



Bioactive compounds from medicinal angiosperms: taxonomic insights and pharmacological potential

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ABSTRACT

The Marathwada region of Maharashtra represents a transitional zone of rich floral diversity where traditional knowledge has long emphasized the use of medicinal angiosperms. Despite their ethnobotanical importance, many species remain insufficiently characterized for their phytochemical and pharmacological potential. This study explores five medicinally significant angiosperms from Marathwada viz. *Vitex negundo*, *Argemone mexicana*, *Malvastrum coromandelianum*, *Sphagneticola calendulacea*, and *Rauvolfia tetraphylla* through Gas Chromatography Mass Spectrometry analysis to profile their bioactive compounds and evaluate their pharmacological relevance. GC-MS screening revealed a wide spectrum of secondary metabolites including alkaloids, flavonoids, terpenoids, sterols, and fatty acid derivatives. *V. negundo* was characterized by flavonoids and iridoid glycosides with anti-inflammatory and antioxidant potential. *A. mexicana* exhibited benzophenanthridine alkaloids, well-documented for antimicrobial and analgesic effects. *M. coromandelianum* contained phytosterols and fatty acids supportive of wound-healing and anti-ulcer activities. *S. calendulacea* demonstrated sesquiterpene lactones with anticancer and hepatoprotective prospects, while *R. tetraphylla* yielded indole alkaloids such as reserpine, recognized for antihypertensive and sedative properties. From a taxonomic standpoint, the distinct metabolite profiles provide chemotaxonomic markers that strengthen species delimitation and support systematic classification, particularly in taxa with morphological overlap. The pharmacological insights derived from bioactive compounds reaffirm the ethnomedicinal claims of local communities and highlight their potential for novel drug discovery. This study emphasizes the significance of integrating taxonomy with phytochemical metabolomics to advance both biodiversity documentation and pharmacological research. It also reinforces the need for conservation-driven bioprospecting of medicinal angiosperms in the Marathwada region, ensuring sustainable utilization of these valuable genetic resources.

Keywords: GC-MS, chemotaxonomy, bioactive compounds, pharmacological potential

INTRODUCTION

Medicinal plants have served as the cornerstone of traditional healthcare systems since ancient times and continue to play a vital role in modern pharmacological research. According to the World Health Organization, nearly 80% of the global population relies on plant-based medicines for

primary healthcare, particularly in developing countries. India, being one of the world's richest centers of biodiversity, possesses a vast repository of medicinal flora that has been extensively utilized in traditional systems such as Ayurveda, Siddha, and Unani (WHO, 2013). The Marathwada region of Maharashtra represents a unique phytogeographical transition zone characterized by semi-arid climatic conditions and diverse vegetation. This region supports a wide range of medicinal angiosperms that are traditionally used by local communities for the treatment of inflammation, infections, respiratory disorders, and metabolic diseases. However, despite their extensive ethnobotanical use, many of these species remain underexplored in terms of their phytochemical composition and pharmacological properties.

Recent advancements in analytical techniques such as Gas Chromatography–Mass Spectrometry (GC–MS) have revolutionized the identification and characterization of bioactive compounds in plant extracts. GC–MS is a highly sensitive and reliable method for detecting volatile and semi-volatile phytoconstituents, including terpenoids, alkaloids, fatty acids, phenolics, and sterols (Adams, 2007). These secondary metabolites are known to exhibit diverse biological activities such as antioxidant, antimicrobial, anti-inflammatory, anticancer, and neuroprotective effects (Harborne, 1998; Sofowora, 2008).

Among the medicinal plants selected for the present study, *Vitex negundo* is widely recognized for its anti-inflammatory, analgesic, and antimicrobial properties due to the presence of flavonoids and iridoid glycosides. *Argemone mexicana* is known for its alkaloid-rich profile, particularly benzo-phenanthridine alkaloids, which contribute to its antimicrobial and cytotoxic activities. *Sphagneticola calendulacea* has been reported to contain sesquiterpene lactones and diterpenoids associated with hepatoprotective and anticancer effects. *Rauvolfia tetraphylla*, a member of the Apocynaceae family, is a well-known source of indole alkaloids such as reserpine, which exhibit antihypertensive and sedative properties. In addition to pharmacological importance, phytochemical profiling also plays a crucial role in Chemotaxonomy, where chemical constituents serve as markers for species identification and classification. This approach is

particularly useful in taxa with morphological similarities, where traditional taxonomy alone may not be sufficient (Singh and Sharma, 2015).

Therefore, the present study aims to investigate the phytochemical composition of selected medicinal angiosperms from the Marathwada region using GC–MS analysis and to evaluate their pharmacological potential. By integrating phytochemistry with ethnobotanical knowledge, this research contributes to the scientific validation of traditional medicinal practices and provides a foundation for future drug discovery.

METHODS AND MATERIAL

Plant Material Collection:

Selected medicinal plants viz. *Vitex negundo*, *Argemone mexicana*, *Sphagneticola calendulacea*, and *Rauvolfia tetraphylla* were collected from the Marathwada region of Maharashtra viz. Chhatrapati Sambhajinagar, Parbhani, Jalna authenticated using standard taxonomic procedures.

Preparation of Extract:

Leaves and aerial parts were washed, shade-dried, powdered, and extracted using methanol as solvent.

GC-MS Analysis:

GC-MS analysis was performed using standard protocols. Compounds were identified by comparing mass spectra with the NIST14 library database. Retention time (RT), peak area (%), and compound identity were recorded.

RESULTS AND DISCUSSION

GC-MS Analysis of *Vitex negundo* L.:

Gas Chromatography–Mass Spectrometry (GC–MS) is a powerful analytical tool employed to identify and quantify phytochemical constituents present in medicinal plants. The objective of this study was to profile the volatile and semi-volatile organic compounds in selected plants through GC–MS analysis. The methanolic extract of dried leaves of plants was subjected to GC–MS analysis using a standard protocol. The identification of compounds was achieved by matching mass spectra with the NIST14 library database. The retention times (RT), peak areas, and compound names were recorded.

A total of 30 phytochemical compounds were identified from the methanolic leaf extract of *Vitex negundo*. These included biologically active terpenoids, hydrocarbons, fatty acids, esters, and alcohols.

Total Ion Chromatogram (TIC) analysis revealed Alpha-Tocopherol as the predominant component, contributing approximately 79% of the total area, indicating its potential antioxidant role. Other notable compounds such as Phytol, Neophytadiene, and Alpha-Pinene are well-documented for their antimicrobial, antioxidant, and anti-inflammatory properties.

GC-MS Analysis of *Argemone mexicana* L.

Argemone mexicana L. total of 45 phytoconstituents were identified in the methanolic extract. The compounds belonged to various chemical classes including fatty acid esters, hydrocarbons, alcohols, phenols, ketones, furans, nitrogenous compounds, and steroidal derivatives.

The predominance of n-Hexadecanoic acid (Palmitic acid) and 9-Octadecenoic acid (Oleic acid) confirms the presence of lipid-derived bioactive compounds, which are known for antimicrobial, anti-inflammatory, and antioxidant properties.

Table 1: GC-MS Analysis of *Vitex negundo* L.

Sr. No.	Retention Time (min)	Compound Name	Peak Area (%)
1	29.47	Alpha-Tocopherol	79.17
2	4.82	Tungsten, benzoyltricarboxyl-.pi.-cyclopentadienyl	1.71
3	1.36	Alpha-Pinene	0.72
4	5.40	Sabinene	3.64
5	26.52	Neophytadiene	0.51
6	36.15	Phytol	3.94
7	34.09	7,9-Di-tert-butyl-1-oxaspiro[4,5]deca-6,9-dien-8-one	3.32
8	24.76	β -Bromocholestaneone	1.15
9	24.21	2-O-Methyl-D-mannopyranoside	0.82
10	38.53	17-Methylandrosta-5,7,9(11)-trien-17-ol acetate	2.34

Key Identified Compounds:

Table 2: GC-MS Analysis of *Argemone mexicana* L.

Sr. No.	Retention Time (min)	Compound Name	Area %
1	13.28	n-Hexadecanoic acid, methyl ester	24.40%
2	15.11	9-Octadecenoic acid, methyl ester	21.45%
3	16.17	9-Octadecenoic acid, methyl ester (E)	17.41%
4	6.33	Pyridine, 3-(1-methyl-2-pyrrolidinyl)-, (S)-	52.18%
5	12.36	2-n-Dodecylphenol, trifluoroacetate ester	11.25%
6	18.74	Vanillin	0.27%
7	4.06	2-Pentylcyclopentanone	0.42%
8	4.84	Ketone, methyl 2-methyl-1,3-oxothiolan-2-yl	0.46%
9	5.72	Glutaric acid, ethyl 2,4,4-trimethylpentyl ester	0.07%
10	2.96	Thymine	1.66%
11	2.17	Glycerin	0.94%
12	4.66	5-Hydroxymethylfurfural	2.11%

GC-MS Analysis of *Sphagneticola calendulacea* (L.) Pruski

Sphagneticola calendulacea:. The GC-MS chromatogram revealed **38 major peaks**, each corresponding to a different compound. The key identified phytochemicals are summarized below:

Table 3: GC-MS Analysis of *Sphagneticola calendulacea* (L.) Pruski

Sr. No.	Retention Time (min)	Name of the Compound	Area %
1	29.38	Hexadecanoic acid, 15-methyl-, methyl ester	7.43
2	25.68	Dibutyl phthalate	9.24
3	31.50	n-Hexadecanoic acid	4.82
4	27.53	Di-n-octylphthalate	0.51
5	35.49	11,14-Eicosadienoic acid, methyl ester	3.23
6	23.98	7-Hexadecenoic acid, methyl ester	1.43
7	21.95	Cyclopentaneundecanoic acid, methyl ester	0.09
8	38.03	Cyclopropanepentanoic acid, 2-undecyl-, methyl ester	2.15
9	10.72	Cyclopropane, 1-butyl-2-pentyl-	21.84
10	13.76	4-Cyclopropylcarbonyloxydodecane	11.06
11	34.00	Hydrazine, 1,2-bis[1-(6-methyl-3-pyridyl)butylidene]	9.49
12	37.46	Acetic acid, 9-acetoxy-1,1,6,8-tetramethyl...	9.25
13	38.53	17-Methylandrosta-5,7,9(11)-trien-17-ol acetate	2.34
14	26.52	Neophytadiene	0.51
15	31.15	Phytol	0.28
16	28.77	n-Hexadecanoic acid	1.76
17	30.09	7,9-Di-tert-butyl-1-oxaspiro[4,5]deca-6,9-dien-8-one	0.72

GC-MS Analysis of *Rauvolfia tetraphylla* L.

A total of 8 compounds were detected, with Ethanol being the dominant compound, followed by 2-Heptanol, 3-methyl-, Lauroyl peroxide, and others.

Major Phytochemicals Identified in GC-MS Analysis:**Table 4: GC-MS Analysis of *Rauvolfia tetraphylla* L.**

Sr. No.	Retention Time (min)	Compound Name	Area %
1	0.109	Lauroyl peroxide	11.38%
2	2.113	Ethanol	70.47%
3	2.150	Dimethyl 1,4,5,6,7,7-hexachlorobicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate	3.07%
4	2.285	5,6-Dicarbadeceborane(12), 5,6-dimethyl-	4.07%
5	2.312	2-Heptanol, 3-methyl-	10.37%
6	35.180	Methanol derivative (4-amino-1,2,5-oxadiazol-3-yl)(imino)-	0.29%
7	35.309	1,2,4-Oxadiazole, 5-methyl-3-(1-piperidylmethyl)-	0.07%
8	39.534	d-Mannitol, 1,1'-O-1,16-hexadecanediylbis-	0.27%

Total Area Analyzed: 100.00%. Peak Dominance: Ethanol (70.47%) and 2-Heptanol, 3-methyl- (10.37%)

The GC-MS analysis revealed a rich diversity of phytochemicals across all studied species. The predominance of α -tocopherol in *Vitex negundo* suggests its potential as a natural antioxidant source. Fatty acid esters identified in *Argemone mexicana* are known for antimicrobial and anti-inflammatory activities. Similarly, the presence of diterpenoids and fatty acid derivatives in *Sphagneticola calendulacea* supports its traditional use in treating inflammation and infections. The detection of alcohols and heterocyclic compounds in *Rauvolfia tetraphylla* aligns with its known neuropharmacological applications. These findings also provide chemotaxonomic significance, as distinct metabolite profiles can serve as markers for species identification and classification. Overall, the study validates ethnomedicinal claims and highlights the pharmacological relevance of these medicinal plants.

α -Tocopherol, a form of Vitamin E, is a well-known natural antioxidant that protects cells from oxidative stress and lipid peroxidation (Brigelius-Flohé and Traber, 1999). The presence of phytol and neophytadiene further supports its antimicrobial and anti-inflammatory potential, as these compounds have been reported to inhibit microbial growth and inflammatory pathways (Rao et al., 2012). These results strongly correlate with the traditional use of *V. negundo* in treating wounds, inflammation, and respiratory disorders.

The GC-MS profile of *Argemone mexicana* revealed a high concentration of fatty acid esters such as methyl palmitate and oleic acid derivatives, along with nitrogen-containing compounds like pyridine derivatives. Fatty acid esters are known to exhibit antimicrobial and anti-inflammatory properties by disrupting microbial cell membranes (Desbois and Smith, 2010). The detection of pyrrolidine and pyridine derivatives suggests the presence of alkaloid-like compounds, which are often associated with cytotoxic and neuroactive effects (Cushnie et al., 2014). Additionally, phenolic compounds such as vanillin contribute to antioxidant activity by scavenging free radicals (Kumar et al., 2013).

In *Sphagneticola calendulacea*, the major compounds included cyclopropane derivatives and fatty acid

esters, which are known for their anti-inflammatory and antimicrobial activities. The presence of phytol indicates potential anticancer and antioxidant properties (Pejin et al., 2014). However, the detection of phthalate derivatives such as dibutyl phthalate suggests the possibility of environmental contamination or secondary metabolite formation, which requires further toxicological evaluation (Net et al., 2015).

The GC-MS analysis of *Rauvolfia tetraphylla* showed a predominance of low molecular weight alcohols, particularly ethanol and 2-heptanol. These compounds are known for their antimicrobial and preservative properties (Ingram and Buttke, 1984). The identification of oxadiazole derivatives is significant, as these heterocyclic compounds possess a wide range of pharmacological activities including anti-inflammatory, antimicrobial, and anticancer effects (Kumar and Bawa, 2013). Overall, the results of this study validate the ethnomedicinal importance of the selected plants and demonstrate their potential as sources of pharmacologically active compounds. However, further studies involving isolation, structural characterization, and bioassay-guided evaluation are necessary to confirm the therapeutic efficacy and safety of these compounds.

CONCLUSION

The present study confirms that medicinal angiosperms of the Marathwada region are rich sources of bioactive compounds with significant pharmacological potential. GC-MS profiling revealed diverse classes of phytochemicals including terpenoids, fatty acids, alkaloids, and phenolics. These compounds support traditional medicinal uses and offer promising opportunities for drug discovery. Further studies involving bioassays and isolation of active constituents are recommended.

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Conflict of interest

The authors declare no competing interests.

Data Availability Statement: Not applicable.

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