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Chemical Characterization of *Dillenia pentagyna* Bark Powder Using GC–MS Analysis

[*1] Dipali Samir Warange

[*1] Assistant Professor, Department of Botany, M.B. More Foundation's Arts, Commerce and Science Women College, Dhatav-Roha, Raigad, Maharashtra, India.

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***Corresponding Author**
Dipali Samir Warange
Assistant Professor, Department of Botany, M.B. More Foundation's Arts, Commerce and Science Women College, Dhatav-Roha, Raigad, Maharashtra, India.

Abstract
The objective of this study was to analyze and characterize the phytochemical constituents present in the bark powder of *Dillenia pentagyna* using Gas Chromatography–Mass Spectrometry (GC–MS). The plant species holds local medicinal significance, but comprehensive chemical profiling is limited. A total of twenty-five compounds were detected, including sulfoxides, esters, siloxanes, aromatic derivatives, triazoles, steroids, and various trimethylsilyl (TMS) derivatives. Major constituents included Methyl 2-hydroxyethyl sulfoxide (38.00%) and Ethanol (24.12%), while several minor bioactive compounds were identified at higher retention times. The findings provide a detailed chemical profile that may support future pharmacological explorations of the species.

Keywords: *Dillenia pentagyna*, GC–MS, phytochemicals, bark powder, chemical profiling.

1. Introduction

Medicinal plants play a significant role in traditional healing systems due to their rich repository of secondary metabolites. *Dillenia pentagyna*, widely distributed across India and neighboring regions, is known for traditional uses involving its bark, fruits, and leaves. Local healers and rural communities have utilized its bark for treating pain, inflammation, and general health ailments. Despite its ethnomedicinal relevance, scientifically validated chemical profiling is relatively sparse.

Gas Chromatography–Mass Spectrometry (GC–MS) is an advanced analytical tool widely used for detecting volatile and semi-volatile phytochemicals. It integrates two powerful analytical techniques-gas chromatography for compound separation and mass spectrometry for compound identification. The technique is particularly useful for detecting organic acids, esters, alkaloids, siloxanes, aromatic compounds, and steroidal derivatives.

The present study aims to chemically characterize the constituents in *Dillenia pentagyna* bark powder through GC–MS analysis. The results help form a chemical basis for understanding its medicinal potential. The analysis strictly follows the GC–MS output available from the provided sample file.

2. Materials and Methods

2.1 Sample Information

The sample consisted of bark powder labeled as sample18_Dillenia pentagyna_bark powder. The analysis was performed by the designated laboratory using method file *Phytochemical profile extract.qgm*.

- **Sample ID:** 1584
- **Sample Type:** Unknown
- **Injection Volume:** 1.00 µL
- **Dilution Factor:** 1
- **Vial No.:** 6

2.2 Instrumentation: GC–MS

The analysis employed a standard GC–MS system configured for phytochemical screening. The Total Ion Chromatogram

(TIC) was recorded, and mass spectral data were matched using the NIST14 library.

2.3 Compound Identification

Each chromatographic peak was identified based on:

- Retention time (min)
- Peak area (%)
- Mass spectral matching
- Similarity index (SI) from NIST14
- Molecular formula and structure suggestions

Only the compounds with sufficient similarity matches were reported.

3. Results

3.1 Total Ion Chromatogram (TIC)

The chromatogram shows two major peaks at retention times 1.434 min and 1.496 min, followed by numerous smaller but diverse phytochemical constituents eluting after 28 min, particularly between 31–33 min.

3.2 Identified Compounds

Table 1: GC–MS Identified Compounds in *Dillenia pentagyna* Bark Powder

Peak No.	R. Time (min)	Area%	Identified Compound
1	1.434	38.01	Methyl 2-hydroxyethyl sulfoxide
2	1.496	24.13	Ethanol
3	28.675	1.06	2,6-Nonadienoic acid, methyl ester derivative
4	31.145	1.37	Cyclotetrasiloxane, octamethyl-
5	31.330	1.50	1,2-Bis(trimethylsilyl)benzene
6	31.545	1.64	1,4-Bis(trimethylsilyl)benzene
7	31.595	1.17	Triazole-carboxylic acid derivative
8	31.625	1.04	Tetramethyl-benzochromenone derivative
9	31.668	2.40	Phosphinolineethanol oxide derivative
10	31.845	2.15	1,2-Bis(trimethylsilyl)benzene
11	31.940	2.53	Perhydro-htx-8-one derivative
12	31.982	1.14	17a-Allyl-aza-androst-one derivative
13	32.060	2.22	Hydroxymethandienone derivative (TMS)
14	32.126	1.87	1,4-Bis(trimethylsilyl)benzene
15	32.161	1.18	Cycloheptatrienone derivative
16	32.215	2.66	1,2-Bis(trimethylsilyl)benzene
17	32.345	1.90	Sebacic acid di-ester derivative
18	32.419	2.30	3,4-Dimethylbenzoic acid (TBDMS)
19	32.466	1.10	Benzo(a)heptalen-one derivative
20	32.540	1.79	Glutaric acid di-ester derivative
21	32.613	1.73	Silicic acid diethyl bis(trimethylsilyl) ester
22	32.810	1.29	Adipic acid derivative
23	32.895	1.22	Bromo-nitro quinoline derivative
24	32.971	1.08	Tris(tert-butyldimethylsilyloxy)arsane
25	33.105	1.50	Cyclobarbital

3.3 Classification of Compounds

Table 2: Chemical Classification of Identified Compounds

Class	Representative Compounds (from GC–MS)
Sulfoxides	Methyl 2-hydroxyethyl sulfoxide
Alcohols	Ethanol
Esters	Nonadienoic acid ester, glutaric acid esters, adipic acid derivatives, sebacic acid esters
Siloxanes & Silyl Derivatives	Cyclotetrasiloxane, TMS derivatives, TBDMS derivatives
Aromatic Compounds	Trimethylsilyl benzenes, methyl-benzoate derivatives
Heterocyclics	Triazole derivatives, pyranone derivatives
Steroid-like Compounds	Androstene derivative
Halogenated Aromatics	Bromo-nitro quinoline derivative
Others	Barbiturate derivative, phosphinoline derivative

4. Discussion

The GC–MS profile demonstrates substantial chemical diversity in the bark powder of *Dillenia pentagyna*. The chromatogram is dominated by two early-eluting compounds: Methyl 2-hydroxyethyl sulfoxide (38%) and Ethanol (24%), suggesting the presence of polar and volatile compounds.

The mid-range and late-eluting constituents (28–33 min) reveal a broad spectrum of:

- Esters,
- Siloxane-based derivatives,
- Aromatic silyl compounds,
- Heterocyclic structures such as triazoles,
- And complex steroidal derivatives.

The presence of esters and aromatic TMS derivatives indicates secondary metabolites or derivatization products commonly seen in bark extracts during GC–MS analysis. The identification of sebacic acid, adipic acid esters, and benzoic acid derivatives may indicate lipid-derived breakdown products or plant wax components. Steroidal and heterocyclic constituents, even in low percentages, are noteworthy as bark tissues often contain triterpenoids, alkaloids, or nitrogenous

secondary metabolites. The findings provide a preliminary chemical fingerprint of *Dillenia pentagyna* bark powder, forming a foundation for future phytopharmacological evaluations.

Conclusion

The GC–MS analysis of *Dillenia pentagyna* bark powder revealed a total of twenty-five identifiable compounds. The chemical composition is dominated by sulfoxides, esters, siloxanes, aromatic derivatives, and minor steroidal and heterocyclic compounds. This chemical profile is valuable for establishing the phytochemical characteristics of the species and may serve as a baseline for further bioactivity studies and medicinal plant research.

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