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Commentary

Insights into Advantages and Limitations of Network Pharmacology in Traditional Chinese Medicine

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In recent years, network pharmacology, which integrates multiple interdisciplinary fields such as systems biology, bioinformatics, and network science, has emerged as a powerful tool in traditional Chinese medicine (TCM) research. It offers fresh perspectives for investigating complex systems in TCM and furnishes new technological support for guiding rational clinical medication practices and advancing the development of new pharmaceuticals.

We recently read an article published in *Future Integrative Medicine* by Yang *et al*.,[1] which systematically explored the mechanism of Shufeng Jiedu Capsules in treating influenza for the first time using network pharmacology, bioinformatics, and molecular docking techniques. The authors identified core active compounds such as kaempferol, luteolin, isorhamnetin, and β-sitosterol, which exert anti-influenza effects through key targets including Tumor Necrosis Factor, AKT Serine/Threonine Kinase 1, and Epidermal Growth Factor Receptor. The article effectively demonstrates the systematic and integral characteristics of network pharmacology in TCM research. In addition, this research model, centered around network pharmacology, offers a valuable reference for subsequent related research and establishes an exemplary model for similar studies.

As an emerging discipline, TCM network pharmacology (TCM-NP) elucidates the interaction between TCM and the human body at the systems level, reflecting the holistic philosophy of TCM. Active compound discovery is a central focus: based on chemical analysis, networks such as "compound–target" and "disease–target" can be constructed to predict pharmacological targets and pathways. Thus, TCM-NP shifts active component research from being experiment-dominated to a more efficient strategy combining computational simulation, database mining, and predictive modeling, greatly improving both accuracy and efficiency. Beyond compound identification, TCM-NP plays a pivotal role in investigating pharmacological mechanisms. By integrating bioinformatics and systems biology, it enables multi-component, multi-target, and multi-pathway analysis of prescriptions, thereby offering mechanistic insights into classical TCM theories such as medicinal properties and compatibility. Additionally, TCM-NP has been applied in safety evaluation, helping uncover adverse reactions and toxic mechanisms of TCM.

In recent years, more researchers have applied TCM-NP to study TCM. On the one hand, in terms of active component discovery, Chinese medicine prescriptions are the main research object. Xu *et al.*[2] utilized TCM-NP combined with high-throughput UPLC-Q-TOF/MS and molecular docking techniques to predict potential active components of the Dampness-Expelling Detoxification Formula. Li *et al*.[3] combined TCM-NP with molecular biology experiments to predict the potential compound of Lei-gong-gen formula granule for treating hypertension. On the other hand, although Chinese medicine prescriptions are still the main research object in the study of pharmacological mechanisms, there is also much research on TCM monomer compounds and single herbs. In a monomer compound study, Deng *et al.*[4] integrated TCM-NP with single-cell multiomics sequencing to explore the anti-tumor mechanism of cycloastragenol, an effective active molecule in Astragalus membranaceus. In the study of a single herb, Li *et al.*[5] used TCM-NP to investigate the molecular mechanism of Cordyceps sinensis in treating diabetic nephropathy. In the safety evaluation of Chinese medicine, Jiang *et al.*[6] integrated network pharmacology with cellular biology to explore the key components and targets involved in the hepatotoxicity induced by Polygonum multiflorum. In addition, elucidating TCM theories and revealing formula compatibility principles are essential for applying TCM-NP to explore pharmacological mechanisms. He *et al.*[7] used TCM-NP to investigate the therapeutic effect of Codonopsis Radix on different gastric diseases, providing a scientific basis for understanding the strategy of "same treatment for different diseases" in TCM. Furthermore, the research and development of new TCM drugs is another main direction of TCM-NP application. For example, Chen *et al.*[8] applied TCM-NP to discover the potential and underlying mechanisms by which Tongguanteng Injection might treat prostate cancer in the secondary development of Chinese herbal compounds.

TCM-NP is improved and developed while being widely used. Through the above research cases, it is not difficult to find that multi-disciplinary integration is the primary trend in the development of TCM-NP, and the combination with artificial intelligence (AI) is one of the most crucial development directions. The advantage of AI in processing complex data enables it to effectively consolidate multi-source data, including literature, clinical data, multi-omics data, and public online databases, dynamically identifying potential drug tar-

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gets and biomarkers, thereby enhancing the accuracy and efficiency of TCM-NP research. The UNIQ system, an AI-based Molecular Network Navigation System for Western and Chinese medicine developed by Li Shao et al., is a pioneering example and is at the forefront of AI applications in TCM-NP.[9] t realizes the systematic analysis of the biological network basis of disease and syndrome, as well as the overall analysis of the multi-component regulatory mechanism of TCM. With the development of related technologies, combining TCM-NP with multi-omics and single-cell sequencing methods is another development trend, and the article published by Deng *et al*.[4] is a good example. Combining TCM-NP with microflora research, exploring the interaction between TCM and microflora, and revealing pharmacological mechanisms is a new application direction for TCM-NP.[10] In addition, examining the quality markers of TCM is also a new direction for application. TCM-NP can be used to find the related compounds that affect the quality of TCM and understand their molecular mechanisms to control the quality of TCM more efficiently and safely. For example, Wang *et al*.[11] combined TCM-NP with pharmacokinetics and bioactivity evaluation to explore the quality markers of the Danlou tablet.

Moreover, optimizing data and network analysis algorithms is also a developing trend. On the one hand, as demonstrated in the aforementioned research cases, through the combination of TCM-NP and analytical technology, such as liquid chromatography and mass spectrometry, to analyze and identify relevant Chinese medicine components, ensuring the integrity and authenticity of the data while integrating multiple databases provides the relative completeness of data collection. On the other hand, through the optimization of the network analysis algorithm, such as weighted analysis according to the concentration of components, the results of TCM-NP are more consistent with the characteristics of TCM.

Although TCM-NP shows promising prospects, it remains constrained by several limitations. It relies heavily on databases such as TCMSP and STRING, which often contain incomplete or inconsistent data, leading to unreliable results. In addition, the absence of standardized research criteria may exclude bioactive compounds and restrict comprehensive profiling. Most conclusions are based on computational predictions that cannot fully represent the complexity of biological systems, underscoring the need for rigorous experimental validation. Furthermore, TCM-NP does not adequately reflect core principles of TCM or account for dosage and pharmacokinetics, which are critical to therapeutic effects.

Overall, TCM-NP has transformed traditional single-target research paradigms by providing a holistic framework to elucidate bioactive compounds, mechanisms of action, and multi-target therapeutic effects of Chinese herbal medicines. Despite current limitations in data quality and methodological standardization, ongoing integration with multi-omics technologies, AI, and advanced analytical algorithms will further establish TCM-NP as a cornerstone of modern TCM research and drug development.

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Conflict of interest

None.

Author contributions

Study concept and design (ML), funding acquisition (ML), drafting of the manuscript (ML, XZ), critical revision of the manuscript for important intellectual content (ML, XZ, JC, HZ), and study supervision (ML, XZ). All authors have contributed significantly to this study and approved the final manuscript.

References

[1] Yang M, Zhao C, Chen T, Xu X, Liu Q. The Molecular Mechanism of Shufeng Jiedu Capsules in the Treatment of Influenza: A Comprehensive Analysis Based on Network Pharmacology, Bioinformatics, and Molecular Docking. Future Integr Med 2024;3(3):160–171. doi:10.14218/FIM.2024.00030.

[2] Xu H, Li S, Liu J, Cheng J, Kang L, Li W, *et al*. Bioactive compounds from Huashi Baidu decoction possess both antiviral and anti-inflammatory effects against COVID-19. Proc Natl Acad Sci U S A 2023;120(18):e2301775120. doi:10.1073/pnas.2301775120, PMID:37094153.

[3] Li Q, Lan T, He S, Chen W, Li X, Zhang W, *et al*. A network pharmacology-based approach to explore the active ingredients and molecular mechanism of Lei-gong-gen formula granule on a spontaneously hypertensive rat model. Chin Med 2021;16(1):99. doi:10.1186/s13020-021-00507-1, PMID:34627325.

[4] Deng G, Zhou L, Wang B, Sun X, Zhang Q, Chen H, *et al*. Targeting cathepsin B by cycloastragenol enhances antitumor immunity of CD8 T cells via inhibiting MHC-I degradation. J Immunother Cancer 2022;10(10):e004874. doi:10.1136/jitc-2022-004874, PMID:36307151.

[5] Li Y, Wang L, Xu B, Zhao L, Li L, Xu K, *et al*. Based on Network Pharmacology Tools to Investigate the Molecular Mechanism of Cordyceps sinensis on the Treatment of Diabetic Nephropathy. J Diabetes Res 2021;2021:8891093. doi:10.1155/2021/8891093, PMID:33628839.

[6] Jiang HY, Gao HY, Li J, Zhou TY, Wang ST, Yang JB, *et al*. Integrated spatially resolved metabolomics and network toxicology to investigate the hepatotoxicity mechanisms of component D of Polygonum multiflorum Thunb. J Ethnopharmacol 2022;298:115630. doi:10.1016/j.jep.2022.115630, PMID:35987407.

[7] He RP, Jin Z, Ma RY, Hu FD, Dai JY. Network pharmacology unveils spleen-fortifying effect of Codonopsis Radix on different gastric diseases based on theory of “same treatment for different diseases” in traditional Chinese medicine. Chin Herb Med 2021;13(2):189–201. doi:10.1016/j.chmed.2020.12.005, PMID:36117498.

[8] Chen X, Luo Z, Liu X, Li X, Li Q, Zhang W, *et al*. Marsdenia tenacissima (Roxb.) Moon injection exerts a potential anti-tumor effect in prostate cancer through inhibiting ErbB2-GSK3β-HIF1α signaling axis. J Ethnopharmacol 2022;295:115381. doi:10.1016/j.jep.2022.115381, PMID:35595220.

[9] Zhang P, Zhang D, Zhou W, Wang L, Wang B, Zhang T, *et al*. Network pharmacology: towards the artificial intelligence-based precision traditional Chinese medicine. Brief Bioinform 2023;25(1):bbad518. doi:10.1093/bib/bbad518, PMID:38197310.

[10] Liu J, Li B, Zhou X, Liu G, Li C, Hu Z, *et al*. Uncovering the mechanisms of Zhubi decoction against rheumatoid arthritis through an integrated study of network pharmacology, metabolomics, and intestinal flora. J Ethnopharmacol 2025;336:118736. doi:10.1016/j.jep.2024.118736, PMID:39186991.

[11] Wang Q, Chen G, Chen X, Liu Y, Qin Z, Lin P, *et al*. Development of a three-step-based novel strategy integrating DMPK with network pharmacology and bioactivity evaluation for the discovery of Q-markers of traditional Chinese medicine prescriptions: Danlou tablet as an example. Phytomedicine 2023;108:154511. doi:10.1016/j.phymed.2022.154511, PMID:36334388.