

## DRUG DESIGNING IN AYURVEDA

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## ABSTRACT

Ayurveda, the ancient Indian medical tradition, emphasizes the harmony of the body, mind, and spirit. Ayurvedic medicine, with its holistic approach to healing, has been a cornerstone of traditional Indian healthcare for thousands of years. Recent advances in drug design techniques offer the opportunity to bridge Ayurveda's age-old wisdom with modern biomedical science. This essay examines the fundamentals of Ayurvedic medicine creation, emphasizing the fusion of conventional wisdom with cutting-edge scientific techniques. This study emphasizes the importance of Ayurveda in drug discovery and development by examining several Ayurvedic formulations, their pharmacological characteristics, and their possible applications in modern medicine. According to the findings, Ayurveda's extensive pharmacopoeia can be a useful tool for developing innovative medication formulations, which will benefit integrative medicine. Reviving interest in the pharmaceutical industry and providing

distinctive therapeutic treatments for a variety of human illnesses can be achieved through the replication and adaptation of earlier science to contemporary drug development procedures.

**KEYWORDS:** Ayurveda, Ayurvedic discovery, drug design, herbal medicine, Reverse pharmacology, integrative medicine, traditional knowledge, drug development.

## INTRODUCTION

With roots extending back more than 3,000 years, Ayurveda, which means "the science of life," is one of the oldest recognized medicinal systems. Its foundation is the idea of maintaining equilibrium between the three doshas (*Pitta*, *Kapha*, and *Vata*), which control mental and physical processes. In Ayurvedic medicine, drugs are created utilizing natural

ingredients with an emphasis on their overall benefits rather than their discrete chemical properties. By demonstrating the potential of Ayurvedic formulations in current drug discovery, this work seeks to close the gap between conventional Ayurvedic practices and contemporary pharmacological research.

In Ayurveda Drug is defined as Any substance that is used to prevent, diagnose, treat or relieve symptoms. drug designing in ayurveda is important because it is not just efficient in preventing, treating, and diagnosing the illness, but also in enhancing "quality of life" Every new medicine has enormous potential to improve people's lives and quality of life.

Drug resistance, chronic illnesses, and lifestyle disorders are all increasing alarmingly in the modern world. Ayurveda has a lot to offer in terms of holistic and natural treatments, which are in high demand. This article explores the Ayurvedic principles of drug design and shows how molecular docking, bioinformatics, and other drug discovery tools are implementing these ideas into modern pharmaceutical techniques.

## MATERIALS AND METHODS

### 1. Ayurvedic Principles of Drug Design

The principles of "*Rasa*," "*Guna*," "*Veerya*," "*Vipaka*," and "*Prabhava*," which control the pharmacological effects of natural substances, are the basis of Ayurvedic medicine design. These concepts help in recognizing the medicinal potential of herbs and other natural items. Ayurvedic drug development focuses on formulations rather than single isolated compounds, emphasizing the synergistic action of multiple ingredients to balance the *doshas*.<sup>[1]</sup>

Numerous herbs, minerals, and animal products are included in hundreds of Ayurvedic classics including the *Sushruta Samhita* and *Charaka Samhita*. These blends are intended to help the body regain equilibrium by means of immunomodulation, detoxification, and renewal. What Ayurveda has to offer:

- The classical texts of Ayurveda, such as *Brihatrayee*, *Laghutrayee* and *Rasa Classics* form the foundation of its principles,
- Ayurveda is based on the fundamental principles of balancing the three doshas—*Vata*, *Pitta*, and *Kapha*—also *Panchamahabhuta*, *Prakriti parikshan*, and *Dashavidha parikshya Bhava* to maintain health and prevent disease through individualized therapeutic approaches.
- In Classic formulations in Ayurveda, there are >100000 formulation are designed using

precise combinations of herbs to promote overall well-being and strengthen immunity, and their efficacy has been supported by various contemporary studies. Also *Pancha Vidha Kashaya Kalpana* refers to the five fundamental forms of Ayurvedic medicinal preparations, crucial for therapeutic interventions. These include *Swarasa* (fresh juice), *Kalka* (herbal paste), *Kwatha* (decoction), *Hima* (cold infusion), and *Phanta* (hot infusion). Each form is designed to extract active compounds from herbs in different concentrations, catering to individual dosha imbalances and specific health conditions.

- The growing availability of Ayurvedic databases and digital platforms allows researchers to access and analyze classical knowledge, bridging the gap between traditional practices and modern scientific methodologies. For eg. API-326 Ayu plants, AFI-636 Formulation and Materia medica of ayurveda.
- Recent developments in Ayurveda, such as **Ayugenomics**, aim to integrate traditional Ayurvedic principles with modern genomics to explore personalized medicine based on genetic makeup and dosha classification. Another innovation, **Ayusoft**, is a software tool developed to digitize classical Ayurvedic texts, enabling researchers and practitioners to access, analyze, and apply traditional knowledge more effectively using modern computational techniques.

## 2. Phytochemical Analysis and Isolation of Active Compounds

The first step in drug development is identifying bioactive compounds from Ayurvedic herbs. Techniques like High-Performance Liquid Chromatography (HPLC), Gas Chromatography-Mass Spectrometry (GC-MS), and Liquid Chromatography-Mass Spectrometry (LC-MS) are commonly employed for phytochemical profiling of Ayurvedic plants such as *Curcuma longa* (Turmeric), *Withania somnifera* (Ashwagandha), and *Bacopa monnieri* (Brahmi).<sup>[2]</sup>

Phytochemical analysis helps isolate alkaloids, flavonoids, glycosides, and other bioactive constituents that contribute to the pharmacological activity.<sup>[3]</sup>

## 3. Drug development pathway

### a. In Vivo & In Vitro test

The drug development pathway in Ayurveda, while rooted in traditional formulations, follows a systematic process for modern validation. Initially, **in vitro (cell culture)** studies are conducted to evaluate the pharmacological properties and potential bioactive compounds of Ayurvedic herbs. This is followed by **in vivo (animal models)** testing in animal models to

assess efficacy, safety, and toxicity in a biological system. These tests are also used to evaluate the pharmacodynamics, pharmacokinetics, and bioavailability of Ayurvedic drugs.

For example, Ashwagandha has demonstrated significant anti-inflammatory and adaptogenic effects in rodent models, supporting its traditional use for stress management and cognitive enhancement.<sup>[4]</sup>

#### **b. Human testing**

Once preclinical results are favourable, the formulations proceed to **human testing** through clinical trials, ensuring the therapeutic benefits and safety profiles are validated in human populations. Clinical drug development in Ayurveda follows the standard phases seen in modern medicine. In **Phase 1** trials, the primary goal is to assess the **safety** and tolerability of Ayurvedic formulations in a small group of healthy volunteers. **Phase 2** trials expand the sample size to evaluate the **efficacy** and determine optimal dosing in patients with the target condition. Finally, **Phase 3** trials involve a larger, more diverse population to confirm the drug's **safety and efficacy**, often comparing it with standard treatments.<sup>[5]</sup>

Ayurvedic drugs such as *Triphala* have been evaluated in small-scale clinical trials, showing efficacy in conditions like digestive disorders and irritable bowel syndrome. However, more randomized controlled trials (RCTs) with larger sample sizes are required to meet the standards of modern medicine.<sup>[6]</sup>

#### **c. Data Review**

After data collection, a comprehensive **data review** is performed, assessing both clinical outcomes and safety records to ensure the drug meets modern healthcare standards.

#### **d. Post-marketing surveillance**

**Post-marketing surveillance** is then implemented to monitor long-term efficacy and adverse reactions, ensuring ongoing safety in broader populations. It plays a crucial role in refining treatment guidelines and ensuring the formulation's overall risk-benefit profile remains favorable.

### **4. Reverse pharmacology: A Road to ayurvedic discovery**

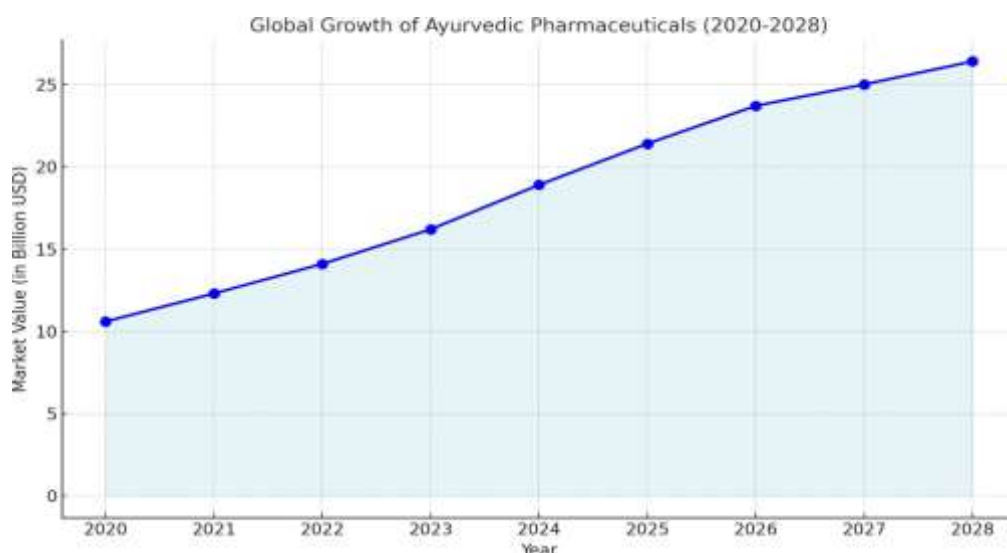
A reverse pharmacology approach involves integrating clinical observations and documented clinical experiences into leads by conducting transdisciplinary exploratory studies and then developing these into drug formulations through robust preclinical and clinical trials, a

rigorous scientific approach of integrating documented clinical experiences.<sup>[7]</sup>

The traditional knowledge-inspired reverse pharmacology described here relates to reversing the routine ‘laboratory-to-clinic’ progress to ‘clinics-to-laboratories’.

## 5. Global Growth of Ayurvedic Pharmaceuticals

Ayurvedic pharmaceuticals are experiencing significant global growth due to increasing demand for natural and holistic treatments. According to market reports, the global Ayurvedic products market was valued at approximately USD 10.6 billion in 2020 and is expected to grow at a compound annual growth rate (CAGR) of around 16% from 2021 to 2028.<sup>[8]</sup> This growth is attributed to the rising popularity of herbal supplements and the increasing recognition of Ayurveda in integrative medicine.



## DISCUSSION

### 1. Drug Designing Based on Ayurvedic Principles

The fundamental philosophy of Ayurveda revolves around treating the body as a whole rather than targeting individual symptoms. Ayurvedic formulations such as *Chyawanprash*, *Triphala*, and *Brahmi Rasayana* contain a blend of herbs that work synergistically to restore homeostasis. Modern research has supported this holistic view, with studies showing that polyherbal formulations often exhibit better efficacy and reduced toxicity compared to single-molecule drugs.<sup>[9]</sup>

For instance, *Triphala*, a combination of three fruits (*Embllica officinalis*, *Terminalia chebula*, and *Terminalia bellirica*), has been shown to have a potent antioxidant and anti-inflammatory

effect. Modern drug discovery methods have elucidated the molecular mechanisms through which *Triphala* acts, particularly its role in modulating the expression of pro-inflammatory cytokines.<sup>[10]</sup>

## 2. Preclinical and Clinical Studies

Preclinical animal models have shown that Ayurvedic formulations have a broad spectrum of activity, from anti-inflammatory to neuroprotective effects. For example, *Bacopa monnieri* (Brahmi) has shown significant cognitive-enhancing properties in rodent models, making it a potential treatment for Alzheimer's disease.<sup>[11]</sup> Furthermore, clinical trials have provided evidence supporting the efficacy of Ayurvedic compounds in modern healthcare. A clinical trial on *Ashwagandha* showed a significant reduction in cortisol levels in patients with chronic stress.<sup>[12]</sup>

## CONCLUSION

Ayurveda, with its rich history of holistic healing, is increasingly finding validation through modern scientific techniques such as molecular docking and bioinformatics. The integration of traditional knowledge with contemporary drug design offers immense potential for developing novel therapeutics. Ayurvedic formulations are proving their efficacy in treating complex conditions like inflammation, stress, and neurodegeneration. However, challenges remain in terms of standardization, quality control, and the need for large-scale clinical trials. Future efforts should focus on the convergence of traditional wisdom and modern science to develop safe, effective, and affordable healthcare solutions for global populations.

Developing a strategy based on past experiences and key learnings from the past is crucial to making significant progress. In India more than 70% of the population use herbal drugs for their health. There is a vast experience-based evidence for many of these drugs. There are also a number of Institutes/Universities in India carrying out research on herbal drugs and medicinal plants. Using the 'reverse pharmacological' approach, several Institutes carry out basic and clinical research on the potential health benefits of herbal drugs.

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