Commentary Article

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Integrating Systems Biology and Artificial Intelligence in Traditional Pharmacy Research: Advancements, Challenges, and Opportunities

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Abstract

In the age of artificial intelligence (AI) and biomedical big data, network pharmacology represents a breakthrough in traditional medicine (TM) research. The emergence of interdisciplinary frontiers, such as bioinformatics and systems medicine, has led to a new pharmaceutical research generation that emphasize networks and systems (1) (2). In recent years, TM researchers have shown great interest in exploring AI technologies as an emerging discipline (3). The network pharmacology field has proven to be an effective means of elucidating the mechanisms of traditional herbal medicine and traditional pharmacy (4). The primary focus is to modernize TM by incorporating cutting-edge techniques in genomics, metabolomics, and systems biology. This will enable a fresh look at the knowledge and insights offered by TM (5).

Systems biology, which takes a holistic approach, is a crucial research methodology for understanding the TM pharmacology. To successfully integrate systems biology into TM, it is necessary to combine computational technologies with holistic insights (6). By constructing a network of interrelated "herb-compound-target-pathway" relationships, this technique provides a holistic understanding of the mechanisms underlying traditional medicine. The integration of computational techniques into the network pharmacology has led to a significant improvement in the accuracy and efficiency of active constituent screening and target identification, surpassing previous levels of performance (4). On the other hand, there has been a gradual increase in the global studies of traditional medicinal plants due to their natural sources and wide variety. These plants are capable of complementing modern pharmacological approaches (7-10). It's important to point out that TM therapy is distinguished by its comprehensive, customized, multifaceted approach that targets multiple components, pathways, and objectives. A new concept called "network target" has been proposed to investigate the biological foundation of TM in a systematic manner. This concept is based on the multi-target approach of TM and represents a shift from the prevailing research paradigm, which focuses on single targets. There is currently a growing interest in network pharmacology as it relates to TM (1).

By combining experimental research, network pharmacology plays a critical role in driving innovation and advancement in the field of TM. The integration of network pharmacology with TM is seen as valuable in offering insights into the mechanisms of TM and supporting clinical practice (1). It has been found that many diseases, such as hypertension, are most effectively treated through the use of multiple drugs or targeting multiple factors simultaneously (11). Indeed, the prevalence of complex diseases

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poses a serious threat to human health. Drug discovery strategies that rely on single genes, drugs, and targets are inadequate in addressing complex diseases. Consequently, the development of novel multicomponent drugs for management of complex diseases is crucial. A significant scientific challenge in this pursuit is the establishment of an appropriate solution for drug group-target protein network analysis. Herbal medicines, which have served as the foundation of sophisticated TM systems, have yielded several essential drugs that are still consumed today (12).

AI-powered methods (e.g. machine learning and deep learning) have the ability to connect various aspects of TM such as chemical composition, targets, and diseases. Essentially, AI offers novel approaches to examining ancient literature on TM, facilitating the identification of key components in herbs or formulas, elucidating the mechanisms of action to guide the precise application of TM (3). By analyzing network characteristics and conducting literature mining, possible synergistic mechanisms and effective multi-components can tentatively be identified. This study suggests that this approach can serve as an effective strategy for discovery of active substances and elucidating their pharmacological mechanisms in TM (13). Integrating the strengths of both modern and traditional medicine into a unified integrative medicine has the potential to benefit patients around the world (5). The recent progress in phytochemistry, DNA sequencing, high throughput screening, bioinformatics, and systems biology has facilitated the exploration of the chemical composition and molecular mechanisms of TM, thereby providing insights into the early stages of drug discovery. As a result, there is potential for a renaissance in multi-component drug discovery, fueled by the inspiration of TM (11).

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