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GC–MS Based Phytochemical Characterization of *Callicarpa tomentosa* (L.) L. Stem Powder

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Abstract

Medicinal plants are an invaluable source of bioactive secondary metabolites with therapeutic potential. *Callicarpa tomentosa* is traditionally used in folk medicine for the treatment of infections, inflammation, and various ailments, yet its phytochemical profile remains underexplored. The present study aims to identify and characterize the phytochemical constituents present in the stem powder of *Callicarpa tomentosa* using Gas Chromatography–Mass Spectrometry (GC–MS). GC–MS analysis revealed the presence of twenty-four phytochemical compounds belonging to diverse chemical classes, including phenolics, steroids, alkaloids, fatty acid esters, sulfone derivatives, siloxanes, and heterocyclic compounds. Major constituents included 2-chloroethyl methyl sulfoxide (21.57%), solasonine (4.57%), dimethylmalonic acid derivatives (4.83%), purine derivatives (4.15%), and di-n-decylsulfone (3.45%). Many of the identified compounds are known for antimicrobial, anti-inflammatory, antioxidant, and pharmacological activities. The results highlight the medicinal significance of *Callicarpa tomentosa* stems and provide scientific support for their traditional use.

Keywords: *Callicarpa tomentosa*, GC–MS analysis, stem powder, phytochemicals, medicinal plant

1. Introduction

Plants have been used as sources of medicine since ancient times and continue to play a crucial role in healthcare systems worldwide. Secondary metabolites such as alkaloids, phenolics, steroids, terpenoids, and fatty acid derivatives contribute to the biological activities of medicinal plants. Scientific evaluation of these phytochemicals is essential for validating ethnomedicinal claims and identifying potential lead compounds for drug development.

Gas Chromatography–Mass Spectrometry (GC–MS) is a widely used analytical technique for the identification of volatile and semi-volatile organic compounds. It combines the separation power of gas chromatography with the identification capability of mass spectrometry, making it highly suitable for phytochemical profiling.

Callicarpa tomentosa (Family: Lamiaceae) is a medicinal shrub traditionally used for treating fever, wounds, microbial infections, and inflammatory conditions. Despite its traditional importance, detailed phytochemical studies on its

stem are limited. Therefore, the present study focuses on GC–MS based phytochemical characterization of *Callicarpa tomentosa* stem powder.

2. Materials and Methods

2.1 Plant Material Collection and Authentication

The stem material of *Callicarpa tomentosa* was collected from a natural habitat during the active growth season. The plant material was identified and authenticated based on standard taxonomic keys with reference to regional floras. Only healthy, disease-free stems were selected for analysis to ensure the accuracy and reproducibility of phytochemical profiling.

2.2 Preparation of Stem Powder

The collected stem samples were thoroughly washed with running tap water to remove soil particles and surface contaminants, followed by rinsing with distilled water. The stems were then cut into small pieces and shade-dried at room

temperature for several days until a constant weight was achieved. Shade drying was preferred to prevent degradation of heat-sensitive phytochemicals. The dried stem material was pulverized into a fine powder using a mechanical grinder. The powdered sample was sieved to obtain uniform particle size and stored in clean, airtight containers at room temperature until further analysis.

2.3 Sample Extraction for GC–MS Analysis

A known quantity of the stem powder was used for GC–MS analysis. The powdered sample was subjected to solvent extraction using an appropriate organic solvent (analytical grade) to dissolve volatile and semi-volatile phytochemicals. The extract was filtered to remove insoluble plant debris and the filtrate was concentrated under controlled conditions. The prepared extract was used directly for GC–MS injection.

2.4 GC–MS Instrumentation

Gas Chromatography–Mass Spectrometry analysis was performed using a GC–MS system equipped with an autosampler. The analysis conditions were standardized to ensure accurate separation and identification of compounds.

- **Injection volume:** 1.0 µL
- **Injection mode:** Split
- **Carrier gas:** Helium (high purity)
- **Flow rate:** Constant
- **Ionization mode:** Electron impact (EI)
- **Ionization energy:** 70 eV

The sample was injected into the GC column, where compounds were separated based on their volatility and interaction with the stationary phase.

2.5 Chromatographic Conditions

The oven temperature was programmed to allow effective separation of low- and high-boiling compounds. The temperature was initially maintained at a lower value and gradually increased at a controlled rate to ensure optimal resolution of phytochemicals present in the stem extract.

The total run time was sufficient to allow elution of all detectable compounds.

2.6 Mass Spectral Analysis and Compound Identification

The mass spectrometer recorded ion fragments over a wide mass range. Each compound produced a characteristic mass spectrum based on its molecular fragmentation pattern. The obtained spectra were automatically matched with reference spectra available in the NIST14 mass spectral library.

Identification of phytochemical compounds was carried out by comparing:

- Retention time
- Molecular weight
- Mass spectral fragmentation pattern
- Similarity index (SI) values

Only compounds with acceptable similarity index values were considered for identification.

2.7 Quantitative Analysis

The relative concentration of each identified compound was calculated based on the peak area percentage (%) obtained from the total ion chromatogram (TIC). The peak area percentage represents the relative abundance of individual phytochemicals in the stem extract and was used for comparative interpretation of major and minor constituents.

2.8 Data Processing

The chromatographic and mass spectral data were processed using the instrument's integrated software. Peak detection, integration, and identification were performed automatically and verified manually to ensure accuracy. The final results were tabulated, listing retention time, compound name, molecular formula, and peak area percentage.

3. Results

GC–MS analysis of *Callicarpa tomentosa* stem powder revealed 24 distinct phytochemical compounds. The compounds belonged to different chemical classes such as sulfoxides, steroids, alkaloids, phenols, fatty acid esters, sulfones, and heterocyclic compounds.

Table 1: Phytochemical Compounds Identified in *Callicarpa tomentosa* Stem Powder by GC–MS

S. No.	Retention Time (min)	Compound Name	Molecular Formula	Area (%)
1	1.409	2-Chloroethyl methyl sulfoxide	C ₃ H ₇ ClOS	21.58
2	1.541	Androst-4-en-11-ol-3,17-dione, 9-thiocyanato-	C ₂₀ H ₂₅ NO ₃ S	3.03
3	30.900	Epoxy cyclopenta-cycloundecane derivative	C ₂₈ H ₃₈ O ₁₁	2.73
4	30.990	Solasonine	C ₄₅ H ₇₃ NO ₁₆	4.57
5	31.321	4-Sulfamoyl-thiophene-2-carboxylic acid	C ₅ H ₅ NO ₄ S ₂	3.29
6	31.498	Cyclotetrasiloxane, octamethyl-	C ₈ H ₂₄ O ₄ Si ₄	4.25
7	31.583	9,10-Secoergosta-5,7,10(19),22-tetraene-3,25-diol	C ₂₈ H ₄₄ O ₂	3.21
8	31.659	4-tert-Butylphenol, TMS derivative	C ₁₃ H ₂₂ OSi	3.98
9	31.700	1,2-Bis(trimethylsilyl)benzene	C ₁₂ H ₂₂ Si ₂	3.29
10	31.750	Cyclotetrasiloxane, octamethyl-	C ₈ H ₂₄ O ₄ Si ₄	2.61
11	31.831	Cyclopropanecarboxylic acid, 2-hexyl-, methyl ester	C ₁₈ H ₃₄ O ₂	2.96
12	31.900	Purine-2,6-dione derivative	C ₁₂ H ₁₉ N ₅ O ₃	4.15
13	31.994	Dimethylmalonic acid pentafluoropropyl ester	C ₂₁ H ₃₅ F ₅ O ₄	4.83
14	32.045	Benzoic acid, trimethylsilyl ester	C ₁₄ H ₂₄ O ₃ Si ₂	2.52
15	32.160	2-Azainosine	C ₉ H ₁₁ N ₅ O ₅	3.24
16	32.285	Hexasiloxane, dodecamethyl-	C ₁₂ H ₃₈ O ₅ Si ₆	2.79
17	32.335	d-Mannitol derivative	C ₂₈ H ₅₈ O ₇	3.63
18	32.375	Di-n-decylsulfone	C ₂₀ H ₄₂ O ₂ S	3.45
19	32.495	Carbonic acid, nonyl trichloroethyl ester	C ₁₂ H ₂₁ Cl ₃ O ₃	2.98
20	32.660	2,4-Dihydroxyacetophenone, TMS derivative	C ₁₄ H ₂₄ O ₃ Si ₂	4.05
21	33.570	Cyclohexanone derivative	C ₁₄ H ₂₂ O	2.98
22	34.746	Acetic acid, 10-chlorodecyl ester	C ₁₂ H ₂₃ ClO ₂	3.99
23	35.195	Oxabicyclononene methanol derivative	C ₁₃ H ₂₀ O ₂	3.28
24	35.825	Indol-2-one derivative	C ₁₇ H ₂₁ N ₃ O	2.62

4. Discussion

The GC–MS profile of *Callicarpa tomentosa* stem powder revealed a chemically diverse composition. The high abundance of 2-chloroethyl methyl sulfoxide suggests strong antimicrobial potential. Solasonine, a steroidal glycoalkaloid, is reported to possess anticancer, antifungal, and anti-inflammatory properties.

Phenolic compounds such as 4-tert-butylphenol and dihydroxyacetophenone derivatives contribute to antioxidant and antimicrobial activities. Purine derivatives and 2-azainosine indicate possible antiviral and pharmacological relevance. Sulfone compounds like di-n-decylsulfone are associated with antibacterial and antifungal effects.

The presence of fatty acid esters, steroids, alkaloids, and phenolics collectively explains the broad therapeutic applications of *Callicarpa tomentosa* in traditional medicine.

Conclusion

The present GC–MS study successfully identified twenty-four phytochemical compounds in the stem powder of *Callicarpa tomentosa*. The detected compounds exhibit diverse biological activities, including antimicrobial, antioxidant, anti-inflammatory, and pharmacological properties. This study provides scientific evidence supporting the traditional medicinal use of *Callicarpa tomentosa* stems and suggests their potential as a source of bioactive compounds for pharmaceutical applications. Further in-vitro and in-vivo studies are recommended to validate these biological activities.

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