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Letter to Editor

Decoding Biological Networks: A Network Pharmacology Approach Powered by Artificial Intelligence

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Dear Editor,

In recent years, many techniques have been developed to elucidate the complex structure of biological systems that are difficult to analyze and to understand many diseases at the molecular level. These advancements have revealed that drug development approaches that only focus on a single target are often inadequate in the treatment of complex diseases in which multiple genetic and environmental factors have a major impact (1). This has increased the importance of multidisciplinary approaches and led the scientific world to seek more holistic models. Systems biology-based approaches are gaining more and more importance, and the concept of network pharmacology, which evaluates the intrinsic dynamics of biological systems through networks, including multi-component, multi-target and multi-level analyses, is coming to the fore (2). Network pharmacology has become a strategic tool in today's drug discovery processes, especially because it provides the opportunity to evaluate gene, protein and drug interactions at multiple levels (3). However, for this approach to be used efficiently, large and complex datasets need to be processed. At this point, the possibilities offered by artificial intelligence come into play.

Artificial intelligence, especially machine learning and deep learning techniques, make the analysis of biological data much more meaningful and faster. Modeling processes that could take months with traditional methods can now be done in minutes. However, artificial intelligence has become not only an accelerator, but also a tool that can establish new relationships, make predictions and generate hypotheses (4, 5). Network pharmacology aims to analyze the interactions of genes, proteins, metabolites, etc. through networks. However, these networks are often very large and complex, so classical statistical approaches may be insufficient.

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The role of artificial intelligence at this point is critical. Especially in studies conducted in countries with a strong traditional medicine background such as China and India, the effects of herbal compounds on the network have been systematically mapped with the help of artificial intelligence (6). Likewise, evaluating the ethnobotanical knowledge widespread in Anatolia with these methods can make significant contributions to both the preservation of cultural legacy and the discovery of potential therapeutic candidates.

While the potential of AI-supported network pharmacology is high, there are some challenges that slow the progress of this field. First of all, the decision processes of AI algorithms are often "black box" in nature, meaning that they have limited explainability, making biological interpretation difficult (7). Moreover, the quality, standardization and reliability of the data are factors that directly affect model performance. In particular, noise and missing data problems, which are frequently encountered omics datasets can reduce the reliability of AI models (8).

Another important aspect is the need for interdisciplinary collaboration. Developing a common language between biologists, computer scientists, pharmacologists and clinicians is critical for the successful implementation of these models. In this regard, issues such as platforms that encourage open data sharing, the development of modular and explainable artificial intelligence models, and ensuring data privacy within the framework of ethical rules are expected to be on the agenda more in the coming years (9, 10).

Network pharmacology approaches supported by artificial intelligence pioneer the understanding of disease mechanisms at the system level and the development of effective treatment strategies. Especially in the modeling of multi-target and multi-component therapies, this approach offers more holistic and effective solutions compared to classical methods (11). This interdisciplinary field has great potential in terms of scientifically analyzing complex therapeutic elements such as herbal products, developing individualized medicine practices and accelerating drug discovery processes (6).

Through this letter, I hope that more researchers will embrace, support and strengthen international collaborations in this powerful approach that combines artificial intelligence and network pharmacology.

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References

1. Makhoba XH, Viegas C Jr, Mosa RA, Viegas FPD, Pooe OJ. Potential Impact of the Multi-Target Drug Approach in the Treatment of Some Complex Diseases. Drug Des Devel Ther. 2020; 14: 3235-3249.
2. Shah A, Patel V, Jain M, Parmar GR. Network Pharmacology and Systems Biology in Drug Discovery. In: CADD and Informatics in Drug Discovery. 2023; 231-252.
3. Hopkins A. Network pharmacology: the next paradigm in drug discovery. Nat Chem Biol. 2008; 4: 682–690.
4. Bhardwaj A, Kishore S, Pandey DK. Artificial Intelligence in Biological Sciences. Life (Basel). 2022; 12(9): 1430.
5. Han H, Liu W. The coming era of artificial intelligence in biological data science. BMC Bioinformatics. 2019; (Suppl 22): 712.
6. Zhao W, Wang B, Li S. Network pharmacology for traditional Chinese medicine in era of artificial intelligence. Chin Herb Med. 2024; 16(4): 558-560.
7. Hagenbuchner M. The black box problem of AI in oncology. Journal of Physics: Conference Series. 2020; 1662(1): 012012.
8. Baena-Miret S, Reverter F, Vegas E. A framework for block-wise missing data in multi-omics. PLoS One. 2024; 19(7): e0307482.
9. Di Bitonto P, Magarelli M, Novielli P, Romano D, Diacono D, de Trizio L, et al. From data to nutrition: the impact of computing infrastructure and artificial intelligence. Explor Foods Foodomics. 2024; 2: 810–29.
10. Falvo F, Cannataro M. Ethics of Artificial Intelligence: challenges, opportunities and future prospects. IEEE International Conference on Bioinformatics and Biomedicine (BIBM), 2024; 5860-5867.
11. Zhang P, Zhang D, Zhou W, et al. Network pharmacology: towards the artificial intelligence-based precision traditional Chinese medicine. Brief Bioinform. 2023; 25(1): bbad518.