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Review JOAYUSH

Exploring the Intersection of AI Network Pharmacology and Ayurveda: Innovations in Traditional Medicine

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Abstract

Integrative frameworks that integrate traditional medicine and modern computer research are increasingly important for advancing evidence-based, individualized healthcare. One interesting strategy is the combination of Ayurveda, network pharmacology, and artificial intelligence (AI). AI expands the capability by allowing for the quick analysis of biomedical big data, the identification of therapeutic trends, and the optimization of treatment plans. Ayurveda, with its long-standing emphasis on individualized care, holistic balance, and natural remedies, provides a distinct treasury of therapeutic knowledge to supplement these scientific breakthroughs. The presented study investigates the relationship between these three areas, proposing that combining AI with network pharmacology provides a strong foundation for deciphering and evaluating Ayurvedic formulations. Such computational approaches can illuminate molecular pathways, match traditional treatments with modern biological concepts, and provide fresh hypotheses for drug discovery. In turn, Ayurveda provides a holistic framework that is frequently lacking in reductionist biomedical models, with the ability to guide the development of multi-target, customized therapeutic solutions. This multidisciplinary approach seeks to improve the efficacy and legitimacy of Ayurvedic medicines by combining ancient wisdom with modern science. It paves the path for more precise, individualized, and scientifically verified therapies while maintaining their holistic basis. Finally, the combination of Ayurveda, network pharmacology, and AI has the potential to reshape integrative medicine by creating scalable, data-driven, and culturally grounded healthcare solutions. This combination not only improves Ayurveda's global relevance but also helps to build creative methods for solving complicated health concerns in modern clinical practice.

Keywords: Artificial intelligence (AI), ayurveda, network pharmacology, traditional medicine, drug discovery

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INTRODUCTION

Ayurveda, also referred to as the "Science of Life," is an ancient Indian medical system that has been practiced for over 5000 years. It is thought to be among the world's oldest healthcare classifications and has been in use continuously throughout history [1]. By taking a comprehensive approach to health and well-being, Ayurveda places a strong emphasis on establishing balance between the mind, body, and spirit. Its roots are found in Vedic writings like the Atharva Veda, Rig Veda, and Yajur Veda. Ayurvedic texts, such as the Charaka Samhita and the Sushruta Samhita, which were assembled between 1000 and 500 BCE, serve as the foundation for this conventional medical practice [2].

In the recent era, Ayurveda has gained importance in modern health methodologies, and the World Health Organization (WHO) also acknowledges it [3]. Ayurveda employs an integrative approach to the psychological, physiological, and spiritual well-being of an individual. Ayurveda emphasizes the importance of maintaining health by balancing the doshas (bio-energies), dhatus (body tissues), and malas (waste products). To restore this equilibrium, practitioners employ various therapeutic approaches and lifestyle modification [4].

In parallel with the revival of interest in traditional medicine, modern technological advancements such as artificial intelligence (AI) are transforming the landscape of healthcare. Its strength lies in its capacity to examine vast, heterogeneous datasets and spot patterns and relationships. For instance, AI technology can condense a patient's whole medical history into a single number that indicates a likely diagnosis [5].

The ability of AI to manage and interpret complex biological data complements the objective of network pharmacology, an emerging interdisciplinary domain that integrates the concept of network analysis, computational biology, and pharmacology to elucidate the interactions among biological entities at the systems level.

Its primary objective is to examine the complex relationships that exist between metabolites, proteins, other molecular components, and genes in biological networks. Modeling these intricate networks, network pharmacology facilitates a deeper understanding of pharmacological mechanisms and disease progression [6, 7].

The integration of network pharmacology with AI offers a novel scientific framework for evaluating traditional medicine systems like Ayurveda. This approach enables the identification of bioactive compounds and their molecular targets within Ayurvedic formulations. Through network-based modeling, it becomes possible to delineate the structural and functional relationships underlying the pharmacological efficacy of these traditional medicines.

Moreover, these methodologies offer scientific validation for Ayurvedic practices by linking traditional claims to defined molecular pathways and biological targets. The integration of AI, network pharmacology, and Ayurvedic principles not only reinforces the scientific credibility of traditional medicine but also facilitates the creation of novel drug discovery approaches and personalized treatment strategies [8].

AI IN AYURVEDA

The integration of AI into Ayurveda is opening new avenues for combining traditional knowledge with modern technology. AI is increasingly being used to analyze classical Ayurvedic texts, identify active compounds in herbs, and develop safer, more effective plant-based medicines [9]. Given the global shift toward digital healthcare, there is a growing need to strategically integrate AI into Ayurveda to remain competitive in the international market [10].

Machine learning and AI tools have been applied in various diagnostic methods, such as facial recognition for Prakriti analysis, questionnaire-based Prakriti prediction, and pulse diagnosis, like Nadi Tarangini. Devices such as the Ayurvedic Tridosha Scanner have also been developed to assess doshic balance and physiological status through sensor-based testing (Table 1) [11, 12].

Treatments in addition to diagnostic tools, digital platforms like the Traditional Knowledge Digital Library (TKDL), AYUSH Research Portal, DHARA, and Ayusoft provide valuable resources to support Ayurvedic research, diagnosis, and treatment planning [13].

Table 1. AI-based tools and techniques in ayurvedic diagnosis.

S.N.	Tools/ techniques	Ayurvedic diagnostic method	Technology used	Key features	Reference
1	Facial Recognition Model	Akriti Pariksha (Face Analysis)	Computer vision, Image Processing	Identifies Prakriti based on facial features (skin, hair, eyes, nose, lips) using labelled datasets	[11]
2	Question-based Model	Prashna Pariksha (Questioning)	Machine Learning, Ensemble Techniques	Predicts Prakriti using a 25-question survey and ensemble learning algorithms	[14]
3	Nadi Tarangini (NT)	Nadi Pariksha (Pulse Diagnosis)	Sensor-based Analysis, Signal Processing	Record and analyse pulse to assess organ function and disease stages, and provide lifestyle guidance	[12]
4	Electro Tridosha Graphy (ETG)	Tridosha Assessment	Pulse Testing, Sensor Technology	Evaluates Doshas, Dhatus, and Malas using 7 sensors, and generates a comprehensive diagnostic report	[5]

AI IN AYURVEDIC DRUG DISCOVERY

AI can accelerate the discovery of bioactive compounds from traditional Ayurvedic plants by predicting their potential therapeutic effects. When combined with network pharmacology, AI techniques can improve our understanding of how Ayurvedic formulations work at the molecular level.

AI-driven network target identifications aim to solve two main problems:

- identifying genes associated with specific symptoms or disease phenotypes, and
- Predicting molecular targets related to Ayurvedic herbs or polyherbal formulations.

Predicting Genes Linked to Symptoms or Phenotypes

Gene prediction algorithms based on biological networks often use the concept of multilevel modular relationships and analyze the network's structure (topology). Early approaches applied traditional machine learning techniques, such as regression analysis and random walk algorithms, to link genes with disease or syndromes. One of the most notable models is the CIPHER algorithms, which offer a framework for applying AI to biological networks at both detailed (micro) and system-wide (macro) levels [15].

Building on this, the CIPHER-SC [16] uses single-cell data and applies graph convolutional neural networks to predict disease-related genes within multilayer biological networks. These AI-based models demonstrate strong potential for identifying targets relevant to complex Ayurvedic formulations, thereby offering insights into their molecular mechanisms.

Predicting Targets Associated with Ayurvedic Herbs or Formulations

From a methodological perspective, two types of machine learning approaches are used for predicting compound-target interactions

- Traditional methods that rely on network topology (e.g., regression model), and
- Advanced deep learning models

DrugCIPHER is one of the most well-known systems in this area. It uses a network-based regression analysis to precisely identify compounds that are associated with targets. [17, 18]. While traditional methods focus on network structure, deep learning models go further by integrating diverse datasets – such as drug activity profiles, disease associations, and structural similarities of compounds to achieve more accurate predictions [19].

CASE STUDIES AND RECENT DEVELOPMENTS

A potent method for confirming the conventional claims of Ayurvedic medications in recent years is network pharmacology. The intricate relationships between Ayurvedic formulations and biological systems have been effectively investigated by researchers using network analysis techniques and computational modelling, providing insight into the therapeutic efficacy and mechanisms of action of

these formulations. Numerous case studies have shown how network pharmacology can be used to support traditional Ayurvedic uses with scientific proof and validate their claims.

Ayurvedic medicines used to treat cancer were the subject of the case study. The capability of network pharmacology to understand the mechanism of action of Triphala, an Ayurvedic medicine, was demonstrated by researchers. Key chemicals and pathways implicated in Triphala's anti-cancer properties were identified using a network-based approach that integrated data on the plant's chemical composition and interactions with target proteins. This groundbreaking work could lead to new leads and targets for many diseases, providing new opportunities to understand the pharmacodynamics of Ayurvedic medications, such as triphala (Table 2) [20].

Table 2. An overview of case studies in network pharmacology in Ayurvedic formulation.

S.N.	Formulation	Target disease/ condition	Key targets/ pathways	Findings	References
1	Triphala	Cancer	Anti-cancer pathways	Identified the mechanism of action and potential new leads for cancer treatments	(20)
2	Triphala	cardio-cerebral vascular disorders (CCVDs)	PTGS2, MMP9, and IL6	Suppressed expression of targets suggested novel CCVD therapeutics	[21]
3	Nisha Amalaki	Type-2 diabetic mellitus (T2DM)	as regulation of cell cycle, inflammation, insulin resistance, apoptosis, and glucose and lipid metabolism,	Linked to multiple biological processes, validated anti-diabetic properties	[22]
4	Nisakathakadi Kashaya (NK)	Diabetes	DPP4 inhibition, diabetes gene network	Demonstrated DPP4 inhibitory potential, modulated diabetes related pathways	[23]
5	Saraswatarishta (SWRT)	Neurological disorders	blood-brain barrier penetration, CNS gene targets	Neuroprotective effects, correlated with neurological disease	[24]

Another study investigated the protective mechanism of triphala, a traditional medicinal compound, against cardio-cerebral vascular disorders (CCVDs) using a network pharmacology-based methodology. Key targets (PTGS2, MMP9, and IL6) and possible treatment pathways were found by examining compound-target gene networks and pathways. The results were corroborated by in vitro studies, which showed that triphala suppresses the expression of PTGS2, MMP9, and IL6. This work reveals possible targets for creating novel CCVD therapeutics and delivers insightful information about the constituents and pharmacological mechanisms of triphala (Table 2) [21].

Researchers examined the pharmacological mechanism of Nisha Amalaki, a herbal combination used to treat Type 2 diabetes mellitus (T2DM) (Table 2) [22]. A protein-protein interaction network was examined, and possible targets of Nisha Amalaki were found using a network pharmacology-based methodology. Numerous biological pathways and processes, including insulin resistance, inflammation, apoptosis, glucose and lipid metabolism, and cell cycle regulation, were identified by enrichment analysis as being linked to its anti-diabetic properties.

A different investigation examined the potential of Nisakathakadi Kashaya (NK), an Ayurvedic anti-diabetic formulation, as a DPP4 inhibitor and its ability to modulate gene networks linked to diabetes. The DPP4 inhibitory potential of Nisakathakadi Kashaya was investigated, and bioactive compounds were identified using in vitro and in silico techniques. Nisakathakadi Kashaya's connections with diabetes-related proteins and pathways were discovered by network pharmacology analysis. The study sheds light on the potential for managing diabetes and the mechanism of action of Nisakathakadi Kashaya (Table 2) [23].

Saraswatarishta (SWRT), an ayurvedic formulation, was examined to check its neuroprotective potential in neurological diseases using network pharmacology. The gene targets and interactions of nine active phytoconstituents and five additives were examined. The phytoconstituents demonstrated possible therapeutic effects, and the networks identified correlations with significant neurological illnesses. The study also discovered signs that the phytoconstituents can penetrate the BBB (blood-brain barrier) and notable expression of gene targets in different areas of the central nervous system (Table 2) [24].

AI'S POTENTIAL APPLICATIONS IN AYURVEDA

Virtual Aides for Health

Chatbots and AI-powered virtual health assistants may serve as individualized health counsellors, providing instant access to Ayurvedic knowledge and advice [25]. People can get help from these virtual assistants in knowing their Prakriti, adopting healthy living habits, and choosing Ayurvedic treatments and remedies.

Integrative Medical Care

Integrating AI with contemporary medicine to create a comprehensive and cooperative approach to healthcare is where Ayurveda's use of AI is expected to grow. Ayurvedic practitioners and contemporary medical professionals can communicate more easily thanks to AI, creating comprehensive treatment plans that take advantage of both systems' advantages for the benefit of patients [26].

Improved Studies and Evidence-Based Procedures

Research on Ayurvedic remedies and their effects can be conducted on a wide scale with the use of AI-powered data analytics. By gathering and evaluating enormous volumes of clinical data, artificial intelligence (AI) can support Ayurvedic evidence-based practice, confirming conventional treatments and enhancing Ayurveda's integration with contemporary healthcare systems [27].

Health Care Prediction

To enable preventative therapies, AI systems can examine a person's health trends over time, forecasting possible imbalances or future medical issues [28].

CONCLUSION

Modernizing traditional medical practices through the integration of Artificial Intelligence, Network Pharmacology, and Ayurveda is beneficial for the effective management of several diseases.

AI and network pharmacology improve the precision, efficacy, and safety of Ayurvedic medicine. This review summarizes the application of AI and network pharmacology with Ayurvedic medicine.

Author Contribution

Original draft preparation, writing, tables, and editing of the manuscript – Ishana Chand, Review and editing of the manuscript – Alok Shiomurti Tripathi, Conceptualization and final approval of the manuscript – Rajiv Gupta.

Conflict of Interest

The authors hereby declare there is no conflict of interest.

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