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Review Article

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"ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING IN AYURVEDIC PHARMACEUTICS: OPPORTUNITIES IN FORMULATION, QUALITY CONTROL AND SAFETY PREDICTION"

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ABSTRACT

Background: Artificial intelligence (AI) and machine learning (ML) are transforming pharmaceutical research. In traditional medicine, most applications so far concern diagnosis and knowledge digitisation, while applications to the manufacture and quality of medicines remain limited, particularly for Ayurveda. **Objective:** To review current applications of AI and ML relevant to Ayurvedic pharmaceutics, drawing on experience in traditional Chinese medicine (TCM) and pharmaceutical sciences, and to propose priority use cases and requirements. **Methods:** A narrative review of reviews and primary studies on AI in traditional medicine, AI-based quality evaluation of herbal materials, computational toxicology, formulation modelling and Indian phytochemical databases. **Results:** A 2025 review of AI in traditional medicine found only two Ayurveda-specific AI studies, both outside pharmaceutics. In TCM, AI-based spectroscopic and imaging methods have reached high accuracy in quality tasks, for example raising adulterant identification from 77.1% to 97.6% with FT-NIR and machine learning, and achieving 99.35% accuracy in species identification with convolutional neural networks. ML models have flagged potentially hepatotoxic constituents in medicinal plants. Artificial neural networks have long been used for formulation optimisation in conventional pharmaceutics. India has curated resources, such as a database of 1,742 medicinal plants, 9,596 phytochemicals and 974 traditional formulations. Barriers include small and heterogeneous datasets, inconsistent terminology, limited external validation and unclear regulation. **Conclusion:** AI could strengthen raw material authentication, fingerprint interpretation, process control and safety screening in Ayurvedic pharmaceutics, but only with standardised, well-annotated datasets and transparent validation.

KEYWORDS: Artificial intelligence; Machine learning; Ayurvedic pharmaceutics; Quality control; Formulation optimisation; Chemometrics; Safety prediction

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INTRODUCTION

AI, and in particular ML, has become a core tool in pharmaceutical research, from target identification and virtual screening to formulation and process control[1]. In traditional medicine, interest has focused on diagnostic pattern recognition, personalised treatment and digitisation of classical knowledge[2,3]. Applications to the medicines themselves, their raw materials, processing and quality, are less developed.

Ayurvedic pharmaceutics faces problems that AI is well suited to address: variable natural raw materials, complex multi-ingredient formulations, empirical process end-points, and large differences between products of the same name[4,5]. This review examines where AI and ML could help, what has been demonstrated in related fields, and what must be in place before such tools can be used reliably.

METHODS OF THE REVIEW

This is a narrative review. Reviews and primary studies were identified through bibliographic databases and publisher platforms using the terms artificial intelligence, machine learning, deep learning, chemometrics, Ayurveda, traditional medicine, herbal medicine, quality control, authentication, formulation and toxicity. Given the small number of Ayurveda-specific studies, evidence from traditional Chinese medicine and conventional pharmaceutics was included to illustrate feasible applications.

CURRENT STATE OF AI IN TRADITIONAL MEDICINE

A 2025 mini-review of AI in Ayurveda, traditional Chinese medicine and Thai traditional medicine found applications in diagnosis, personalised treatment, outcome prediction, herbal pharmacology, knowledge digitisation and telemedicine, but identified only two Ayurveda-specific AI studies and no references on formulation, quality control or herbal identification[2]. The authors highlighted heterogeneous and small datasets, inconsistent ontologies, limited explainability, privacy concerns and unclear regulation as the main barriers. A review of AI in Ayurveda similarly described current concepts and prospects rather than validated pharmaceutical applications[3].

In TCM, AI has advanced further into the pharmaceutical domain, with reviews describing applications in industry modernisation, drug discovery and herbal knowledge mining[6,7], as well as practical guidance for implementing AI in traditional medicine research[8].

OPPORTUNITIES IN AYURVEDIC PHARMACEUTICS

Table 1. Potential applications of AI and ML in Ayurvedic pharmaceutics

Domain	Example application	Evidence from related fields
Raw material authentication	Detection of adulterants and substitutes using near-infrared spectra and ML	FT-NIR with pattern recognition raised adulterant identification accuracy from 77.06% to 97.58%
Quality grading of powders	Multi-sensor fusion models for powdered herbal drugs	Classification of *Panax notoginseng* powder quality with AI sensory and multi-source fusion
Species and part identification	Image-based deep learning	CNN species identification accuracy up to 99.35% reported in TCM materials
Fingerprint interpretation	Chemometric and ML analysis of HPTLC or HPLC fingerprints	Pattern-recognition approaches for authenticity and origin
Safety screening	Prediction of hepatotoxic constituents	ML identified potentially hepatotoxic metabolites in *Polygonum multiflorum*; structure-based DILI prediction
Formulation optimisation	Neural network models relating composition and process to product properties	Long-established in conventional pharmaceutics
Process control	Quality-by-design and process analytical technology for granulation and drying	Proposed for conversion of *kwatha* to granules

1. Raw material authentication

Adulteration and substitution of raw herbs are among the main threats to the quality of Ayurvedic medicines. In TCM, combining Fourier-transform near-infrared spectroscopy with ML algorithms such as support vector machines and artificial neural networks raised identification accuracy for a seed drug and its adulterants from 77.06% to 97.58%[9], and multi-sensor fusion has been used to grade herbal powders[10]. Image-based deep learning has achieved high accuracy in species identification and origin tracing[11]. Similar models trained on authenticated Ayurvedic raw materials could support rapid incoming-material checks in manufacturing units.

2. Interpretation of fingerprints

Chromatographic fingerprints of polyherbal formulations are complex and are often interpreted visually. ML and chemometric methods can compare fingerprints with reference batches, detect missing ingredients and quantify similarity. Validated HPTLC methods for formulations such as *Mahasudarshan churna*[12] provide the type of data on which such models could be trained. Large inter-brand variation in marker content[5] illustrates the problems such tools could detect.

3. Safety screening

Computational toxicology can screen constituents for hepatotoxicity and other risks before laboratory testing. In a case study of *Polygonum multiflorum*, machine learning models identified potentially hepatotoxic constituents[13], and structure-based models have been developed to predict drug-induced liver injury[14]. Applied to Ayurvedic plants, such models could prioritise constituents for testing and support pharmacovigilance signal assessment.

4. Formulation and process optimisation

Artificial neural networks have long been used in conventional pharmaceutics to model the relationship between formulation variables, process parameters and product properties[15]. Ayurvedic processes such as *bhavana*, *puta* and *kupipaka* involve many variables and empirical end-points. Logging process data, such as temperature profiles in furnaces or energy input in triturators, and linking them to instrumental product attributes would allow models to predict when a process is complete and to keep batches consistent. Quality-by-design frameworks proposed for converting *kwatha* into granules[16] provide a natural structure for such work.

5. Knowledge mining

Curated databases make classical knowledge computable. One Indian database links 1,742 medicinal plants, 9,596 phytochemicals, 1,124 therapeutic uses and 974 traditional formulations[17]. Combined with pharmacopoeial data[18], such resources can support hypothesis generation, for example identifying constituents shared across formulations with the same indication. Network pharmacology and AI-based target prediction should, however, be treated as hypothesis-generating rather than as evidence of efficacy.

BARRIERS AND REQUIREMENTS

- **Data quality and size.** Models need large, well-annotated datasets from authenticated materials and characterised products. Most current datasets are small and heterogeneous[2,11].
- **Terminology.** Consistent ontologies for plants, parts, processes and formulations are needed so that data from different sources can be combined.
- **Validation.** External validation on independent samples and laboratories is essential; accuracy in a controlled laboratory study does not guarantee performance in routine use[11].
- **Explainability.** Regulators and practitioners need to understand why a model classifies a sample as adulterated or a constituent as toxic.
- **Regulation.** Use of AI in release testing or pharmacovigilance requires regulatory acceptance and documented validation.
- **Ethics and ownership.** Traditional knowledge, practitioner data and patient data require appropriate governance, benefit sharing and privacy protection.

A PRACTICAL ROADMAP

- **Short term:** build reference spectral and image libraries of authenticated raw materials; apply chemometrics to existing HPTLC fingerprints.
- **Medium term:** instrument key processes to record temperature, time and energy data; develop predictive models for process end-points; screen constituents of priority plants with computational toxicology.
- **Long term:** integrate raw material, process, product and pharmacovigilance data in quality management systems with validated AI.

CONCLUSION

AI and ML have so far had little impact on Ayurvedic pharmaceutics, but experience from traditional Chinese medicine and conventional pharmaceutics shows clear opportunities in raw material authentication, fingerprint interpretation, safety screening and process control. Realising these opportunities depends less on algorithms than on standardised, well-annotated data from authenticated materials and characterised processes, rigorous external validation and regulatory engagement. Building these foundations would also strengthen Ayurvedic pharmaceutics independently of AI.

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