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Network Pharmacology in Pharmacognosy and Traditional Health Systems

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ABSTRACT: The traditional approach of the discovery of drugs (one-target, one-drug) has slowly transformed into a network-target, multi-component one, which developed into the concept of network pharmacology. This growing field brings together ideas of pharmacology, systems biology, and computational science to explore multi-molecular dynamics between biological systems. This kind of integrative paradigm exists in addition to Ayurveda - the ancient Indian system of holistic medicine that revolves around creating balance between the physiological, mental and spiritual realms. The traditional approach of single target, single drug drug discovery has slowly evolved to a network target, multi- component paradigm and the concept of network pharmacology has emerged. This is a new field that incorporates pharmacological, systems biology and computational science concepts to study more complicated molecular interactions in the biological systems. This integrative paradigm is a supplement to the Ayurveda - the traditional Indian model of holistic medicine based on the establishment of balance between physiological, mental, and the spiritual spheres. Ayurvedic preparations which are usually a combination of numerous phytoconstituents with various bioactivities have therapeutic effects due to multiple-simultaneous action on different molecular targets. Network pharmacology can give the means to intercept these complex interactions, through the identification of active ingredients, prediction of target-drug interactions, and mapping of biological pathways. There are typically the database development, ADMET screening, proteinprotein interaction studies, molecular docking, and visualization of ingredienttargetdisease networks using important tools such as SwissADME, STRING, Cytoscape, and KEGG pathway analysis. This methodology has over the past years been critical in establishing conventional assertions, streamlined operation of processes and in the rationalization of Ayurvedic treatment scientifically. Network pharmacology combined with bioinformatics also help to predict biomarkers, and to identify new therapeutic courses, hence bridging the gap between ancient knowledge and contemporary biomedical research. Nonetheless, it is known that the chemical nature of polyherbal preparations is complicated, making it difficult to determine pharmacodynamics and pharmacokinetics. Enhancing the collaboration between Ayurveda traditional healers and scientists can speed up the process of innovation and eventually the integration of Ayurveda into the rest of the world. Altogether, network pharmacology is a promising path of evidence-based assessment and development of traditional medicine. Although it varies, workflow typically includes database development, ADMET screening, protein protein interaction studies, molecular docking, and visualizing ingredient target disease networks with main business tools such as SwissADME, STRING, Cytoscape, and the KEGG pathway analysis. This method has proven valuable in the past few years to confirm the traditional assertions, to decipher the action mechanisms and scientifically justify the Ayurvedic remedies.

KEYWORDS: Network Pharmacology, Drug target, Multi target drug discovery, Systems biology

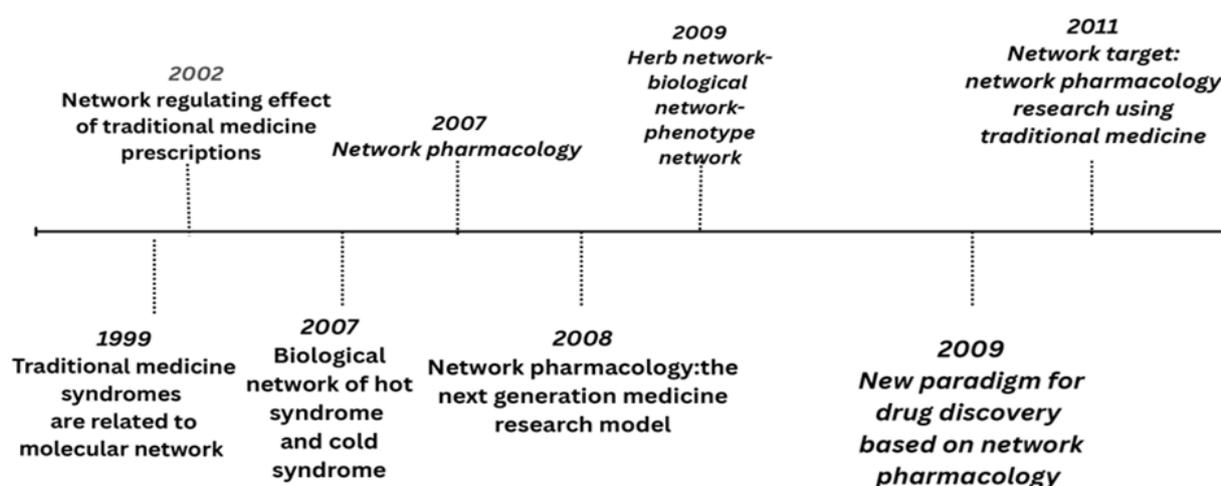
I. INTRODUCTION

The past several years have seen the global health issues escalating in nature and thus there has been a growing need to focus on interacting with key medical issues at an international scale . The study of complex diseases like cancer and diabetes has generated much interest in research since, in most cases, they are a result of failure in whole regulatory systems and not the failure in a specific gene . As such, single molecular target based strategies are not usually sufficient to diagnose and treat such diseases .

The natural products still act as a significant source of contemporary pharmaceutical drug, especially in treating a variety of conditions . In the past, the products have been used as a source of bioactive compounds that are useful in improving human health . The progress in the high-throughput technology has enhanced the assessment of the pharmacological properties of herbal medicines which have facilitated its use in drug discovery . The efficient approach to clarifying the therapeutic actions of bioactive compounds is to forecast the network of genes altered by active plant constituents. For centuries, local communities have relied on medicinal plants to manage their health problems, often without formal

scientific validation. conditions, often without formal scientific validation. Traditional medical systems around the world have used a wide range of plant species for therapeutic purposes. across the world have utilized a wide range of plant species for therapeutic purposes. While medicinal plants play an important role in providing natural and affordable health solutions, improper harvesting practices, overuse and unregulated application have led to the decline and loss of several valuable medicinal plant species natural healthcare solutions, improper harvestin gpractices, overuse, and unregulated application have led to the decline and loss of several valuable medicinal plant species. Traditional medicine is based on a holistic philosophy and emphasizes the use of multicomponent therapies to treat the complex nature of diseases. grounded in a holistic philosophy and emphasizes the use of multi- component therapies to address the complex nature of diseases. One of the most distinctive features of traditional health systems is the use of herbal formulations, which combine multiple plant ingredients to achieve therapeutic balance. characteristics of traditional healthcare systems is the use of herbal formulations, which combine multiple plant ingredients to achieve therapeutic balance. In the era of big data and systems biology, ancient medical knowledge can now be reexamined and modernized by exploring the combinatorial properties of medicinal plants and understanding their underlying mechanisms of action. re-examined and modernized by exploring the combinatorial properties of herbal medicines and understanding their underlying mechanisms of action. [1]

Figure 1. Timeline illustrating the historical development of network pharmacology.



Methodology of Network Pharmacology

Stage	Method / Concept	Description	Key Outcome
Conceptual Development	Molecular Network–TCM Syndrome Hypothesis (1999)	Proposed that TCM syndromes represent dynamic molecular networks of genes, proteins, metabolites, and signaling pathways rather than isolated clinical entities.	Established theoretical link between TCM syndrome differentiation and molecular biology.
	Network-Based TCM Research Framework (2007)	Introduced a structured network framework integrating herbal compounds, molecular targets, and disease processes.	Shifted focus from single targets to holistic network regulation.
	Cold–Hot Syndrome Network Case Studies (2009)	Compared molecular pathways regulated by cold- and hot-natured herbs using network analysis.	Provided molecular validation for classical TCM herb classifications.
	Herb–Biological Network–Phenotype Model (2009)	Developed a multi-layer model linking compound networks with biological and phenotypic networks.	Explained therapeutic effects of herbal formulations at

			systems level.
	Establishment of TCM Network Pharmacology (2011)	Formal recognition of network pharmacology as a discipline emphasizing multi-component and multi-target synergy.	Defined systems-level disease regulation aligned with TCM philosophy.
	Network Target Concept (2011)	Introduced “network targets” representing groups of interacting molecules instead of single proteins.	Enabled holistic interpretation of herbal medicine action.
Disease Gene Identification	CIPHER	Predicts disease-associated genes based on network proximity and phenotype similarity.	Identification of candidate disease genes.
	CIPHER-HIT	Uses modularity analysis to improve disease gene prediction accuracy.	Enhanced prediction through functional gene modules.
Target Prediction	Drug-CIPHER	Maps drugs and herbal compounds to molecular targets within interaction networks.	Prediction of protein targets and affected pathways.
	Com-CIPHER	Identifies co-modules linking drugs, genes, and diseases.	Reveals coordinated molecular mechanisms.
Herbal Network Construction	DMIM	Constructs herb–compound–target networks and performs co-module analysis.	Identification of synergistic herb interactions.
	LWDH	Multi-layer herb–biomolecule–disease network analysis.	Exploration of combinatorial mechanisms of herbal formulas.
Drug/Herb Effect Evaluation	NADA	Evaluates effects of compounds on disease-related molecular networks rather than single targets.	System-wide pharmacological assessment.
Synergy Identification	NIMS	Detects synergistic interactions in multi-component drug or herbal combinations.	Identification of effective compound combinations.
	Network-Based Drug Combination Models	Mathematical and network-based models to assess synergy, additivity, or antagonism.	Quantitative evaluation of combination therapies.
Disease Network Construction	LMMA	Builds disease-specific molecular interaction networks using omics data.	Identification of disease-relevant molecular interactions.
	Disease Pathway Networks	Constructs disease-centric pathway interaction maps.	Identification of key therapeutic pathways.
	ClustEx	Identifies disease-responsive gene modules using clustering techniques.	Functional gene module detection.
Database Utilization	TCMSP, TCMID, BATMAN-TCM, HERB, HerbBioMap	Databases providing compounds, ADME properties, targets, and herb–phenotype associations.	Compound screening and target identification.
	STRING, KEGG, DisGeNET, dbNEI	Protein interaction, pathway mapping, and disease association databases.	Biological interpretation and pathway enrichment.
	ETCM, SymMap, TCM-Mesh	Multi-layer integration platforms linking herbs, targets, diseases, and symptoms.	Systems-level network construction.
Information Extraction	Literature Mining & SMILES Generation	Identification of bioactive compounds and conversion to canonical SMILES.	Input data for target prediction.

	Transcriptomic Analysis	Genome-wide gene expression analysis after herbal treatment.	Mechanistic pathway identification.
Network Construction & Analysis	Cytoscape, VNP, Gephi	Visualization and analysis of compound–target–pathway–disease networks.	Identification of hubs and key nodes.
	PPI Network Analysis	Construction of protein–protein interaction networks to identify hub targets.	Identification of critical therapeutic targets.
	GO & KEGG Enrichment	Functional annotation and pathway enrichment analysis.	Biological interpretation of network targets.
Therapeutic Development	Multi-Target Drug Discovery	Identification of pleiotropic herbal compounds affecting multiple disease pathways.	Improved efficacy and reduced toxicity.
	Polypharmacological Strategies	Rational combination of compounds targeting disease-specific network nodes.	Enhanced therapeutic response.
	Network-Based Drug Repurposing	Identification of new drug–target interactions and toxicity prediction.	Safer and more effective therapies.

II. APPLICATION OF NETWORK PHARMACOLOGY TO TRADITIONAL HERBAL MEDICINE

The integration of network pharmacology with traditional medical systems such as Ayurveda and Traditional Chinese Medicine (TCM) offers a rational framework to decode the pharmacological basis of complex, multi- component formulations. This approach is particularly suited to polyherbal preparations, where numerous phytoconstituents act on multiple molecular targets and pathways in a coordinated manner, rather than following a single drug–single target paradigm. By combining phytochemical databases, target prediction algorithms, protein– protein interaction (PPI) networks, and pathway enrichment analyses, network pharmacology enables the systematic translation of traditional indications into quantifiable compound–target–disease relationships. [2] A representative example in Ayurveda is the investigation of Triphala, a classical rasayana formulation comprising *Emblica officinalis*, *Terminalia chebula*, and *Terminalia bellirica*, which is traditionally used for rejuvenation and as an adjuvant in cancer. In a network pharmacology study, the major phytoconstituents of Triphala were curated from phytochemical and ethnopharmacological resources, followed by in silico prediction of their putative protein targets and construction of a compound–target–disease network. Topological analysis, along with Gene Ontology and KEGG pathway enrichment, revealed that multiple polyphenols and tannins converged on key nodes involved in cell cycle regulation, apoptosis, oxidative stress, and inflammatory signalling, thereby supporting a multi-target, synergistic mechanism for its reported anticancer effects. These findings demonstrate how network pharmacology can rationalize the traditional uses of an Ayurvedic formulation, identify potential biomarkers, and highlight candidate molecules or pathways for further experimental validation in oncology. [3]

In TCM, Qu’s formula, a patented herbal preparation used clinically for endometriosis, provides another clear example of this integrative strategy. In that study, candidate active compounds were first screened using oral bioavailability and drug-likeness criteria, after which their potential targets were integrated with known endometriosis-related genes to build comprehensive compound–target and PPI networks. Subsequent GO and KEGG enrichment analyses indicated that Qu’s formula mainly modulates processes such as immune regulation, apoptosis and proliferation, oxidative stress, and angiogenesis, with hub targets including VEGFA, IL1B, CCL2, CXCL8, and PTGS2 emerging as central nodes in the network. Molecular docking revealed strong binding affinities between key flavonoids (e.g. quercetin) and these hub proteins, and in vitro experiments confirmed downregulation of pro-inflammatory and pro-angiogenic genes, providing experimental support for the network-derived mechanistic hypotheses. Taken together, these studies illustrate how network pharmacology can bridge traditional knowledge with contemporary biomedical science by mapping multi-component herbal formulations onto modern molecular networks. For Ayurveda and other traditional systems, this approach not only helps to validate classical claims and elucidate mechanisms of action, but also facilitates the identification of new therapeutic targets, repurposing opportunities, and lead compounds for drug discovery. In the context of evidence-based modernization of traditional medicine, such application-oriented network pharmacology workflows—incorporating database building, ADMET screening, PPI analysis, molecular docking, and ingredient–

target–disease network construction—provide a robust methodological template for future research on complex herbal formulations. Application of network pharmacology to traditional herbal medicine. The integration of network pharmacology with traditional medical systems such as Ayurveda and Traditional Chinese Medicine (TCM) offers a rational framework to decode the pharmacological basis of complex, multi- component formulations. This approach is particularly suited to polyherbal preparations, where numerous phytoconstituents act on multiple molecular targets and pathways in a coordinated manner, rather than following a single drug–single target paradigm. By combining phytochemical databases, target prediction algorithms, protein– protein interaction (PPI) networks, and pathway enrichment analyses, network pharmacology enables the systematic translation of traditional indications into quantifiable compound–target–disease relationship. [4]

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III. CONFLICT OF INTEREST

The authors have no conflicts of interest regarding this investigation.

IV. ACKNOWLEDGMENTS

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