GMR
The Original

ARTIFICIAL INTELLIGENCE-DRIVEN PHYTOCHEMICAL DISCOVERY AND GENOMIC TARGET IDENTIFICATION FOR PRECISION AYURVEDIC DRUG DEVELOPMENT

Dr Chandni Gupta[1], Shreya N Desai[2], Dr Asha S Raj[3], Dr Ankita Goyal[4], Dr. Shivansh Chandra Sharma [5]

[1]Associate Professor, Dravyaguna, Specialization in MD (Dravyaguna), Atal Medical and Research University, Mandi, Himachal Pradesh, ORCID: 0000-0002-5479-4972, Email ID: kaurachandni17@gmail.com
[2]Master"s in Data Science with Specialization in AI/ML, ORCID: 0009-0003-1513-0174, Email ID: desaishreya001@gmail.com
[3]Associate Professor, Department of Dravyagunavijnana, J S Ayurveda Mahavidyalaya, Nadiad, 387001, MAM University, ORCID: 0000-0002-8902-5698, Email ID: drashasraj@gmail.com
[4]Lecturer, Department of Dravyaguna Vigyan, Specialization in MD Dravyaguna, Guru Ravidas Ayurved University, Hoshiarpur, Punjab, ORCID: 0000-0003-0028-0455, Email ID: ankita.goyal07@gmail.com
[5]Assistant Professor, Department of Kriya Sharir, Manglaytan University, Aligarh - 202146, Email ID: dr.shivanshchandra17892@gmail.com

ABSTRACT

Ayurvedic drug development is increasingly positioned at the intersection of traditional knowledge, phytochemical science, and precision medicine, yet its progress is constrained by complex formulations, variable botanical composition, limited target validation, and fragmented molecular evidence. This review examines how artificial intelligence can accelerate phytochemical discovery, identify genomic targets, and support individualized Ayurvedic therapeutics. Relevant literature on machine learning, deep learning, cheminformatics, molecular docking, network pharmacology, pharmacogenomics, multi-omics, and Prakriti-based stratification was critically synthesized. Current evidence indicates that AI can improve compound annotation, dereplication, bioactivity prediction, drug-likeness assessment, toxicity screening, and lead prioritization while reducing the experimental search space. Network pharmacology and systems biology provide appropriate frameworks for modelling the multi-component, multi-target, and multi-pathway actions of Ayurvedic formulations. Genomic, transcriptomic, proteomic, metabolomic, and epigenomic integration can strengthen target discovery, biomarker identification, mechanistic validation, and responder stratification. Prakriti-informed pharmacogenomics may enhance treatment selection and dosing when constitution-based phenotypes are linked to reproducible molecular signatures. Translation remains limited by inconsistent botanical standardization, heterogeneous datasets, algorithmic opacity, inadequate external validation, population bias, and uncertain regulatory pathways. Progress requires curated interoperable databases, explainable models, laboratory confirmation, prospective clinical trials, pharmacovigilance, and protection of traditional knowledge. Integrating AI with validated Ayurvedic principles can establish a more rigorous, scalable, and clinically credible pathway toward safe, standardized, and personalized phytotherapeutic development across diverse populations and healthcare settings globally.

KEYWORDS: Artificial intelligence, Ayurvedic drug development, Genomic target identification, Phytochemical discovery, Precision medicine

INTRODUCTION

Traditional and modern therapeutic applications of medicinal plants continue to be one of their main sources for bioactive molecules (Latif & Nawaz, 2025). The various secondary metabolites such as flavonoids, terpenoids, phenolic compounds, alkaloids, glycosides, and others exhibit antioxidant, anti-inflammatory, antimicrobial, anticancer, metabolic, and neuroprotective properties (Latif & Nawaz, 2025). Ayurveda relies on the use of medicinal plants and medicinal polyherbal formulations in a personalized approach to the disease taking into account the constitution, disease presentation, diet and lifestyle (Upasani, 2025). This systems-oriented approach can be integrated with precision medicine, but it needs to be translated to the scientific level, which necessitates reproducible identification of the active compounds present in the plasma, molecular targets, mechanisms, safety and treatment response determinants (Khandelwal et al., 2026).

Traditional natural product discovery involves extraction, fractionation, bioactivity-guided screening, isolation, structure elucidation and experimental re-testing (Muthuraj & Chandrasekaran, 2026). These are time-consuming, resource-intensive and hard to scale procedures (Paerhati et al., 2026). Low levels of active metabolites and poor characterization of compound–target relationships are two other constraints for discovery (Varghese et al., 2025). Species, geography, cultivation, harvesting, storage, extraction and processing condition influence the phytochemical composition which affects the efficacy, dosage uniformity, safety and reproducibly (Karthikeyan et al., 2025). Multiple constituents in polyherbal formulations can interact synergically, additively, antagonistically or through pharmacokinetic interactions, which makes it more difficult to understand the effect of the formulation (Spanakis et al., 2025).

These are some of the drawbacks that can be remedied by applying artificial intelligence to analyse large heterogeneous datasets (Gupta et al., 2025). Knowledge mining, metabolite annotation, compound dereplication, virtual screening,

activity prediction, and lead optimization are some of the areas where machine learning, deep learning, and cheminformatics can aid in knowledge mining, metabolite annotation, compound dereplication, virtual screening, activity prediction, and lead optimization (Liu et al., 2025). The phytochemicals can be prioritized based on molecular docking and QSAR modelling using AI tools based on the predicted binding affinity and biological activity (Ydyrys et al., 2025). Pre-experimental estimation of drug-likeness, toxicity and pharmacokinetic parameters can also be used as computational tools (Gholap et al., 2026). The applications of these are applicable to antimicrobial discovery, which can relate plant derived molecules with resistant pathogens (Yin et al., 2026). Similar strategies can facilitate the discovery of phytochemicals as anti-cancer agents (Assi et al., 2026).

Genomic and multi-omics methods bring precision by detecting genes associated with the disease, pathways changed, disease markers, and therapeutic response (Yin et al., 2026). Combining multi-omics with AI can help to elucidate the interactions between different biological systems and understand the mechanisms by which phytochemicals can affect these interactions (Ishtyaq Mahmud & Banerjee, 2026). One of the key applications of AI in network pharmacology is its ability to model multi-component, multi-target, and multi-pathway interactions at various levels of biological complexity, which is particularly salient for Ayurvedic medicines (Cui et al., 2025). These models can aid in target prioritization, identification of biomarkers, optimization of drug formulations, predicting drug responses, and mechanistic understanding of complex herbal treatments (Varghese et al., 2025).

Artificial Intelligence, genomics, and Ayurvedic principles have the potential to converge and contribute to precision Ayurveda by supporting the integration of phytochemical interventions with biological variability and phenotypic types based on Ayurveda (Khandelwal et al., 2026). Using pharmacogenomic analysis can enhance the prediction of efficacy, dosage needs, adverse reactions and interactions among herbs and drugs (Spanakis et al., 2025). Classical manuscripts may be analysed by computational methods to aid in reverse pharmacology and evidence-based repurposing of traditional medicines (Patel et al., 2026). The available evidence is still scattered in the various fields of application, such as in phytochemistry, computational screening, network pharmacology, genomic target identification, and Ayurvedic informatics (Varghese et al., 2025). A significant number of models do not have standard datasets, validation, transparency, or validation of the interactions predicted by the model (Abdallah et al., 2026). Research pertaining to molecular stratification based on Prakriti, interactions of the formulation, regulatory pathways, ethical governance, traditional-knowledge protection, algorithmic bias, and prospective clinical validation are still limited (Ghosh et al., 2025). This review aims to assess the possibilities of introducing the phytochemical discovery and genomic target identification with AI in a systematic and clinically translatable approach to precision Ayurvedic drug development. The integrated AI-driven precision Ayurvedic drug development pathway is shown in figure 1.

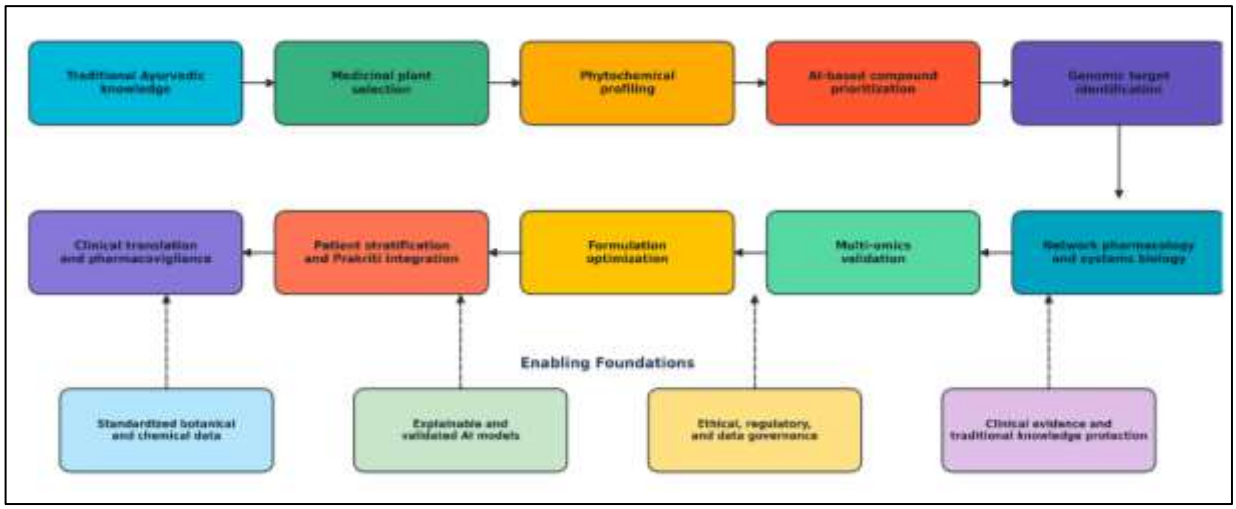

Figure 1. AI-enabled pipeline for precision Ayurvedic drug development

1.1 Objectives of the Review

The present review discusses how AI can be utilized for phytochemical discovery and compound prioritization, and also explores the possibilities of the use of AI in the identification of genomic targets for Ayurvedic drug development. It discusses the potential of network pharmacology, multi-omics and pharmacogenomics for understanding the mechanism and therapeutic effect of Ayurvedic formulations. It also elucidates the methodological, clinical, regulatory and ethical challenges, and suggests directions for the development of precise, safe and clinically translatable Ayurvedic therapeutics.

2. REVIEW

2.1 Phytochemical Diversity and Therapeutic Potential of Ayurvedic Medicinal Plants

Ayurvedic medicinal plants are rich in structurally diverse secondary metabolites such as alkaloids, flavonoids, terpenoids, phenolic compounds, glycosides, tannins and saponins. Plant-based formulations are known to have a wide range of pharmacological activities, attributed to these constituents which can modulate several molecular targets and biological pathways. Variation in the genome of medicinal plants can influence their biosynthetic pathways, metabolite abundance, environmental adaptability, and therapeutic consistency (Devlet & Işık, 2026). Conservation of genetic diversity is therefore important to avoid the loss of valuable chemotypes and ensure the availability of consistent sources for drug discovery.

Phytochemical composition also is affected by environmental conditions. Changes in environmental conditions, such as climate change, habitat loss, temperature, and precipitation can alter the synthesis of bioactive components in plants and decrease the potential for their reproduction (Pandey & Pant, 2026). In the case of polyherbal formulations, the therapeutic effect can also be due to synergic, additive, antagonistic or pharmacokinetic interactions between several compounds.
Pharmaceutical technologies could enhance efficacy and clinical use of phytochemicals that are poorly soluble or unstable. Nanocarriers have the potential to improve the solubility, stability, bioavailability, and targeted delivery of natural compounds (Dohre et al., 2026). Quality control is essential for reliable applications, however. Product consistency is enhanced by botanical authentication, chromatographic fingerprinting, marker-compound quantification, contaminant testing and stability assessment (Gupta et al., 2026). A combination of genetic authentication and analytical and pharmacological profile offers better foundation for precision ayurvedic drug development.

2.2 Artificial Intelligence Technologies for Drug Discovery and Drug Delivery

AI is revolutionizing phytochemical discovery by facilitating the analysis of intricate chemical, biological, and ethnopharmacological data. Patterns in chromatographic, spectroscopic, metabolomic, and bioactivity data could be identified by machine-learning algorithms that may not be discovered by traditional analytical approaches. These methods enable compound classification, peak identification, metabolite identification, quantitative analysis, and even the prediction of biological activity (Srivastava et al., 2025). They are particularly useful for Ayurvedic extracts as they tend to have many structurally similar compounds with similar effects.
The molecular representations can be generated directly from chemical structures, biological sequences and multi-omics profiles with deep-learning models. These models can be used to predict various physicochemical properties, compound–target interactions, toxicity, and therapeutic potential (Vora et al., 2025). Classical manuscripts and scientific literature can also be consulted to derive the name of plants, therapeutic uses, preparation, and disease associations using NLP.
AI aided identification of targets connects phytochemicals to proteins and pathways of diseases. Supervised learning, clustering, and knowledge-graph techniques can prioritize compounds and provide insights into potential new indications for existing natural products (Odah, 2025). Generative models can also yield structures with enhanced potency or selectivity, inspired by those found in nature.
In the field of cancer research, AI's application includes the integration of genomic alterations, molecular networks, and chemical data to prioritize targets of interest that are mechanistically relevant (Khan et al., 2026). Curated datasets, transparent models, external validation, and lab verification are still crucial for guiding the drug discovery process in Ayurveda, but similar principles can be applied. In Table 1, the major applications of AI in drug discovery for Ayurveda are summarized.

Table 1. Major AI Applications Across the Ayurvedic Drug-Discovery Pipeline

AI approach	Input data	Primary application	Expected output	Relevance to Ayurvedic drug development	Key limitations	References
Machine learning	Bioassays, chromatographic data, and molecular fingerprints	Activity and toxicity prediction	Ranked phytochemical candidates	Prioritises promising compounds from large plant libraries	Dependent on data quality and external validation	Muthuraj and Chandrasekaran (2026)
Deep learning	Chemical structures, genomic and multi-omics data	Compound–target and biomarker prediction	Molecular signatures and predictive models	Identifies complex phytochemical–target relationships	Limited interpretability and risk of overfitting	Vora et al. (2025)
Natural-language processing	Ayurvedic manuscripts and scientific literature	Knowledge extraction and indication mapping	Structured plant–compound–disease associations	Converts traditional knowledge into analysable data	Terminological and translation inconsistencies	Patel et al. (2026)
Cheminformatics	Molecular structures and descriptors	Virtual screening, QSAR, and lead optimisation	Drug-like phytochemical leads	Supports rational compound selection	Limited representation of biological complexity	Ydyrys et al. (2025)
Generative artificial intelligence	Molecular graphs and target-binding data	De novo molecular design	Optimized natural-product-inspired structures	Improves potency and selectivity of phytochemical scaffolds	Synthetic feasibility may be uncertain	Paerhati et al. (2026)
Image recognition	Plant and microscopic	Authentication and	Species classification	Strengthens raw-material	Sensitive to image quality	Srivastava et al. (2025)

	images	adulteration detection	and authenticity scores	quality control	and training diversity	
Knowledge graphs	Compound, target, pathway, and disease data	Network mapping and target prioritisation	Compound–target–pathway networks	Models the multi-target effects of Ayurvedic formulations	Dependent on database completeness and validation	Cui et al. (2025)

2.3 In Silico Screening, Molecular Docking, and Drug-Likeness Prediction

An in silico screening method can help in the quick screening of Ayurvedic phytochemicals before expensive experimental screening. Virtual screening is a method to assess a large library of compounds against a selection of molecular targets and rank compounds based on the predicted bioactivity or structural compatibility. Ligand-based methods are used to compare compounds with known active compounds, while structure-based methods assess binding to proteins for which a structure has been solved and/or modelled. AI reinforces these approaches, recognising that there are more complex relationships between molecular structure, target characteristics and pharmacological activity (Khamrayev, 2025).

The molecular docking process can be used to estimate the relative favourability of the compound to bind to the protein binding site and predict how the compound is oriented within the binding site. Can recognise hydrogen bonds, nonpolar contacts, electrostatic contacts and amino acids that recognise a ligand. The network pharmacology integration is useful for the integration of individual compound–target interactions with other pathways and disease mechanisms. In herbal medicine research, integrated network pharmacology and docking techniques are commonly used for the studies of cancer, inflammatory and metabolic diseases (Terkimbi et al., 2026).

The quantitative structure–activity relationship models are used for the estimation of the biological activity from molecular descriptors and biological activity data of the known compounds. Chemical and biological data can be used to extract complex features using deep-learning approaches, enhancing these predictions (Vora et al., 2025). Computational ADMET screening can also be used to find candidates that have poor bioavailability, poor stability, or are even toxic.

There are integrated AI pipelines that integrate docking, activity prediction, selectivity, and pharmacokinetic assessment (Khan et al., 2026). These observations are still preliminary and need confirmation in molecular-dynamics simulations, biochemical assays, in cell and suitable animal models.

2.4 Genomic Target Identification in Precision Drug Development

The molecular basis of the association of phytochemicals with disease mechanisms and variable treatment response can be found through genomic target identification. GWAS can detect variants that are associated with disease susceptibility, disease progression, therapeutic response and adverse effects. This information can be complemented by transcriptomic profiling, which shows differentially expressed genes and pathways between tissues at different stages of disease and/or between patient groups.

AI helps to enhance genomic analysis by processing high-dimensional sequence, expression, epigenetic and functional data. Machine-learning models can prioritise disease-associated genes, predict the effect of variants, classify molecular subtypes and infer the regulatory relationships (Mahmud & Banerjee, 2026). By integrating proteomic, metabolomic, and other multi-omics data, a more comprehensive view of disease biology is provided (Vora et al., 2025). This framework can be used to match plant-derived compounds with defined patient groups and be used to match plant-derived chemicals with molecular abnormalities.

Treatment is not a one-size-fits-all approach in precision medicine, but rather is based on stratification with biomarkers. The Alzheimer Precision Medicine Initiative (APMI) illustrates the ways genomic, biomarker, lifestyle, and clinical information can help to define disease heterogeneity and inform personalised approaches to treatment (Hampel et al., 2019). Such a scheme may be used to determine if there exists a set of repeatable molecular signatures that correspond to the Ayurvedic phenotype of constitution.

AI-driven target discovery for the genome is also making significant strides in cancer therapeutics by leveraging mutations, signalling networks, functional dependencies, and molecular structures (Khan et al., 2026). The therapeutic validity does not depend on genomic association. Functional validation, compound-binding assessment, pathway confirmation, population diversity and prospective clinical evaluation are candidate targets that need to be validated.

2.5 Network Pharmacology and Systems Biology in Ayurveda

Most ayurvedic formulations are multi-component formulations containing multiple phytochemicals, which can target multiple molecular targets, multiple signalling pathways and multiple physiological systems. The single compound – single target paradigm is not sufficient to depict this pharmacological architecture. Network pharmacology is a more suitable approach to mapping relationships between compounds, targets, pathways and diseases. Target identification techniques are also aided by AI, which can determine previously unknown relationships between phytochemicals and proteins linked to disease (Odah, 2025).

The analysis of protein–protein interaction can be used to detect the hub genes, functional modules and signalling nodes that can play a regulatory role in the collective action of polyherbal formulations. By leveraging sequence data, structural features, molecular interactions, and disease relevance, AI models can prioritise druggable targets for further investigation and development (Riaz et al., 2026). Pathway enrichment analysis is then conducted to identify if the predicted targets converge on processes like inflammation, oxidative stress, apoptosis, metabolism, immunity or cellular proliferation.

Systems biology takes this analysis a step further by connecting molecular interactions with the responses at the cellular and organismal levels. Complex therapeutic networks can be better understood using biochemical modelling, with the help of AI algorithms, to differentiate between central mechanisms and incidental associations (Junaid, 2025). However, the results of computational studies are tentative until confirmed by docking, gene-expression studies, biochemical studies, and disease-relevant experimental models.

The development of anticancer drugs illustrates the usefulness of using network analysis, pharmacophore modelling, docking and predictive algorithms to prioritise multi-target compounds (Garg et al., 2024). In the context of Ayurveda, this system of integration can help to understand synergy in formulation and to identify the dominant therapeutic nodes as well as optimise polyherbal formulations based on evidence. The simplified linkage of the phytochemicals with the molecular targets and therapeutic outcomes is shown in figure 2.

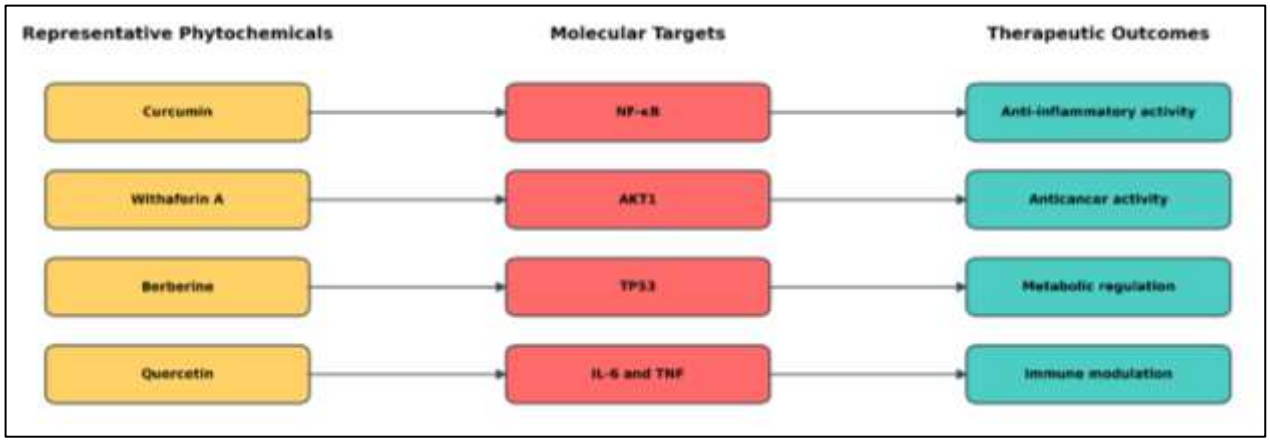

Figure 2. Simplified AI-supported mapping of Ayurvedic phytochemicals

2.6 Multi-Omics Integration for Mechanistic Validation

Multi-omics integration provides a holistic approach to the identification of the mechanism(s) of action of Ayurvedic phytochemicals on disease related biological systems. Genomics detects genetic variation, inherited or acquired, and transcriptomics detects changes in gene expression as a result of treatment. Proteomics identifies the abundance of proteins, their modification and interaction while metabolomics identifies downstream biochemical responses. Epigenomic analysis provides additional data on DNA methylation, chromatin accessibility and regulatory changes.

In this regard, artificial intelligence helps them to be analysed together, even if they are different in size, form and dimension. Coordinated molecular signatures can be discovered by deep-learning and bioinformatics models, which might not be visible in any single layer of data (Thamminaina & Shinde Rutuja, 2026). These signatures could aid the identification of biomarkers linked to disease subtypes, phytochemical sensitivity, toxicity, and/or therapeutic response. In the field of precision oncology, likewise, the integration of multi-omics and radiomics has been shown to enhance patient stratification and prognosis modelling (Camps et al., 2025).

To validate the mechanism, the computations have to be correlated with measurable effects on the biology. Target discovery can be assisted by AI to match genomic alterations with structurally similar compounds and even druggable proteins (Li et al 2026). Phytochemical exposure may lead to a reversal of the disease-associated transcriptomic or proteomic signature, which may be more convincing than docking.

For predicting genes that drive a phytochemical response, AI-driven CRISPR platforms can be used to determine if predicted genes are causally involved. This may help in the selection of the biomarker, optimisation of formulations, dose stratification and reproducibility of precision Ayurvedic therapeutics. Table 2 shows a summary of computation tools and omics tools employed in the validation of phytochemical targets.

Table 2. Computational and Multi-Omics Tools for Phytochemical–Target Validation

Approach	Data type	Main role	Validation output	Key limitation	References
Molecular docking	Protein structures and phytochemical ligands	Predicts binding orientation and affinity	Ranked compound–target interactions	Limited representation of biological dynamics	Terkimbi et al. (2026)
Molecular dynamics	Protein–ligand complexes	Evaluates interaction stability over time	Binding stability and conformational changes	High computational demand	Li et al. (2026)
QSAR modelling	Molecular descriptors and bioactivity data	Predicts biological activity	Activity scores for untested compounds	Dependent on training-data quality	Vora et al. (2025)
ADMET prediction	Chemical structures and pharmacokinetic	Assesses developability and safety	Bioavailability and toxicity profiles	Predictions require experimental	Gholap et al. (2026)

	data			confirmation	
Genomics	DNA variants and disease-associated genes	Identifies molecular targets and responder groups	Actionable genomic targets	Population-specific bias	Mahmud and Banerjee (2026)
Transcriptomics	Gene-expression profiles	Detects pathway changes after treatment	Differentially expressed genes	Sensitive to tissue and timing effects	Camps et al. (2025)
Proteomics	Protein abundance and interaction data	Confirms target and pathway modulation	Protein signatures and network changes	Limited coverage of low-abundance proteins	Thamminaina and Shinde Rutuja (2026)
Metabolomics	Metabolite profiles	Measures downstream biochemical responses	Metabolic biomarkers and pathway shifts	Strongly affected by diet and environment	Vora et al. (2025)
Epigenomics	DNA methylation and chromatin data	Identifies regulatory effects of phytochemicals	Epigenetic response signatures	Causal interpretation remains difficult	Mostafa et al. (2026)
CRISPR validation	Gene-editing and functional assays	Tests the causal involvement of predicted targets	Confirmed gene–response relationships	Off-target effects and delivery barriers	Thomson et al. (2026)

2.7 Prakriti, Pharmacogenomics, and Personalised Ayurvedic Therapeutics

According to Prakriti, each person has a set of more or less fixed constitutional characteristics that can be used to classify individuals, and are used to guide diet, lifestyle, disease evaluation and selection of therapy. Evidence in favour of these phenotypes relating to reproducible genomic, transcriptomic, metabolic, physiological, or clinical features is necessary for their integration in precision medicine. Molecular characterisation, in this case, could thus transform Prakriti from a descriptive concept to a valid classification tool and remain in the Ayurvedic context.

Pharmacogenomics is the study of genetic variations that affect drug metabolism, transport, molecular targets, efficacy and toxicity. AI can be used to process large genotype–phenotype databases and uncover the non-linear relationships between genetic variants and treatment effects (Srivastav et al., 2025). This may be the case for constitution-associated molecular patterns and how they are going to react to certain phytochemicals or polyherbal combinations.

Genomic, biochemical, and clinical data can be combined on the same platform to identify patient subgroups that have different treatment needs, using the biomarkers (Thamminaina & Shinde Rutuja, 2026). These algorithms can then predict the likelihood of benefit, adverse effects, or clinically-relevant interactions with treatment. The concept of personalised oncology demonstrates the use of genomic abnormalities in decision-making for targeted treatment options and monitoring response (Sheikh et al., 2025).

Precision medicine using AI has the potential to enhance the selection of dosages, taking into account metabolic capacity, organ function, comorbidities, co-medications, and molecular biomarkers (Liu & Kuo, 2026). Standardised Prakriti Assessment, wide population databases, validated biomarkers, prospective trials, and interpretable models are, however, required for clinical adoption. Hence, there is a need to integrate Constitutional classification with molecular evidence and not view either one as a standalone system. The framework of Prakriti-informed personalised Ayurvedic treatment is presented in Figure 3.

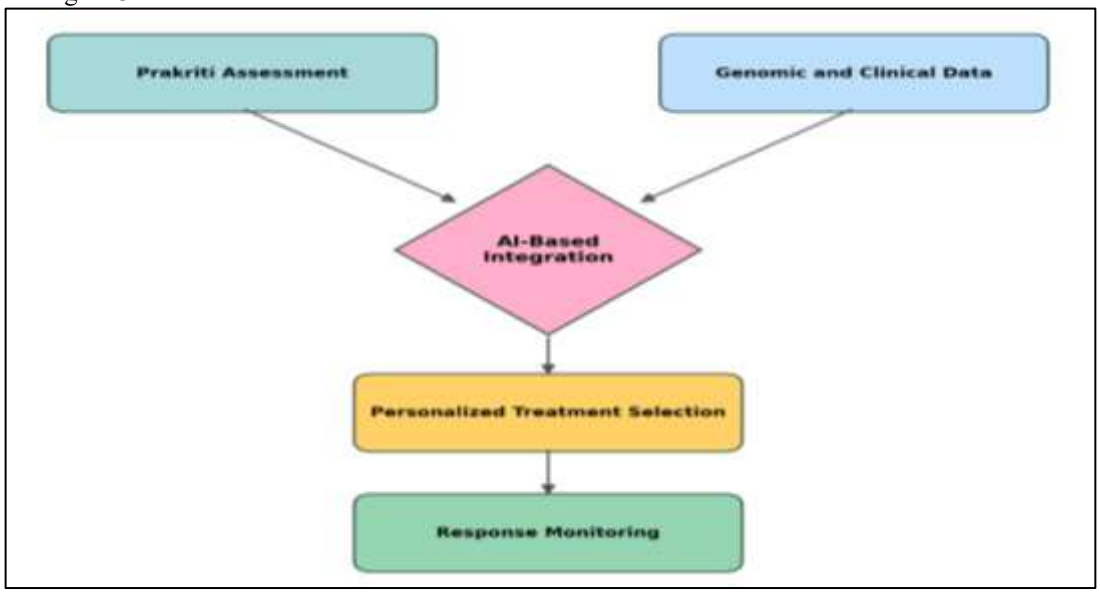

Figure 3. Prakriti-informed precision Ayurvedic therapeutics

2.8 Translational Challenges, Regulatory Considerations, and Future Directions

The challenges of clinical translation include issues with data quality, standardisation, and regulatory readiness, which hinder the application of AI in Ayurvedic drug discovery. Earlier collected data might be poorly annotated for phytochemicals, may use different botanical names, may have different experimental conditions, and may have limited variability of populations. Such data can lead to unreliable predictions from the models, unrealised biases or poor out-of-sample performance.

Algorithmic interpretability becomes even more crucial when the results of the computation affect the selection of the target, optimisation of the dose or patient stratification. AI-powered drug development processes should enable traceability of the inputs supplied, the compounds predicted, the molecular targets reached and the therapeutic choices made (Mandar, 2026). Independent external validation is also necessary, as good internal performance does not imply biological validity and clinical generalizability.

The research on precision-therapy suggests that a model built from static or limited datasets may not accurately reflect the molecular diversity and resistance of patients, leading to lower reliability in the model. The study of precision-therapy has shown that models created from static or limited data sets may not accurately represent the molecular diversity and resistance of patients, reducing the reliability of the model. Model calibration and clinical relevance may be enhanced by longitudinal clinical data and real-world evidence. Smart delivery platforms can improve the stability, targeting and controlled release of phytochemicals, but they will need to be regulated for their own materials, manufacturing, biodistribution and toxicity (Bae et al., 2025).

Privacy, informed consent, genomic discrimination, algorithmic bias, equitable access and accountability for AI-supported decisions are all issues that require ethical governance. Clear guidelines for clinical responsibility and data protection are also necessary for pharmacogenomic applications (Srivastav et al., 2025). The interoperability of databases, interpretable models, future validation, pharmacovigilance, transparent regulatory bodies, and safeguarding of traditional knowledge are necessary for future advances. The main requirements for clinical translation of the AI-based Ayurvedic therapeutics are presented in Table 3.

Table 3. Translational Requirements for Precision Ayurvedic Drug Development

Domain	Current challenge	Potential consequence	Recommended action	References
Botanical standardization	Variable species identity, cultivation, harvesting, and processing	Inconsistent phytochemical composition and efficacy	Apply genetic authentication, chemical fingerprinting, and batch testing	Gupta et al. (2026)
Data quality	Fragmented and poorly annotated datasets	Unreliable model training and weak reproducibility	Develop curated, interoperable phytochemical and genomic databases	Mandar (2026)
Algorithmic transparency	Black-box predictions and limited interpretability	Reduced clinical trust and regulatory acceptance	Use explainable AI and traceable decision pathways	Srivastav et al. (2025)
Experimental validation	Heavy reliance on in silico findings	Uncertain biological and therapeutic relevance	Confirm predictions through biochemical, cellular, and animal studies	Riaz et al. (2026)
Clinical validation	Limited prospective human evidence	Restricted translation into practice	Conduct biomarker-guided clinical trials in diverse populations	Liu and Kuo (2026)
Population diversity	Underrepresentation of genomic and constitutional variation	Biased predictions and reduced generalizability	Include diverse ethnic, genomic, and Prakriti groups	Sheikh et al. (2025)
Regulatory oversight	Unclear standards for AI-enabled phytotherapeutics	Delayed approval and inconsistent quality control	Establish product-specific regulatory and reporting frameworks	Mao et al. (2025)
Pharmacovigilance	Limited post-marketing safety surveillance	Delayed detection of adverse effects and interactions	Integrate digital monitoring and real-world safety reporting	Spanakis et al. (2025)
Ethical governance	Privacy, consent, bias, and accountability concerns	Loss of trust and inequitable access	Adopt transparent governance and data-protection standards	Srivastav et al. (2025)
Traditional knowledge protection	Risk of biopiracy and inappropriate commercialisation	Loss of community rights and benefit sharing	Enforce attribution, consent, and equitable benefit-sharing mechanisms	Khandelwal et al. (2026)

CONCLUSION

This review confirms that an AI-enabled precision Ayurvedic drug development can be a credible framework using the convergence of AI, phytochemical science, genomic target identification, network pharmacology and multi-omics. AI has the potential to speed up the identification of compounds, predictions of activity, target prioritisation, and lead optimisation, and diminish the need for lengthy conventional screening. Network-based approaches are particularly well-suited for the study of Ayurvedic formulations since they can describe the various interactions among the components of a formulation and the various targets that the formulation may affect. Mechanistic interpretation, biomarker discovery and patient stratification may be enhanced by genomic, transcriptomic, proteomic, metabolomic and epigenomic data. Pharmacogenomics based on prakriti can also help with personalised medicine in conjunction with molecular signatures that can be reproduced, if the classifications are based on the constitution. The lack of botanical standardisation, incompleteness of data, use of experimental data that is not validated, the opacity of the algorithms, the bias of the study population, and the unclear regulatory process all fall short of clinical translation. The next steps are the development of a curated interoperable database, an interpretable model, laboratory validation, prospective clinical trials, pharmacovigilance, and safeguarding traditional knowledge. A translational approach is therefore coordinated and can be harnessed to transform Ayurvedic wisdom into precision therapeutics that are safer, standardised, mechanistically validated and clinically applicable.

REFERENCES

1. Abdallah, E. M., Alhudhaibi, A. M., Dahab, M., Al Noman, A., Sharma, P. D., Taha, T. H., & Nawaz, M. (2026). The WHO priority list of antibiotic-resistant bacteria: challenges and opportunities for next-generation antimicrobial development. Frontiers in Pharmacology, 17, 1699987.
2. Assi, R. A., Saktiawati, A. M. I., Kurnaz, I. A., Lobine, D., Anywar, G., Cloete, K. J., ... & Enany, S. (2026). Sustainable Strategies in Tuberculosis Management: Bridging Ethnobotanical Pharmacology, Advanced Drug Delivery, and AI-Driven Innovation. Journal of Evidence-Based Medicine, 19(1), e70121.
3. Bae, H., Ji, H., Konstantinov, K., Sluyter, R., Ariga, K., Kim, Y. H., & Kim, J. H. (2025). Artificial intelligence-driven nanoarchitectonics for smart targeted drug delivery. Advanced Materials, 37(42), e10239.
4. Camps, J., Jiménez-Franco, A., García-Pablo, R., Joven, J., & Arenas, M. (2025). Artificial intelligence-driven integration of multi-omics and radiomics: A new hope for precision cancer diagnosis and prognosis. Biochimica et biophysica acta (BBA)-Molecular basis of disease, 1871(6), 167841.
5. Cui, G., Li, M., Guo, W., Gao, M., Zhu, Q., & Liao, J. (2025). AI-driven network pharmacology: Multi-scale mechanisms of traditional Chinese medicine from molecular to patient analysis. Computational and Structural Biotechnology Journal, 27, 5087.
6. Devlet, A., & Işık, M. (2026). Harnessing and Preserving the Genetic Diversity of Medicinal Plants: A Comprehensive Approach to Conservation, Climate Adaptation, and Drug Discovery. In Genetic Diversity in Medicinal Plants: Challenges, Threats, and Future Applications (pp. 395-427). Singapore: Springer Nature Singapore.
7. Dohre, P. D., Verma, V. S. V., Singh, N. S., Singh, N. S., & Kumar, D. K. (2026). Phytopharmacology in the Nanotech Era: Bridging Natural Compounds with Pharmaceutical Nanocarriers. Journal of Pharmacology, Genetics and Molecular Biology, 45-67.
8. Garg, P., Singhal, G., Kulkarni, P., Horne, D., Salgia, R., & Singhal, S. S. (2024). Artificial intelligence–driven computational approaches in the development of anticancer drugs. Cancers, 16(22), 3884.
9. Gholap, A. D., Khuspe, P. R., & Mane, D. V. (2026). Artificial intelligence-driven discovery of anticancer phytochemicals: from plants to lead compounds. In Emerging Trends in Phytotherapy of Cancer (pp. 441-460). Academic Press.
10. Ghosh, S., Singha, V., Datta, S., Singha, P. S., & Ghosh, D. (2025). A current review on the development of antimicrobial drugs from bioactive phytocompounds using artificial intelligence. MGM Journal of Medical Sciences, 12(1), 155-165.
11. Gupta, A., Soni, D., Chauhan, D. N., Kulshrestha, M. K., & Chauhan, N. S. (2026). Quality Approaches for Phytochemicals. In Phytoceuticals for Sustainable Medication (pp. 173-196). Singapore: Springer Nature Singapore.
12. Gupta, M. K., Pattnaik, S., & Sudandiradoss, C. (2025). Artificial intelligence driven based diagnostics with combined surgical and non-surgical management of uterine fibroids: a narrative review. Middle East Fertility Society Journal, 30(1), 64.
13. Hampel, H., Vergallo, A., Perry, G., Lista, S., & Alzheimer Precision Medicine Initiative (APMI). (2019). The Alzheimer's precision medicine initiative. Journal of Alzheimer's Disease, 68(1), 1-24.
14. Ishtyaq Mahmud, M., & Banerjee, T. (2026). Artificial Intelligence in genomics: a comprehensive survey of methods, resources, challenges, and prospects. Briefings in Bioinformatics, 27(3), bbag229.
15. Junaid, M. A. L. (2025). Artificial intelligence-driven innovations in biochemistry: A review of emerging research frontiers. Biomolecules and Biomedicine, 25(4), 739.
16. Karthikeyan, M., Mehta, A., Kumar, S. S., Mohan, H., & Usha, B. (2025). Safety, Dosage, and Regulatory Aspects in the Use of Phytochemicals. In Medicinal Plants and Their Bioactives in Human Diseases (pp. 207-233). Cham: Springer Nature Switzerland.
17. Khamrayev, K. (2025, December). AI-Driven Drug Discovery: Accelerating the Path to New Therapies. In 2025 3rd International Conference on IoT, Communication and Automation Technology (ICICAT) (pp. 1-8). IEEE.
18. Khan, M. S., Saeed, M., Arham, M., Zafar, I., Hussian, M., Jamal, A., ... & Kang, K. S. (2026). Next-Generation Artificial Intelligence Strategies for Mechanistic Cancer Target Discovery and Drug Development: A State-of-the-Art Review. International Journal of Molecular Sciences, 27(9), 4028.

19. Khandelwal, P., Sandrepogu, J., Tiwari, S. K., Chauhan, S., Bairwa, R., Sharma, H., ... & Gangurde, R. (2026). AI–Ayurveda Convergence: Reimagining Traditional Wisdom Through Ethical Digital Intelligence. Journal of Health Synapse, 30-40.
20. Latif, R., & Nawaz, T. (2025). Medicinal plants and human health: A comprehensive review of bioactive compounds, therapeutic effects, and applications. Phytochemistry Reviews, 1-44.
21. Li, D., Shi, S., Yu, Z., Xu, P., & Zhang, C. (2026). AI accelerate the identification of druggable targets by 3D structures of proteins and compounds. npj Precision Oncology, 10(1), 133.
22. Liu, H., Ma, Y., Chen, W., Gu, X., Sun, J., & Li, P. (2025). Strategies for the drug development of cancer therapeutics. Frontiers in Pharmacology, 16, 1656012.
23. Liu, Z. Y., & Kuo, C. F. (2026). Artificial Intelligence-Driven Personalised Medicine. Hand Clinics.
24. Mandar, B. K. (2026). Artificial Intelligence–Driven Novel Drug Discovery: Target Identification to Translational Impact. Journal of Integrative and Translational Biomedicine, 1(1), 09-14.
25. Mao, Y., Shangguan, D., Huang, Q., Xiao, L., Cao, D., Zhou, H., & Wang, Y. K. (2025). Emerging artificial intelligence-driven precision therapies in tumor drug resistance: recent advances, opportunities, and challenges. Molecular cancer, 24(1), 123.
26. Mostafa, M. A., Abdellatif, A. A., & Omar, M. A. (2026). Epigenetic Mechanisms of Natural Compounds. In Bridging Traditions for a New Era in Personalized Natural Medicine (pp. 147-174). CRC Press.
27. Muthuraj, R., & Chandrasekaran, J. (2026). Nature meets machine: the AI renaissance in natural product drug discovery. Natural Products and Bioprospecting, 16(1), 37.
28. Odah, M. (2025). Artificial intelligence meets drug discovery: A systematic review on ai-powered target identification and molecular design.
29. Paerhati, Y., Aikebaier, A., Dilimulati, D., Baishan, A., Yusufujiang, N., Qiu, X., ... & Zhou, W. (2026). Rethinking nature's pharmacy: AI era and natural product drug discovery. Pharmaceuticals, 19(2), 301.
30. Pandey, S., & Pant, P. (2026). Climate Change and the Future of Healing: Tracking Genetic Erosion and Phytochemical Shifts in Medicinal Plants. In Genetic Diversity in Medicinal Plants: Challenges, Threats, and Future Applications (pp. 63-87). Singapore: Springer Nature Singapore.
31. Patel, T., Rohit, P., Mahavar, D., & Parmar, H. (2026). AI-Driven Reverse Pharmacology & Accelerated Drug Repurposing Using Ancient Indian Manuscripts–A Comprehensive Review. Biopress Journal of Advanced Pharmacology (BJAP), 2(03), 42-66.
32. Riaz, M. U., Naeem, M. S., Zohaib, M., Ahmad, B., Ijaz, M. T., Tahir, M. U., ... & Kharl, H. A. A. (2026). AI IN TARGET IDENTIFICATION AND VALIDATION. PharmA AI: Revolutionizing Drug Discovery and Healthcare with Artificial Intelligence.
33. Sheikh, R., Dean, C. J., Akhlaq, M., Naveed, S. A., ur Rehman, A., Hamza, A., ... & Iram, M. (2025). AI-Driven Personalized Cancer Treatment: Integrating Genomic Data for Targeted Therapy Decisions. Pak-Euro Journal of Medical and Life Sciences, 8(3), 609-620.
34. Spanakis, M., Tzamali, E., Tzedakis, G., Koumpouzi, C., Pediaditis, M., Tsatsakis, A., & Sakkalis, V. (2025). Artificial intelligence models and tools for the assessment of drug–herb interactions. Pharmaceuticals, 18(3), 282.
35. Srivastav, A. K., Mishra, M. K., Lillard Jr, J. W., & Singh, R. (2025). Transforming pharmacogenomics and CRISPR gene editing with the power of artificial intelligence for precision medicine. Pharmaceutics, 17(5), 555.
36. Srivastava, M., Nandan, S., Zaidi, A., Samani, A. S., Shukla, V., Aslam, H., ... & Shanker, K. (2025). Artificial intelligence driven applications in analytical chemistry, drug discovery, and food science: advancements, outlook, and challenges. ChemistrySelect, 10(16), e202404446.
37. Terkimbi, S. D., Mujinya, R., Kayanja, K. L., Sunday, B. Y., Dangana, R. S., Paul-Chima, U. O., ... & Kibirige, J. (2026). Integrative network pharmacology and molecular docking approaches in herbal medicine research. a systematic review of applications, advances, and translational potential. F1000Research, 14, 1384.
38. Thamminaina, A., & Shinde Rutuja, P. (2026). Artificial Intelligence–Driven Identification of Biomarkers for Precision Medicine Advancements Through Bioinformatics in Healthcare Applications. Artificial Intelligence and Machine Learning in Neurology, 2, 555-579.
39. Thomson, T., Li, G., Strilchuk, A., Cui, H., Wang, B., & Li, B. (2026). Harnessing artificial intelligence to advance CRISPR-based genome editing technologies. Nature Reviews Genetics, 27(3), 212-230.
40. Upasani, S. A. (2025). Scope of Artificial Intelligence in Healthcare Systems with Contemporary and Ayurvedic Perspective: A Narrative Review. Indian Journal of Ayurveda and Integrative Medicine KLEU, 6(2), 94-102.
41. Varghese, R., Shringi, H., Efferth, T., & Ramamoorthy, S. (2025). Artificial intelligence driven approaches in phytochemical research: trends and prospects. Phytochemistry Reviews, 24(5), 3649-3664.
42. Vora, N., Shah, S., Patel, P., & Shah, M. (2025). Artificial intelligence and multi-omics in drug discovery: A deep learning-powered revolution. Cure & Care, 100011.
43. Ydyrys, A., Nurtayeva, M., & Yerkebayeva, M. (2025). Advancing Medicinal Plant Research with Artificial Intelligence: Key Applications and Benefits.
44. Yin, Z., Chen, C., Wu, X., Luo, W., Quaresma, P., & Dai, J. (2026). AI-Driven Plant-Derived Anti-Infectives: Integrating Traditional Wisdom into Precision Medicine Against AMR. Life, 16(4), 540.