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Editorial

Network Pharmacology-Based Approach in Drug Discovery

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The natural remedies from traditional medicine, such as Ayurveda, are re-emerging as potential and attractive approaches in developing new drugs (Patwardhan and Mashelkar, 2009). The conventional Ayurvedic formulations contain many bio-actives and are multi-targeted, thereby regulating a variety of disease targets. However, the mechanism and scientific rationale remain largely unexplored (Chandran et al., 2015). A multi-target, multi-ingredient formulation approach may be a better option than a single gene/single target/single-drug approach for holistic management of disease associated with complications. This multi-targeted approach can help control lifestyle diseases such as obesity, cardiovascular disease, diabetes and malignancy. Furthermore, the selection of multi-ingredient formulation can deal with various targets due to the structural diversity and may act as synergistic (Hopkins, 2007; Zimmermann et al., 2007). Henceforth, developing Ayurvedic formulations with appropriate scientific proof of standard, safety, synergistic, and efficacy may provide an affordable and better alternative. It is now possible to study complicated interactions between the bioactive constituents and the genes/targets responsible for the diseases with the help of Network Pharmacology.

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Network Pharmacology is a revolutionary technique that combines computational biology and systems biology to investigate multi-component and multi-targeted formulations (Zhang et al., 2019). The advances in computational, omics technology and systems biology have provided a new perspective in identifying numerous target modulations for a particular disease (Gu et al., 2013). For example, Asarone is reported to regulate multiple targets and cell signalling pathways such as activation/upregulation of 5' AMP-activated protein kinase (AMPK), E-cadherin, apoptosis along with inhibition/downregulation of matrix metalloproteinases (MMP), protein kinase B (Akt), heterogeneous nuclear ribonucleoprotein A2/B1 (hnRNP A2/B1), N-cadherin, vascular endothelial growth factor (VEGF), p53 related proteins and arrest of the cell cycle showing its potential in different types of cancer and other diseases (Das et al., 2019; Chellian et al., 2017; Das et al., 2021; Zhang et al., 2020; Liu et al., 2020). Furthermore, the use of virtual high-throughput screening to study the interactions between the ligand molecule (phytoconstituent) and selecting the right target has improved the effectiveness of the drug discovery process.

The network pharmacology technique has been adopted to understand better the mechanisms of Traditional Chinese Medicines (TCM), as observed with the increasing number of studies. Recently, Tao et al., 2020 explored the active constituents and demonstrated the mechanism of the Huashi Baidu formula (HSBDF) using network pharmacology and docking study for severe acute respiratory syndrome Coronavirus 2 (SARS-CoV-2) (Tao et al., 2020). Zhang et al., 2019 provided a summary of the various tools and databases currently used in TCM research. It paved a new direction for studying the mechanisms and safety behind TCM use (Zhang et al., 2019). A recent study carried by Karthikkeyan et al., 2020 adopted the bioinformatics-based network pharmacology approach in understanding the mechanism of action of liquorice metabolites (Karthikkeyan et al., 2020). However, investigations focusing on Ayurvedic formulations are limited. Hence, this computer-based network and the molecular docking study can provide quick information about bio-actives and targets underlying various pathophysiological processes for constructing interactive pharmacology networks. In addition, it can be used as a validation/prediction tool before starting wet-lab studies.

Conflicts of Interest

The author reports no conflicts of interest.

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