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Original Article

COMPREHENSIVE PHYTOCHEMICAL MAPPING OF INDIAN FLORA: LC–MS/MS-BASED IDENTIFICATION OF BIOACTIVE METABOLITES

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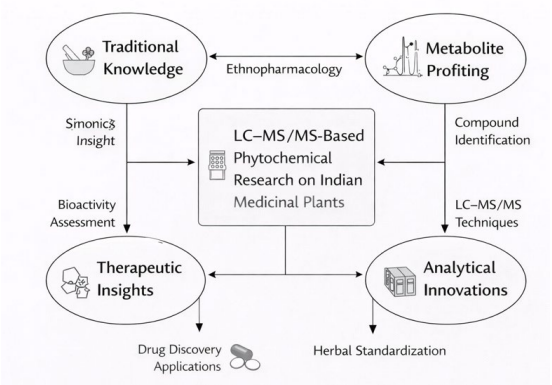
ABSTRACT

Indian medicinal plants constitute a rich source of structurally diverse bioactive metabolites with significant therapeutic relevance. Advances in analytical technologies, particularly liquid chromatography–tandem mass spectrometry (LC–MS/MS), have greatly enhanced the identification and characterization of complex phytochemical profiles. This review critically summarizes published literature on LC–MS/MS-based phytochemical investigations of Indian medicinal plants, focusing on the identification of major classes of secondary metabolites, including flavonoids, alkaloids, phenolic acids, terpenoids, glycosides, and saponins. Evidence from multiple studies demonstrates that LC–MS/MS enables high-resolution metabolite annotation and provides molecular-level insights that support traditional medicinal applications. The review highlights the role of metabolomics-driven approaches in linking ethnopharmacological knowledge with chemical evidence and discusses their significance in drug discovery, quality control, and standardization of herbal formulations.

Keywords: Indian Medicinal Plants, Phytochemical Profiling, LC–MS/MS Analysis, Bioactive Metabolites, Secondary Metabolites, Metabolomics



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Transparency: The authors affirm that this manuscript presents an honest, accurate, and transparent account of the study. All essential aspects have been included, and any deviations from the original study plan have been clearly explained. The writing process strictly adhered to established ethical standards.

INTRODUCTION

India is globally recognized for its extensive medicinal plant diversity and long-standing traditional medical systems. A large proportion of herbal medicines derive their therapeutic efficacy from secondary metabolites such as flavonoids, alkaloids, phenolic acids, terpenoids, and glycosides. While ethnobotanical knowledge provides valuable information on plant usage, scientific validation of these claims requires detailed phytochemical characterization.

Conventional phytochemical screening techniques often fail to capture the full complexity of plant metabolomes. In this context, LC–MS/MS has emerged as a powerful analytical platform capable of resolving structurally diverse metabolites within complex plant matrices. By enabling high-throughput, sensitive, and accurate metabolite identification, LC–MS/MS has become central to modern phytochemical and metabolomics research. This review aims to consolidate existing LC–MS/MS-based studies on Indian medicinal plants and to highlight their contributions to phytochemical mapping and therapeutic understanding.

LC–MS/MS IN PHYTOCHEMICAL RESEARCH

LC–MS/MS combines chromatographic separation with mass-based detection, allowing simultaneous analysis of multiple metabolite classes. Literature reports demonstrate that the use of both positive and negative electrospray ionization modes significantly enhances metabolite coverage. Fragmentation data generated through tandem mass spectrometry further support compound annotation by providing structural information.

Several studies have successfully employed LC–MS/MS to profile complex herbal extracts, revealing metabolites that are often undetectable using traditional analytical approaches. Database-assisted annotation and spectral libraries have further strengthened the reliability of LC–MS/MS-based phytochemical identification.

MAJOR CLASSES OF BIOACTIVE METABOLITES IDENTIFIED

FLAVONOIDS AND PHENOLIC COMPOUNDS

Flavonoids and phenolic acids are among the most frequently reported phytochemicals in LC–MS/MS-based studies of Indian medicinal plants. These compounds are widely associated with antioxidant, anti-inflammatory, cardioprotective, and neuroprotective activities. Their abundance in medicinal plants underscores their importance in redox regulation and cellular protection.

ALKALOIDS

Alkaloids identified through LC–MS/MS analyses exhibit diverse pharmacological properties, including antimicrobial, analgesic, anticancer, and neuroactive effects. Literature evidence suggests that LC–MS/MS is particularly effective in detecting low-abundance alkaloids and distinguishing structurally similar compounds.

TERPENOIDS AND GLYCOSIDES

Terpenoids represent a structurally diverse class of metabolites frequently reported in metabolomics studies. They are associated with anti-inflammatory, anticancer, and antiviral activities. Glycosides, although less abundant, contribute significantly to therapeutic efficacy through their role in bioavailability and biological modulation.

SAPONINS

LC–MS/MS-based studies have also reported the presence of saponins in several Indian medicinal plants. These compounds are known for their immunomodulatory, cytoprotective, and membrane-stabilizing properties, supporting their traditional medicinal applications.

THERAPEUTIC RELEVANCE AND ETHNOPHARMACOLOGICAL CORRELATION

A consistent observation across reviewed studies is the strong correlation between traditionally reported medicinal uses and the presence of pharmacologically relevant metabolites identified by LC–MS/MS. This chemical validation strengthens the credibility of ethnopharmacological knowledge and highlights the value of metabolomics in bridging traditional medicine and modern drug discovery.

Figure 1

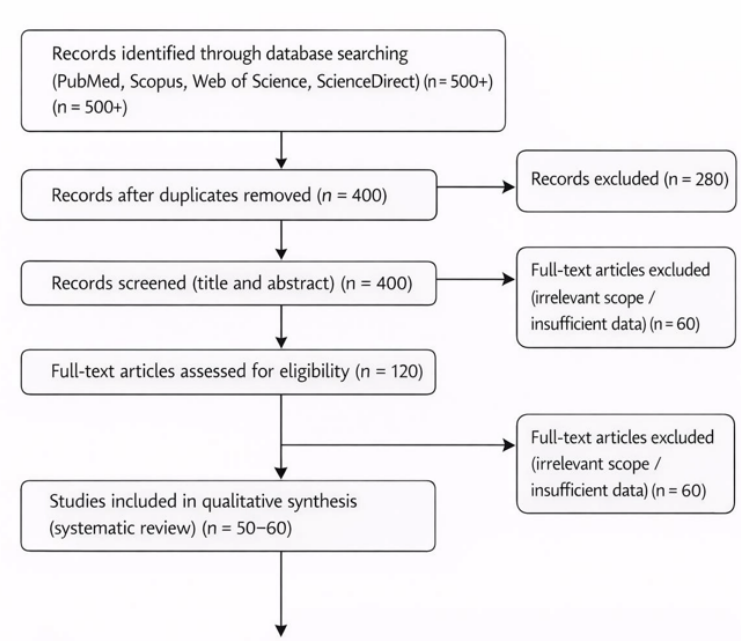

Figure 1 PRISMA Flow Diagram Illustrating the Selection Process of Studies Included in the Systematic Review

Methods:

Literature Search Strategy

A comprehensive literature search was carried out across major scientific databases including PubMed, Scopus, Web of Science, and ScienceDirect. Search terms included combinations of:

"Indian medicinal plants," "LC–MS/MS," "phytochemical profiling," "metabolomics," "bioactive metabolites," and "secondary metabolites."

Only peer-reviewed articles published in English were considered.

Inclusion Criteria

Studies were included if they:

Reported LC–MS/MS-based phytochemical or metabolomic analysis

Focused on Indian medicinal plants

Identified or discussed bioactive secondary metabolites

Were original research articles or high-quality reviews

Exclusion Criteria

Studies were excluded if they:

Did not involve LC–MS/MS analysis

Lacked phytochemical relevance

Were conference abstracts, editorials, or non-peer-reviewed sources

Study Selection Process

Titles and abstracts were screened initially, followed by full-text assessment of eligible studies. Relevant data related to plant species, metabolite classes, analytical approaches, and therapeutic relevance were extracted and synthesized qualitatively.

APPLICATIONS IN DRUG DISCOVERY AND HERBAL STANDARDIZATION

LC–MS/MS-based phytochemical mapping has important implications for natural product research. It facilitates the identification of lead compounds, supports quality control of herbal formulations, and aids in standardization by ensuring chemical consistency. The integration of metabolomics data with biological assays further enhances the translational potential of medicinal plant research.

CHALLENGES AND FUTURE PERSPECTIVES

Despite its advantages, LC–MS/MS-based phytochemical analysis faces challenges such as limited spectral databases for plant metabolites and difficulties in absolute compound identification without reference standards. Future research should focus on expanding metabolite libraries, integrating multi-omics approaches, and linking metabolomic profiles with clinical outcomes to fully exploit the therapeutic potential of Indian medicinal plants.

CONCLUSION

This review highlights the significant contribution of LC–MS/MS-based approaches to the comprehensive phytochemical mapping of Indian medicinal plants. The identification of diverse bioactive metabolites provides molecular support for traditional medicinal claims and advances natural product-based drug discovery. LC–MS/MS-driven metabolomics represents a powerful and indispensable tool for modern herbal research, offering new opportunities for therapeutic innovation and standardization.

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