly in the mechanistic understanding of TCM syndromes and herbal formulations, novel drug discovery, and the delivery of high-quality, patient-centered clinical care¹⁴.

We hope this theme issue offers a platform for researchers to obtain valuable insights into the AI-based natural medicines and TCM modernization. We would like to take this opportunity to thank the authors for their tireless efforts and valuable insights in making this work a reality.

Conflict of interest

These authors have no conflict of interest to declare.

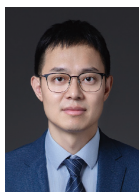
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