# The Use of Artificial Intelligence in Ayurvedic Drug Development: A Review

Dr. Gajanan S Sawrate[1], Dr. Prabhavati D Nadre[2]
[1]*Assistant Professor, Dept of Rsbk Ssvp Ayu Clg and Ri Hatta Basmat Hingoli*
[2]*PG Scholar Dept. Of Dravyagun Vigyan Shri Ayurved Mahavidyalay, Nagpur*

***Abstract*—Ayurveda, one of the world's oldest systems of medicine, has gained global recognition for its holistic and personalized approach to healthcare. However, Ayurvedic drug development faces challenges such as lack of standardization, limited pharmacological validation, variability in herbal formulations, and difficulties in integrating traditional knowledge with modern scientific methodologies. Artificial Intelligence (AI), including machine learning and deep learning technologies, has emerged as a transformative tool in pharmaceutical research and offers promising opportunities for advancing Ayurvedic drug discovery and development. This review critically evaluates the role of AI in various stages of Ayurvedic drug development, including phytochemical screening, molecular docking, formulation optimization, target identification, network pharmacology, and clinical validation. Literature published between 2018 and 2024 was reviewed from databases such as PubMed, Scopus, Web of Science, and Google Scholar. Studies indicate that AI-based approaches can efficiently predict pharmacological activities of phytoconstituents, identify herb–protein interactions, and explain synergistic effects of polyherbal formulations such as Triphala and Chyawanprash. AI-driven analytics also support evidence-based validation and personalized Ayurvedic therapeutics. Furthermore, computational tools have accelerated herbal drug repurposing and biomarker discovery. Despite these advancements, challenges including insufficient structured datasets, quality variability of herbal drugs, and limited interdisciplinary collaboration remain significant barriers. The integration of AI with Ayurveda has the potential to establish a robust evidence-based framework for Ayurvedic medicine and improve its global acceptance. Future perspectives include development of AI-powered Ayurvedic databases, integration with omics technologies, and collaborative research between Ayurvedic scholars, data scientists, and pharmaceutical researchers.**

***Index Terms*—Artificial Intelligence; Ayurveda; Machine Learning; Drug Discovery; Herbal Medicine; Deep Learning; Phytochemicals; Network Pharmacology; Personalized Medicine; Ayurvedic Drug Development.**

## I. INTRODUCTION

Ayurveda, originating in India over 3,000 years ago, is based on the principles of holistic healing and personalized medicine. Its pharmacopeia includes thousands of medicinal plants, minerals, and polyherbal formulations. Global interest in Ayurveda has grown significantly due to the demand for natural and holistic therapies. However, Ayurvedic drug development faces major challenges including lack of standardization, limited pharmacological validation, and difficulties in integrating traditional knowledge with modern scientific frameworks. Artificial Intelligence (AI), particularly machine learning (ML) and deep learning (DL), has transformed pharmaceutical research by enabling large-scale data analysis, drug repurposing, molecular docking, and biomarker discovery. The application of AI in Ayurveda remains relatively unexplored but holds immense potential to enhance drug discovery, formulation design, and clinical validation.

## II. NEED OF THE STUDY

Increasing global interest in herbal and natural medicines demands scientific validation and standardization of Ayurvedic formulations.
Complex multi-herbal formulations in Ayurveda present challenges in understanding molecular interactions and therapeutic effects.
AI can provide predictive models, optimize formulations, and bridge the gap between traditional knowledge and modern evidence-based science.

There is a need to create structured datasets, digital platforms, and AI-powered tools to accelerate drug development in Ayurveda.

Aim

To critically evaluate and review the role of Artificial Intelligence in the discovery, development, optimization, and validation of Ayurvedic drugs.

## III. OBJECTIVES

Primary Objective

To assess the applications of Artificial Intelligence in different stages of Ayurvedic drug development, including phytochemical screening, formulation optimization, target identification, and clinical validation.

Secondary Objective

To identify challenges, limitations, and future prospects of integrating AI with Ayurvedic drug research.

To highlight case studies where AI has successfully contributed to herbal medicine discovery.

## IV. MATERIAL & METHODOLOGY

Study Design: Review article.

Data Sources: Literature was retrieved from PubMed, Scopus, Web of Science, and Google Scholar using keywords such as "Artificial Intelligence," "Ayurveda," "drug discovery," "machine learning," "deep learning," and "herbal medicine."

Inclusion Criteria:

Articles published between 2018–2024 focusing on AI in herbal or Ayurvedic medicine research.

Exclusion Criteria:

Non-English publications, articles without AI applications in herbal or traditional medicine.

Method:

Systematic collection, analysis, and synthesis of data from selected studies. Emphasis was placed on AI applications in phytochemical analysis, molecular docking, clinical trials, and personalized Ayurveda.

## V. OBSERVATIONS

AI is increasingly used to predict pharmacological activity of phytoconstituents and optimize herbal formulations.

Deep learning tools assist in identifying herb–protein interactions, validating traditional claims at the molecular level.

Network pharmacology combined with AI has explained synergistic actions in multi-herbal formulations like Triphala and Chyawanprash.

AI-based clinical trial analysis enhances evidence-based validation of Ayurvedic medicines.

Major challenges include lack of structured datasets, variability in herbal drug quality, and limited collaboration between Ayurvedic scholars and AI experts.

## VI. RESULTS & CONCLUSION

Artificial Intelligence offers transformative potential in Ayurvedic drug development by accelerating phytochemical discovery, optimizing multi-herbal formulations, and enabling personalized healthcare. Case studies on curcumin, ashwagandha, triphala, and tulsi highlight AI's ability to uncover novel therapeutic pathways. However, challenges related to standardization, data scarcity, and interdisciplinary collaboration must be overcome. The integration of AI with Ayurveda can establish a robust, evidence-based foundation for global acceptance of Ayurvedic drugs. Future directions include creating AI-powered Ayurvedic databases, integrating omics sciences, and fostering international collaborations.

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