Received: 17 Oct 2026	Revised: 15 Nov 2026	Accepted: 15 Dec 2026

Review Article

AJDP
Nature has the Power to Heal

ISSN: 3048-5614

"ARTIFICIAL INTELLIGENCE AND CHEMINFORMATICS IN DRAVYAGUNA RESEARCH: CURRENT APPLICATIONS, DATA RESOURCES AND LIMITATIONS"

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FUNDING INFORMATION:
Not Applicable

How to cite this article:
Abhay Gandhi, "Artificial intelligence and cheminformatics in Dravyaguna research: current applications, data resources and limitations" Asian Journal of Dravyaguna and Pharmacology. 2026;3(4):12-15.
Sri. 2026.1006.ajdp.04.04

ABSTRACT
Artificial intelligence (AI) and cheminformatics are increasingly applied to Ayurvedic pharmacology. Curated phytochemical databases, target-prediction tools, protein interaction networks and machine-learning models make it possible to model the chemistry and actions of Ayurvedic drugs at a scale not previously possible. This review describes the main data resources and applications relevant to Dravyaguna, illustrates them with examples, and examines their limitations. IMPPAT 2.0 links 4,010 Indian medicinal plants to 17,967 phytochemicals and their therapeutic uses. PhytoMolecularTasteDB links Ayurvedic plants to taste-active molecules, and the Traditional Knowledge Digital Library has digitised classical formulations, a resource used mainly for patent protection. Machine learning has recovered the three extreme Prakriti types from phenotypic traits in a validated study. Advances outside Ayurveda show what is possible: a deep-learning model identified halicin, a structurally novel antibiotic, after screening large chemical libraries, and AlphaFold made accurate protein structure prediction widely available. Five limitations stand out. Databases describe what a plant may contain rather than what a classical preparation delivers. Predicted properties are treated as facts. Training data are biased towards well-studied compounds and targets. Models are rarely validated prospectively. And classical knowledge is not yet available in structured, machine-readable form. We recommend building structured digital representations of classical Dravyaguna properties, linking them to chemically characterised preparations, requiring prospective experimental validation of predictions, and adopting open, versioned data standards. Used in this way, AI could help test Dravyaguna concepts at scale rather than simply generate untested hypotheses.

KEYWORDS: Artificial intelligence, machine learning, cheminformatics, IMPPAT, Ayurveda, Dravyaguna, databases, drug discovery, Prakriti

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INTRODUCTION

Dravyaguna describes thousands of drugs by a small set of properties – rasa, guna, virya, vipaka, prabhava and karma – and combines them into formulations according to explicit principles. This is, in effect, a large, structured knowledge system, and it invites computational treatment. At the same time, cheminformatics and artificial intelligence (AI) have transformed drug discovery: curated chemical databases, target-prediction tools, interaction networks and machine-learning models now allow researchers to model the chemistry and actions of plants at scale.[1–3] Recent advances outside traditional medicine, such as deep-learning discovery of antibiotics[4] and accurate prediction of protein structures,[5] show how powerful these tools can be.

This review describes the main data resources and computational applications relevant to Dravyaguna, illustrates them with examples, and examines the limitations that currently restrict their value.

METHODS

This is a narrative review. We examined databases, tools and published applications of cheminformatics and machine learning relevant to Ayurvedic drugs and concepts, together with landmark AI studies in drug discovery.

DATA RESOURCES

Table 1 lists key resources.

Table 1. Data resources relevant to computational Dravyaguna research.

Resource	Content	Use and caution
IMPPAT 2.0	4,010 Indian medicinal plants, 17,967 phytochemicals, 1,095 therapeutic uses[1]	Plant–compound–use links; compounds are not quantified and not specific to preparations
TCMSP	Systems pharmacology database of Chinese herbs with predicted ADME properties[6]	Predicted bioavailability; thresholds often used uncritically
PhytoMolecularTaste DB	431 Ayurvedic plants linked to 438 taste-active molecules[7]	Links rasa to chemistry[8]
Traditional Knowledge Digital Library	Digitised classical formulations from Ayurveda, Unani, Siddha and Yoga; used by patent offices[9]	Built for patent protection; access restricted
SwissTargetPrediction	Similarity-based prediction of protein targets[2]	Predictions require experimental confirmation
STRING	Protein–protein association networks[3]	Biased towards well-studied proteins; version-dependent

The Traditional Knowledge Digital Library deserves particular mention. Developed by India's Council of Scientific and Industrial Research, it translated classical formulations into several languages and classified them so that patent examiners could find prior art, and access agreements with the European and other patent offices led to the withdrawal or rejection of many applications based on traditional knowledge.[9] It shows that classical Ayurvedic knowledge can be structured digitally at scale, although it was not designed for research use.

APPLICATIONS

Classifying and predicting from classical properties

Statistical analysis of a taste–action database of 183 Ayurvedic plants showed that taste significantly predicted recorded actions, suggesting that classical properties can serve as features in predictive models.[8] Linking plants to their taste-active molecules[7] provides a bridge between classical properties and chemistry that machine-learning models could exploit.

Prakriti

In a study of 147 healthy individuals of the three extreme Prakriti types from a genetically homogeneous population, unsupervised clustering of phenotypic traits recovered three groups that matched the Prakriti classes, and supervised models classified individuals accurately and were validated in a second population.[10] This demonstrates that a central Ayurvedic concept can be operationalised with machine learning, which opens the way to studying how Prakriti relates to drug response.

Target prediction and network pharmacology

The most common application in Ayurveda research is network pharmacology, in which constituents from databases are mapped to predicted targets and interaction networks.[1–3] As discussed in a companion review, this approach is valuable for generating hypotheses but is prone to problems of preparation mismatch, promiscuous compounds and lack of validation.[11,12]

Lessons from AI in drug discovery

Two landmark studies show what AI can achieve when trained and validated rigorously. A deep neural network trained on experimental growth-inhibition data identified halicin, a structurally novel antibiotic active against several drug-resistant pathogens and effective in mouse infection models, and further predictions from a screen of the ZINC15 library yielded additional structurally distinct antibacterial compounds.[4] AlphaFold predicted protein structures with accuracy approaching experimental methods.[5] In both cases, success depended on large, high-quality training data and on experimental confirmation of predictions.

LIMITATIONS

Table 2 summarises the main limitations of current computational work in Dravyaguna.

Table 2. Limitations of AI and cheminformatics in Dravyaguna research.

Limitation	Explanation
Preparation mismatch	Databases list constituents a plant may contain, not what a classical preparation delivers or in what amounts[1,13]
Predicted values treated as facts	Predicted ADME properties and targets are used as inputs without validation[2,6]
Data bias	Well-studied compounds and proteins dominate, so they appear important regardless of the question[3,12]
Lack of validation	Predictions are rarely tested prospectively in experiments or clinical studies[11]
Unstructured classical knowledge	Classical properties, indications and formulation rules are not available in open, structured, machine-readable form
Identity uncertainty	Data may be attached to plant names whose botanical identity is disputed
Reproducibility	Database versions and model settings are often not reported

The contrast with successful AI studies is instructive. Halicin was discovered by a model trained on measured antibacterial activity and confirmed in the laboratory.[4] Most Ayurvedic applications, by contrast, combine predicted data with predicted data and stop before experimental testing. AI amplifies the quality of its inputs; with poor or unvalidated inputs it produces confident but unreliable outputs.

RECOMMENDATIONS

- Create an open, structured, machine-readable database of classical Dravyaguna properties (rasa, guna, virya, vipaka, prabhava, karma), with textual sources and variant readings.
- Link classical drugs to authenticated botanical identities and to chemically characterised classical preparations.[13]
- Generate high-quality experimental data on classical preparations for model training, rather than relying on predicted values.
- Require prospective experimental validation of AI predictions before claims of efficacy.[4,11]
- Report data sources, versions, model settings and code for reproducibility.
- Use AI to test Dravyaguna hypotheses, such as whether rasa or virya predicts targets or physiological effects.[8]

A DRAVYAGUNA PERSPECTIVE

Dravyaguna is a property-based system for predicting the actions of drugs and combinations, which is precisely the kind of problem machine learning addresses. The opportunity is not to replace classical reasoning with algorithms but to test it: to ask, with data from thousands of drugs, how well classical properties predict measured actions, where they fail, and what they add to chemical information. Answering these questions would strengthen both Ayurveda and computational pharmacology.

LIMITATIONS OF THIS REVIEW

The field is changing rapidly, and new tools, including large language models applied to classical texts, may not be covered. This review is narrative

rather than systematic.

CONCLUSION

AI and cheminformatics offer Dravyaguna powerful tools for organising knowledge, generating hypotheses and potentially discovering new drugs. Their current use in Ayurveda is limited by mismatches between databases and classical preparations, reliance on predicted data, bias and a lack of validation. Structured classical knowledge, high-quality experimental data and prospective validation would allow these tools to test, rather than merely decorate, the classical science of drugs.

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