

Modernization Research of Traditional Chinese Medicine Compound Prescriptions Driven by Artificial Intelligence: From Intelligent Design and Mechanism Prediction to Precise Application

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Abstract This article provides a comprehensive review of the advancements in the application of artificial intelligence (AI) technology in the modernization of traditional Chinese medicine (TCM) compound prescriptions, and emphasizes recent research developments, including intelligent design, prediction of mechanisms of action, and precise application of TCM compound prescriptions. The integration of multi-omics data, deep learning algorithms, and knowledge graph technologies has established novel technical avenues for the modernization research of TCM. This study systematically analyzes the advantages and challenges associated with AI technologies in the research of TCM compound prescriptions, highlighting issues such as data heterogeneity, limited interpretability of AI models, and the absence of standardized procedures. Furthermore, this article examines the prospective developmental trajectories within this field, highlighting the importance of synergistic collaboration between AI and traditional pharmacology to improve the clinical applicability and effectiveness of TCM. The objective is to offer valuable insights into the modernization of TCM driven by AI and to stimulate further research in this area.

Key words Artificial intelligence (AI), Traditional Chinese medicine (TCM) compound prescription, Intelligent design, Mechanism prediction, Precise application

1 Introduction

Traditional Chinese medicine (TCM) compound prescriptions, which serve as the foundation of TCM treatment, have been extensively utilized for a wide range of diseases over millennia. Nevertheless, these compound prescriptions comprise complex and diverse herbal components containing numerous active substances. The interactions among these substances and their mechanisms of action remain incompletely understood, presenting substantial challenges to contemporary scientific investigation and clinical practice. This complexity has impeded the modernization of TCM and hindered the development of universally applicable standardized treatment protocols.

In recent years, the rapid advancement of AI and computing technologies has offered novel approaches to addressing the aforementioned challenges. AI is capable of processing vast quantities of data, uncovering latent patterns, and predicting the efficacy of compound prescriptions based on drug components and historical usage data. Through AI-driven methods, researchers can intelligently design compound prescriptions, optimize the combination of medicinal materials, maximize therapeutic efficacy, and minimize adverse effects, thereby facilitating the transition from empirical treatment to evidence-based medicine. Furthermore, the application of AI in TCM encompasses the prediction of pharmacological mechanisms and the assessment of clinical efficacy. For example, machine learning algorithms have the capability to analyze clinical data, identify potential biomarkers, and elucidate the mechanisms through which TCM exerts its effects. Such systematic research not only enhances the understanding of TCM but also contributes to the development of standardized clinical application guidelines,

thereby facilitating the integration of TCM with modern medical practices.

The advent of omics technologies, including genomics, proteomics, and metabolomics, has significantly enhanced the scope of TCM research. These technologies elucidate the effects of TCM at the molecular level within organisms. When integrated with AI analysis, they facilitate the elucidation of the multi-target and multi-pathway mechanisms underlying compound prescriptions, thereby establishing a robust scientific foundation and advancing the development of precision medicine in TCM. The modernization of TCM, driven by AI and omics technologies, is anticipated to improve the precision and effectiveness of treatments. As technological advancements continue, the development of personalized TCM treatment plans will become feasible, integrating traditional wisdom with contemporary technological innovations. This integration is expected to enable TCM to assume a more prominent role within the modern healthcare system.

In conclusion, the integration of AI with contemporary scientific methods has introduced transformative opportunities for the research and application of TCM. By utilizing these advanced technologies, researchers and clinicians can improve the understanding, efficacy, and safety of TCM, thereby facilitating its recognition and application within the global healthcare system. This article seeks to examine the current applications and future prospects of AI in the modernization of TCM, highlighting its innovative potential.

2 Current situation and challenges of modernization of TCM compound prescriptions

2.1 Complexity and research difficulties of TCM compound prescriptions The complexity of TCM compound prescriptions primarily arises from their multi-component and multi-target na-

ture, which significantly complicates the elucidation of their mechanisms of action. In contrast to single-component drugs, which typically have well-defined pathways of action, TCM compound prescriptions comprise multiple medicinal materials, each containing various active ingredients that interact synergistically. This complexity presents a significant challenge for researchers attempting to elucidate the pharmacological effects of the compound. Conventional *in vitro* experiments and animal model approaches are frequently inefficient and costly, thereby constituting bottlenecks in research progress. For example, while *in vitro* studies can offer preliminary insights, they often fail to accurately replicate the compound's comprehensive interactions within the living organism. Although animal models can represent systemic effects, they present challenges such as high variability and ethical constraints, which affect the reproducibility and generalizability of findings. Consequently, there is an urgent need for innovative approaches to effectively capture the multi-level and multidimensional interactions inherent in compound prescriptions. Although advanced technologies, including systems biology and network pharmacology, provide novel approaches for elucidating complex mechanisms of action, the absence of standardized methods and cross-disciplinary validation continues to pose significant challenges^[1–2].

2.2 Limitations of traditional research methods Traditional methods in TCM research lack systematic analytical tools, which hinders comprehensive analysis of the action networks of compound prescriptions. Additionally, clinical data are fragmented and lack uniform standards, complicating the replication of research findings. For example, in clinical trials, inconsistencies in patient selection, dosage, and treatment duration often lead to ambiguous or contradictory results. Furthermore, traditional experience-based efficacy evaluations lack robust statistical validation, thereby diminishing the scientific credibility of the treatment outcomes. In clinical practice, variations in operational methods among TCM practitioners contribute to inconsistent therapeutic effects, complicating the establishment of standardized, evidence-based conclusions. The utilization of contemporary data analysis and AI technologies in the field of TCM remains in its early stages. Furthermore, practitioners and researchers in this field often lack adequate professional training and access to necessary resources. Consequently, the modernization of TCM faces a significant challenge in harmonizing traditional methods with modern scientific approaches. There is an urgent need to develop a standardized framework to effectively bridge this divide^[3–4].

3 Application of AI technology in the research framework of TCM compound prescriptions

3.1 Integration of multi-omics data and AI analysis The integration of multi-omics data, encompassing genomics, metabolomics, and proteomics, constitutes the foundation for developing AI models aimed at investigating TCM compound prescriptions. By

utilizing these diverse data types, researchers can achieve a more comprehensive understanding of the complex interactions within biological systems. For example, genomics elucidates genetic susceptibilities that may influence disease states; metabolomics illustrates dynamic alterations in metabolic processes following intervention with TCM; and proteomics further clarifies the expression of key proteins and their roles in treatment. The integration of these datasets enables the development of advanced AI algorithms, including deep learning models, capable of identifying potential associative patterns between TCM compound prescriptions and specific diseases. Notably, algorithms such as DeepTCM have been effectively employed to predict the efficacy of TCM compound prescriptions across various diseases by analyzing complex signaling pathways^[5]. This AI-based analysis not only improves the predictive accuracy of TCM applications but also facilitates the advancement of personalized medicine by enabling the customization of treatment plans based on patients' multi-omics data. Nevertheless, standardizing data across different studies and ensuring the interpretability of AI models remain significant challenges widely recognized within clinical practice and the medical community^[6].

3.2 Knowledge graphs and knowledge representation of TCM compound prescriptions

The construction of knowledge graphs is a transformative method for representing knowledge associated with TCM compound prescriptions. This approach integrates information on medicinal material components, biological targets, and their related pathways. Knowledge graphs facilitate the structural representation of relationships among diverse entities, thereby enabling researchers to systematically investigate the complex networks underlying the functions of TCM. Through the application of natural language processing (NLP) technology, researchers are able to extract valuable information from both ancient texts and contemporary literature, thereby enhancing the knowledge base of TCM compound prescriptions. For example, the development of the traditional formula-disease relationship (TFDR) corpus exemplifies how NLP can be employed to annotate and analyze the relationships between TCM compound prescriptions and diseases, facilitating the automatic extraction of critical data from unstructured biomedical literature^[7]. This approach not only improves the accessibility of knowledge regarding TCM but also aids in the identification of novel therapeutic targets and mechanisms of action. Furthermore, knowledge graphs can be integrated with AI algorithms to facilitate the detection of potential synergistic interactions among various herbal components, thereby optimizing the composition of compound prescriptions to enhance therapeutic efficacy. AI-driven knowledge expression systems are advancing the practice of TCM towards evidence-based medicine, enhancing the understanding of its mechanisms of action. As this field progresses, the construction of more sophisticated knowledge graphs and their comprehensive integration with AI technologies will be essential for promoting the modernization of TCM and its clinical

applications^[8].

4 Intelligent design and optimization of TCM compound prescriptions

4.1 Exploration of AI-based compatibility rules The application of AI in the design and optimization of TCM compound prescriptions has fundamentally transformed the compatibility of medicinal materials and their therapeutic effects. Machine learning algorithms, particularly those utilizing deep learning techniques, have been employed to analyze classical TCM prescriptions and elucidate the complex compatibility principles underlying the formulation of new prescriptions. The FordNet system, when combined with deep learning techniques, integrates phenotypic and molecular data to recommend TCM prescriptions that align with clinical symptoms while considering molecular interactions and pathways. This approach not only improves the accuracy of prescription recommendations but also enables the prediction of the efficacy of novel prescriptions based on historical data derived from tens of thousands of electronic health records^[9]. Furthermore, reinforcement learning techniques have been employed to optimize the combination of medicinal materials, with the objective of maximizing therapeutic efficacy while minimizing adverse effects. This optimization process involves the dynamic adjustment of the proportions and selection of medicinal materials through iterative learning based on the outcomes of previous combinations and their synergistic properties. Such an approach represents a significant advancement in the modernization of TCM, transitioning from empirical methods to data-driven strategies, thereby improving the precision and effectiveness of herbal treatments^[10].

4.2 Virtual screening and active ingredient prediction AI has been instrumental in the virtual screening of active ingredients in TCM, facilitating the identification of bioactive compounds and their interactions with specific biological targets. Notably, AI models employing molecular docking and dynamic simulation techniques have demonstrated exceptional performance in predicting the activity of TCM components against diverse disease targets. For example, research demonstrates that AI-driven models are capable of predicting interactions between TCM components and dipeptidyl peptidase-IV (DPP-IV), a target of significant relevance in diabetes management^[11]. Additionally, high-throughput screening techniques facilitate the expedited evaluation of numerous compounds. The integration of serum metabolomics and network pharmacology facilitates the identification of active compounds within complex herbal mixtures and elucidates their pharmacodynamic properties and therapeutic mechanisms. Moreover, molecular docking studies have validated these predictions, reinforcing the role of AI in improving the precision and efficiency of TCM research. This approach also contributes to the advancement of novel therapeutic agents derived from traditional formulations^[12]. This innovative approach not only streamlines the drug discovery process but also facilitates the design of personalized

TCM formulations tailored to specific clinical requirements.

5 AI prediction of the mechanism of action of TCM compound prescriptions

5.1 Integration of AI with network pharmacology The integration of AI with network pharmacology has emerged as a potent approach for elucidating the complex mechanisms underlying TCM compound prescriptions. AI-driven network pharmacology enables the analysis of multidimensional interactions among multiple components of TCM and their biological targets, thereby uncovering the multi-target mechanisms of action of these compound prescriptions. Utilizing technologies such as graph neural networks (GNNs), researchers have developed drug-disease interaction networks to predict the efficacy of specific TCM prescriptions across various diseases. This approach not only enhances the understanding of the pharmacological mechanisms underlying TCM but also facilitates the identification of novel indications for existing prescriptions. Recent studies have demonstrated the efficacy of network pharmacology in predicting active ingredients and their corresponding targets, thereby offering a systematic framework for exploring mechanisms of action. The integration of AI with network pharmacology represents a significant advancement in the modernization of TCM, facilitating the elucidation of complex interactions within compound prescriptions and the optimization of therapeutic strategies^[13-14].

5.2 Prescription-disease association prediction model AI models utilizing clinical data have demonstrated significant potential in predicting the efficacy of TCM compound prescriptions for specific diseases. Through the application of machine learning algorithms to analyze large-scale datasets encompassing patient demographics, clinical outcomes, and treatment responses, these models can identify patterns that are challenging to detect using conventional analytical methods. For example, models can assess the efficacy of TCM prescriptions in treating diseases such as diabetic nephropathy and ulcerative colitis, while also correlating specific medicinal components with their pharmacological properties. Transfer learning technology enhances the model's generalizability across different diseases and improves its clinical applicability. Systematic data analysis has facilitated the development of robust predictive models, which serve as a foundation for clinical decision-making and enhance the application of personalized TCM. This approach not only underscores the value of AI in advancing research on TCM but also promotes the integration of traditional and modern medical practices. AI-driven predictive models enable precision treatment, improve patient outcomes, and contribute to the advancement of integrative medicine^[15-16].

6 Precise application and individualized treatment of TCM compound prescriptions

6.1 AI-assisted clinical decision support system The integration of AI into clinical decision support systems (CDSS) has

substantially advanced the personalization of treatment strategies, particularly highlighting its significant utility in the development of TCM compound prescriptions. AI systems are capable of analyzing extensive datasets, including genomics and metabolomics, to recommend tailored TCM prescriptions based on patients' individual characteristics. By utilizing patients' genetic information, AI algorithms can identify genetic variations that influence drug metabolism and efficacy, optimize combination regimens of TCM, and thereby improve therapeutic outcomes. AI-assisted CDSS are also capable of monitoring patients' responses in real time, dynamically adjusting treatment plans, and ensuring the sustainability and safety of therapeutic effects. This adaptability is especially important because the effects of TCM formulae differ among individuals due to variations in metabolism and the diverse presentations of their conditions. The continuous feedback mechanism established through AI not only improves clinical efficacy but also fosters a more responsive medical environment, thereby facilitating treatment optimization based on real-time data and clinical observations^[17].

6.2 Prediction of the efficacy and safety of TCM compound prescriptions AI possesses considerable potential in predicting the efficacy and safety of TCM compound prescriptions, which is crucial for their clinical application. Utilizing machine learning techniques, AI models can analyze historical clinical data to forecast potential adverse reactions and drug interactions associated with specific prescriptions. By identifying potential risks arising from the interaction between a patient's medical history and currently administered medications, AI has improved the safety of TCM treatments. Furthermore, the integration of blockchain technology has facilitated the sharing and verification of therapeutic effect data across diverse medical systems, thereby ensuring the transparency and traceability of the therapeutic outcomes associated with TCM compound prescriptions. This integrated strategy not only strengthens the clinical credibility of TCM but also fosters collaborative research among multiple stakeholders, thereby facilitating the ongoing refinement and validation of the therapeutic properties of TCM compound prescriptions. The incorporation of AI prediction and blockchain technology constitutes an innovative strategy to enhance trust and safety in the future clinical application of TCM, ultimately offering patients more personalized and secure treatment options^[18].

7 Challenges and future directions

7.1 Data quality and standardization issues The application of AI in TCM encounters significant challenges related to data quality and standardization. The heterogeneity of data concerning TCM compound prescriptions, including variations in herbal components, diverse preparation methods, and differing individual patient responses, impedes the predictive accuracy of AI models. Additionally, missing data adversely impacts the reliability of these models and the associated clinical outcomes. Therefore, it is

imperative to establish a unified standard for data collection and annotation within the field of TCM. Standardizing the procedures for data acquisition, processing, and sharing not only enhances data quality but also facilitates interoperability among diverse AI systems. Developing a comprehensive database encompassing clinical, pharmacological, and chemical information will provide a robust foundation for AI applications. Concurrently, it is necessary to establish a standardized and unified terminology and classification system for the components and effects of TCM. This standardization will improve the consistency and accuracy of AI analysis and facilitate the advancement of precision medicine and personalized treatment^[19–20].

7.2 Model interpretability and clinical acceptance The integration of AI models into clinical practice, particularly in the field of TCM, is frequently impeded by issues related to interpretability. Many AI systems function as "black boxes", with opaque decision-making processes, which engender skepticism among clinicians regarding AI-generated recommendations and consequently limit their routine use. Enhancing the interpretability of these models is therefore essential to facilitate their widespread clinical adoption. By employing explainable artificial intelligence (XAI) techniques, including local interpretable model-agnostic explanations (LIME) and Shapley additive explanations (SHAP), the contribution of each input feature to the model's predictions can be elucidated, thereby enhancing physicians' comprehension and validation processes. XAI not only improves the transparency of models but also aligns with medical ethical standards, thereby ensuring the accountability and reliability of AI applications. As AI becomes increasingly prevalent in the medical domain, prioritizing the development of models with high interpretability is essential for fostering physicians' trust and enhancing patient outcomes^[21–22].

8 Conclusions

The incorporation of AI technology into the modernization research of TCM compound prescriptions signifies a significant paradigm shift within medical research. This article systematically examines the multifaceted roles of AI in intelligent design, mechanism prediction, and precise application. While AI holds considerable potential to improve the efficacy and safety of TCM prescriptions, it also presents challenges, including issues related to data quality and model interpretability, which require prompt attention. Data quality constitutes the cornerstone of the efficacy of AI algorithms. The intricate interactions among components and the variability among patients in TCM necessitate the collection of high-quality, comprehensive, and representative data, alongside the development of a standardized data format and rigorous data validation protocols. Furthermore, the interpretability of the model is of paramount importance. Although AI has the capability to identify complex underlying patterns, its "black box" nature undermines clinical trust and acceptance. Therefore, the development of models that are both accurate and transparent is essential to support

physicians in making informed decisions and to facilitate the integration of AI into clinical practice. Clinical validation functions as a critical link in translating theoretical concepts into practical applications. This process necessitates the collaborative efforts of AI specialists, clinical physicians, and TCM practitioners to design rigorous clinical trials tailored to the unique TCM characteristics. Such collaboration enhances the understanding of AI-assisted TCM applications and facilitates the seamless integration of traditional practices with modern technological advancements.

In the future, interdisciplinary collaboration and technological innovation are expected to propel the expansive potential of AI in the field of TCM. By integrating pharmacology, data science, and the insights of traditional medicine, this approach seeks to develop more precise and personalized treatment strategies, facilitate the convergence of ancient Chinese medical practices with modern technology, and contribute to global health initiatives.

In conclusion, AI offers potent tools for the modernization of TCM compound prescriptions. The full potential of AI can be realized only through the rational integration of the strengths of various stakeholders and the resolution of challenges related to data, modeling, and clinical application. Cross-disciplinary collaboration will not only expedite the modernization of TCM but also enhance the global medical system, thereby inaugurating a new era of innovative healthcare that honors and preserves traditional practices.

References

- [1] LIU YF, HU ZG, XU J, *et al.* Application of phylogenomics in Chinese medicine resources[J]. *China Journal of Chinese Materia Medica*, 2019, 44(5): 891–898. (in Chinese).
- [2] XIAO H, HUANG J, MENG XR, *et al.* Oral absorption and effect of macromolecules in traditional Chinese medicine: A new perspective and research mode of phase structure[J]. *China Journal of Chinese Materia Medica*, 2023, 48(2): 285–291. (in Chinese).
- [3] DU HT, WANG L, DING J, *et al.* Application status and challenges of molecular docking in development of traditional Chinese medicine[J]. *China Journal of Chinese Materia Medica*, 2024, 49(3): 671–680. (in Chinese).
- [4] ZHOU E, SHEN Q, HOU Y. Integrating artificial intelligence into the modernization of traditional Chinese medicine industry: A review[J]. *Frontiers in Pharmacology*, 2024, 15: 1181183.
- [5] QIAN Y, WANG X, CAI L, *et al.* Model informed precision medicine of Chinese herbal medicines formulas – A multi-scale mechanistic intelligent model[J]. *Journal of Pharmaceutical Analysis*, 2024, 14(4): 100914.
- [6] NIU Q, LI H, TONG L, *et al.* TCMFP: A novel herbal formula prediction method based on network target's score integrated with semi-supervised learning genetic algorithms[J]. *Briefings in Bioinformatics*, 2023, 24(3): bbad102.
- [7] YEA S, JANG H, KIM S, *et al.* Annotated corpus for traditional formula-disease relationships in biomedical articles[J]. *Scientific Data*, 2025, 12(1): 26.
- [8] GAO Q, WU H, CHEN M, *et al.* Active metabolites combination therapies: Towards the next paradigm for more efficient and more scientific Chinese medicine[J]. *Frontiers in Pharmacology*, 2024, 15: 1392196.
- [9] ZHOU W, YANG K, ZENG J, *et al.* FordNet: Recommending traditional Chinese medicine formula via deep neural network integrating phenotype and molecule[J]. *Pharmacological Research*, 2021, 173: 105752.
- [10] CHENG YY, WANG Y, LIU L, *et al.* Theoretical innovation of component-based Chinese medicine and its exemplary practice: The study on creating Guanxinning Tablets[J]. *China Journal of Chinese Materia Medica*, 2022, 47(17): 4545–4550. (in Chinese).
- [11] LIU H, YU S, LI X, *et al.* Integration of deep learning and sequential metabolism to rapidly screen dipeptidyl peptidase (DPP)-IV inhibitors from *Gardenia jasminoides* Ellis[J]. *Molecules*, 2023, 28(21): 18.
- [12] WEI Y, XUAN Y, WANG W, *et al.* Rapid and cost-effective screening of therapeutic targets for isouquercitrin in insulin resistance using virtual methods and fiber SPR biosensing[J]. *Biomedical Optics Express*, 2025, 16(3): 1090–1103.
- [13] ZHAO L, ZHANG H, LI N, *et al.* Network pharmacology, a promising approach to reveal the pharmacology mechanism of Chinese medicine formula[J]. *Journal of Ethnopharmacology*, 2023, 309: 116306.
- [14] ZHU PP, LI G, YANG HJ. Trend analysis and regulatory strategies for traditional Chinese medicine formula granules[J]. *China Journal of Chinese Materia Medica*, 2024, 49(15): 4249–4260.
- [15] WANG FL, WANG YH, HAN L, *et al.* Renoprotective effect of Yiqi Yangyin Huayu Tongluo Formula against diabetic nephropathy in diabetic rats[J]. *Evidence-Based Complementary and Alternative Medicine*, 2018: 4276052.
- [16] ZHENG S, XUE T, WANG B, *et al.* Chinese medicine in the treatment of ulcerative colitis: The mechanisms of signaling pathway regulations[J]. *American Journal of Chinese Medicine*, 2022, 50(7): 1781–1798.
- [17] TSCHOCHOHEI M, ADAMS LC, BRESSEM KK, *et al.* AI-enabled clinical decision support systems: Challenges and opportunities[J]. *Bundesgesundheitsblatt-Gesundheitsforschung-Gesundheitsschutz*, 2025, 68(8): 872–879. (in German).
- [18] GU ZX, WANG ZH, ZHANG XQ, *et al.* Research advances in the study of traditional Chinese medicine formula granules on signaling pathway-mediated disease mechanisms[J]. *Frontiers in Pharmacology*, 2025, 16: 1609211.
- [19] ZHANG Y, LI X, SHI Y, *et al.* ETCM v2.0: An update with comprehensive resource and rich annotations for traditional Chinese medicine[J]. *Acta Pharmaceutica Sinica B*, 2023, 13(6): 2559–2571.
- [20] ZHOU C, SUN X, CHANG J, *et al.* Gavage strategy for decoction formula of traditional Chinese medicine in osteosarcoma model mice[J]. *Journal of Visualized Experiments*, 2024, (208): e66177.
- [21] JABBOUR S, FOUHEY D, SHEPARD S, *et al.* Measuring the impact of AI in the diagnosis of hospitalized patients: A randomized clinical vignette survey study[J]. *Journal of the American Medical Association*, 2023, 330(23): 2275–2284.
- [22] NAZIR MI, AKTER A, HUSSEN WADUD MA, *et al.* Utilizing customized CNN for brain tumor prediction with explainable AI[J]. *Helvion*, 2024, 10(20): e38997.