

**PHYTOCHEMICAL FINGERPRINTING FOR EARLY DETECTION OF TOXICITY IN
MEDICINAL PLANTS: AN INTEGRATED DRAVYAGUNA AND MODERN
TOXICOLOGICAL PERSPECTIVE****Dr. Priya Singh^{*1}, Dr. Sachin Kumar Singh²**¹Associate Professor, Department of Dravyaguna Vigyan, Shri Krishna Ayurvedic Medical College & Hospital Rauna Khurd, Chhapra, Varanasi, Uttar Pradesh Pin -221101.²MBBS, MD (PG-JR-I), Department of Forensic Medicine & Toxicology, SRMS-IMS, Bareilly, UP.***Corresponding Author: Dr. Priya Singh**

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ABSTRACT

Medicinal plants possess complex and dynamic phytochemical profiles that contribute to their therapeutic activity as well as, in certain circumstances, their toxicological potential. Variations in plant species, geographical origin, season, cultivation conditions, harvesting stage, processing and storage can alter the qualitative and quantitative composition of secondary metabolites. Conventional quality control approaches based on individual marker compounds may therefore be insufficient to represent the overall chemical complexity of medicinal plants. Phytochemical fingerprinting, using chromatographic and spectrometric techniques such as TLC/HPTLC, HPLC, GC-MS, LC-MS/MS and NMR, provides a broader approach for characterizing the chemical profile of herbal materials. WHO recognizes chromatographic fingerprinting and spectroscopic/spectrometric approaches among methods used for quality control of herbal materials and products. The integration of phytochemical fingerprints with toxicological markers may facilitate the early recognition of potentially unsafe samples before clinical toxicity becomes evident. Evidence from medicinal plants containing aristolochic acids demonstrates how chromatographic fingerprinting and multivariate analysis can assist in detecting toxic constituents, while mass-spectrometric approaches have been used for characterization of other toxic phytochemical groups such as pyrrolizidine alkaloids. This review discusses the conceptual relationship between Ayurvedic Dravya identification, Rasa-Panchaka, phytochemical markers and modern toxicological profiling, and proposes an integrated framework for safety-oriented phytochemical fingerprinting of medicinal plants.

KEYWORDS: Dravyaguna, phytochemical fingerprinting, medicinal plants, herbal toxicity, HPTLC, HPLC, LC-MS/MS, toxicological biomarkers, phytochemical markers, quality control.**INTRODUCTION**

Medicinal plants constitute an important source of therapeutic agents and are extensively used in traditional systems of medicine. Ayurveda recognizes medicinal substances not merely on the basis of botanical identity but through an integrated assessment involving Dravya, Rasa, Guna, Virya, Vipaka and Karma. Correct identification and appropriate selection of a medicinal plant are therefore fundamental to therapeutic efficacy and safety.^[1]

Modern herbal quality control has traditionally emphasized botanical identification, physicochemical

parameters and selected chemical markers. However, a medicinal plant contains hundreds of chemically diverse constituents, and the concentration of these constituents can vary considerably. Consequently, the measurement of a single marker may not always adequately represent the complete chemical identity or safety profile of the drug.^[2,3]

The European Medicines Agency recognizes the use of active and analytical markers for quality assessment and recommends appropriate chromatographic fingerprinting where relevant to demonstrate consistency and stability of herbal preparations. This becomes particularly

important from a toxicological perspective. A plant may contain therapeutically useful constituents together with potentially harmful compounds. Moreover, adulteration, substitution, environmental contamination and variation in cultivation or processing may alter its chemical profile.^[2,4]

Therefore, phytochemical fingerprinting can be considered a bridge between botanical identification and toxicological safety assessment.^[5]

Major advantages of Phytochemical Fingerprinting

- Authentication of medicinal plant material
- Detection of substitution and adulteration
- Assessment of batch-to-batch consistency
- Monitoring of geographical and seasonal variation
- Detection of changes during processing and storage

- Identification of potentially toxic constituents
- Comparison of genuine and abnormal samples
- Generation of chemical profiles for quality databases.^[3,6,7]

Ayurvedic Perspective: Dravya Identification and Safety

Ayurvedic Dravyaguna emphasizes the identification and characterization of medicinal substances through multiple attributes.^[1,8]

a. Classical framework

Dravya → Rasa → Guna → Virya → Vipaka → Karma

b. Modern analytical science provides another layer

Botanical identity → Phytochemical fingerprint → Marker compounds → Toxic constituents → Biological/toxicological response.

These two approaches need not be viewed as competing systems. Rather, they can be integrated.

Classical Parameter	Possible modern analytical correlation
Dravya	Botanical/molecular authentication
Rasa	Phytochemical composition influencing sensory characteristics
Guna	Physicochemical and pharmacological characteristics
Virya	Pharmacological activity and bioactive constituent profile
Vipaka	Metabolic transformation and post-absorptive effects—conceptual correlation
Karma	Pharmacological/toxicological biological response
Shodhana/Sanskara	Changes in chemical fingerprint
Matra	Dose-response and exposure
Desha	Chemotypic/geographical variation
Kala	Seasonal phytochemical variation

This should be presented as a conceptual correlation, rather than claiming that one Ayurvedic parameter is directly equivalent to a modern biochemical measurement.^[8]

Phytochemical Fingerprinting Techniques

1. TLC and HPTLC

TLC/HPTLC is particularly useful for routine herbal authentication because it can provide a visual chemical profile consisting of multiple bands.

The fingerprint can be compared between.

- Authentic and suspected samples
 - Different geographical samples
 - Different harvesting seasons
 - Different batches
 - Processed and unprocessed drugs
- WHO specifically includes TLC/HPTLC among chromatographic approaches used in quality control of herbal material.
 - An unusual band, loss of an expected band, or significant change in fingerprint intensity can trigger secondary investigation using more specific analytical techniques^{6,9}.

2. HPLC and HPLC-DAD Fingerprinting: - HPLC provides a more quantitative and reproducible chromatographic profile.^[2,4]

It can be used for

- Marker quantification
 - Fingerprint generation
 - Identification of abnormal samples
 - Comparison of batches
 - Detection of specific toxic phytochemicals.
- A particularly relevant example is aristolochic acid. Research has demonstrated that HPLC-DAD fingerprinting combined with multivariate analysis could help evaluate the potential presence of aristolochic acids in medicinal herbal samples. The authors also noted that suspected positives require confirmatory analytical approaches such as mass spectrometric hyphenation.^[10]
 - This provides an important model for the concept proposed in this article.

Fingerprint → suspicious chemical pattern → targeted toxic constituent analysis → confirmation → safety decision

3. LC-MS/MS and High-Resolution Mass Spectrometry: - LC-MS/MS provides greater molecular specificity and sensitivity than conventional fingerprinting.^[11]

It is particularly useful for detecting

- Alkaloids
- Glycosides

- c) Phenolics
- d) Toxic metabolites
- e) Pyrrolizidine alkaloids
- f) Aristolochic acid derivatives
- g) Other low-abundance constituents.
- Mass spectrometry has become an important analytical tool for pyrrolizidine alkaloids, which have been associated with hepatotoxic, genotoxic and embryotoxic effects.^[11,12]
- High-resolution LC-MS/MS can additionally support non-targeted profiling, where unknown chemical differences between samples can be investigated rather than limiting analysis to predefined compounds.

4. NMR-Based Fingerprinting: - NMR metabolomics provides a relatively comprehensive representation of metabolites present in a plant extract.^[13,14]

Its potential applications include

- a) Chemo type differentiation,
- b) Authentication
- c) Metabolic profiling
- d) Detection of abnormal samples
- e) Comparison of toxic and non-toxic varieties.

For complex medicinal plants, NMR can therefore complement chromatographic approaches.

5. Factors Responsible for Phytochemical Variation^[7]

The chemical fingerprint of a medicinal plant can be influenced by.

a. Intrinsic factors

- Species
- Variety
- Genetic composition
- Plant part
- Developmental stage

b. Extrinsic factors

- Desha
- Soil
- Temperature
- Rainfall
- Altitude
- Light exposure
- Water availability
- Agricultural practices
- Post-harvest factors
- Collection time
- Drying
- Processing
- Storage
- Moisture
- Temperature
- Packaging

Proposed “Phytochemical Safety Fingerprint” Model

One of the novel aspects of this review can be a proposed model.

PSF – Phytochemical Safety Fingerprint

It may consist of four layers.

Layer 1 – Identity

Botanical + macroscopic + microscopic authentication



Layer 2 – Chemical Fingerprint

TLC/HPTLC/HPLC/GC-MS/LC-MS/NMR



Layer 3 – Toxicological Markers

Known toxic constituents + contaminants + degradation products

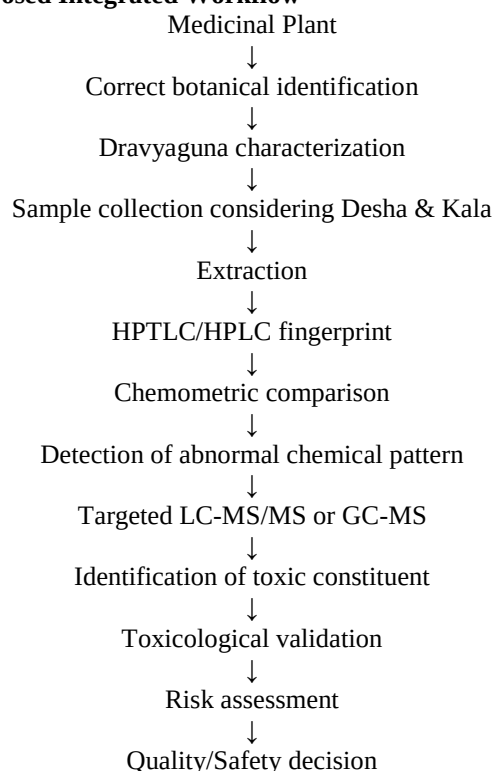


Layer 4 – Biological Confirmation

Cytotoxicity / genotoxicity / hepatotoxicity / nephrotoxicity / other relevant assays

Final output: - Identity + Chemical profile + Toxic-marker profile + Biological response = Safety profile. This could become the distinctive conceptual contribution of your article.

Proposed Integrated Workflow



Challenges and Limitations^[15]

- Although phytochemical fingerprinting has considerable potential, several limitations should be recognized.
- A chemical difference does not automatically indicate toxicity.
- Fingerprinting cannot replace validated toxicological testing.
- Unknown peaks require structural identification.
- Different extraction methods may produce different fingerprints.
- Reference fingerprints need to be standardized.

- Natural phytochemical variability must be distinguished from abnormal contamination.
- Chemo-metric models require appropriate training and validation.
- Toxicity may depend on dose, exposure duration and susceptible individuals.
- Synergistic or antagonistic interactions among constituents may complicate interpretation.
- Thus, fingerprinting should be considered a screening and quality-assurance tool, rather than a standalone toxicity assay.

CONCLUSION

Phytochemical fingerprinting offers an important analytical bridge between medicinal plant identification, chemical standardization and toxicological safety. Rather than relying exclusively on a single marker compound, fingerprinting captures a broader chemical pattern and can reveal deviations associated with species substitution, adulteration, environmental variation, processing or the presence of potentially toxic constituents.^[2,4,6]

Evidence from aristolochic acids demonstrates that chromatographic fingerprinting can be combined with multivariate analysis to screen medicinal herbal materials for toxic chemical signatures, while modern mass spectrometric methods provide increasingly sensitive approaches for targeted detection of toxic phytochemical groups such as pyrrolizidine alkaloids.^[10,11]

From an Ayurvedic perspective, integrating Dravya identification, Rasa-Panchaka, Desha, Kala and Sanskara with modern phytochemical and toxicological techniques offers a promising framework for safety-oriented Dravyaguna research. The proposed Phytochemical Safety Fingerprint may serve as a conceptual model in which chemical profiling acts as an early-warning step, followed by targeted identification and biological toxicological validation.

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