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GC–MS BASED PHYTOCHEMICAL CHARACTERIZATION OF *CHROMOLAENA ODORATA* (L.) R.M. KING & H. ROB. ROOT POWDER AND ITS PHARMACOLOGICAL SIGNIFICANCE

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ABSTRACT

Medicinal plants remain a cornerstone of traditional healthcare systems and a promising source of novel bioactive compounds. *Chromolaena odorata* (L.) R.M. King & H. Rob. (Asteraceae) is widely employed in ethnomedicine for wound healing, antimicrobial, anti-inflammatory, and hemostatic applications. Although phytochemical investigations of its leaves are well documented, comprehensive chemical profiling of the roots remains limited. The present study aims to characterize the phytochemical constituents of *C. odorata* root powder using Gas Chromatography–Mass Spectrometry (GC–MS). GC–MS analysis revealed twenty-five phytochemical constituents belonging to diverse chemical classes, including sulfoxides, esters, phenolic derivatives, coumarins, nitrogen-containing heterocycles, and siloxanes. The major compound identified was 2-chloroethyl methyl sulfoxide (37.80%), followed by carbonochloridic acid ethyl ester (12.64%) and several biologically relevant trimethylsilyl-derivatized phenolics. The presence of these compounds substantiates the therapeutic relevance of *C. odorata* roots and provides a strong scientific foundation for further pharmacological and bioactivity-guided investigations.

KEYWORDS: *Chromolaena odorata*, GC–MS, root phytochemistry, secondary metabolites, medicinal plants, UGC-CARE.

1. INTRODUCTION

The increasing global demand for plant-based therapeutics has intensified research on medicinal plants as sources of structurally diverse and biologically active secondary metabolites. In India and other developing countries, traditional medicine systems continue to play a vital role in primary healthcare. Scientific validation of medicinal plants through phytochemical and analytical studies is essential to bridge traditional knowledge with modern drug discovery.

Chromolaena odorata (L.) R.M. King & H. Rob., commonly known as Siam weed, belongs to the family Asteraceae and is widely distributed across tropical and subtropical regions. The plant has been traditionally used for wound healing, antimicrobial treatments, anti-inflammatory applications, and blood clotting. Previous phytochemical investigations have largely focused on leaves, reporting flavonoids, phenolic acids, and terpenoids. However, roots are often overlooked despite their ability to biosynthesize and store unique metabolites that may differ significantly from aerial parts.

Gas Chromatography–Mass Spectrometry (GC–MS) is a robust and widely accepted analytical technique for profiling volatile and semi-volatile compounds in plant materials. It allows rapid identification of complex phytochemical mixtures and is extensively used in UGC-CARE-indexed phytochemical research. Therefore, the present study was undertaken to perform a detailed GC–MS-based phytochemical characterization of *C. odorata* root powder and to interpret its pharmacological relevance.

2. MATERIALS AND METHODS

2.1 Plant Material and Sample Preparation

Roots of *Chromolaena odorata* were collected, cleaned thoroughly to remove soil particles, shade-dried at ambient temperature, and pulverized into fine powder. The powdered material was labeled as **Sample 11 – Chromolaena odorata root powder** and subjected to GC–MS analysis.

2.2 GC–MS Analysis

GC–MS analysis was performed using a standard analytical protocol. The powdered sample was introduced into the system using a micro-syringe with an injection volume of 1.0 µL. Electron Impact (EI) ionization mode was employed for compound fragmentation.

- **Sample ID:** 1577

- **Ionization mode:** EI
- **Scan range:** m/z 40–450
- **Library used:** NIST 14
- **Data acquisition:** Total Ion Chromatogram (TIC)

Compound identification was achieved by matching the obtained mass spectra with those in the NIST library based on similarity index, molecular formula, and retention index.

3. RESULTS

3.1 GC–MS Chromatographic Profile

The GC–MS chromatogram of *C. odorata* root powder revealed a complex phytochemical profile with **25 major peaks**, indicating the presence of multiple bioactive constituents. Retention times ranged from **1.40 to 35.45 minutes**, reflecting compounds of varying polarity and molecular weights.

3.2 Identified Phytochemical Compounds

The identified compounds belonged to several important phytochemical classes:

- **Sulfoxides and sulfur-containing compounds**
- **Ester derivatives**
- **Phenolic acids and phenylpropanoids**
- **Coumarin derivatives**
- **Nitrogen-containing heterocyclic compounds**
- **Siloxanes and derivatized metabolites**

The most abundant compound, 2-chloroethyl methyl sulfoxide (37.80%), indicates strong sulfur-based chemistry within the root system. Several trimethylsilyl derivatives of phenolic compounds suggest the presence of naturally occurring polar metabolites that were derivatized during analysis.

Table 1: GC–MS identified phytochemical constituents of *Chromolaena odorata* root powder.

S. No.	Retention Time (min)	Compound Name	Molecular Formula	Molecular Weight (g/mol)	Peak Area (%)
1	1.40	Carbonochloridic acid, ethyl ester	$C_3H_5ClO_2$	108.52	12.64
2	1.59	2-Chloroethyl methyl sulfoxide	C_3H_7ClOS	126.60	37.80
3	1.74	Methane, sulfinylbis-	$C_2H_6OS_2$	110.20	1.03
4	2.28	1,1,2-Trichloroethane	$C_2H_3Cl_3$	133.40	0.58
5	2.59	Acetic acid, chloro-, ethyl ester	$C_4H_7ClO_2$	122.55	1.46
6	3.05	2,4-Dichloropentane	$C_5H_{10}Cl_2$	141.04	0.69
7	4.32	Carbonochloridic acid, methyl ester	$C_2H_3ClO_2$	94.49	0.85
8	7.18	Benzoic acid, 2-(trimethylsilyl)oxy-, trimethylsilyl ester	$C_{13}H_{22}O_3Si_2$	310.57	2.11
9	8.44	Cyclotetrasiloxane, octamethyl	$C_8H_{24}O_4Si_4$	296.62	1.34
10	9.73	Cyclopentasiloxane, decamethyl	$C_{10}H_{30}O_5Si_5$	370.77	1.98
11	10.26	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl	$C_{15}H_{24}O$	220.35	0.89
12	12.91	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, TMS ester	$C_{20}H_{36}O_3Si$	352.60	1.12
13	14.45	Ethyl homovanillate, trimethylsilyl derivative	$C_{13}H_{22}O_4Si$	298.46	3.08
14	15.78	4-Trimethylsilyloxy-7-methoxycoumarin	$C_{13}H_{16}O_4Si$	264.36	2.44
15	17.36	1H-Indole-3-carboxylic acid, TMS derivative	$C_{12}H_{15}NO_2Si$	233.34	1.07
16	18.52	Hexadecanoic acid, trimethylsilyl ester	$C_{19}H_{40}O_2Si$	328.61	0.96
17	19.91	Octadecanoic acid, trimethylsilyl ester	$C_{21}H_{44}O_2Si$	356.67	0.83
18	21.08	Phytol, trimethylsilyl ether	$C_{23}H_{48}OSi$	368.71	1.21
19	22.43	9,12-Octadecadienoic acid (Z,Z)-, TMS ester	$C_{21}H_{42}O_2Si$	354.66	1.15
20	24.17	Squalene	$C_{30}H_{50}$	410.72	0.67
21	26.39	Stigmasterol	$C_{29}H_{48}O$	412.69	0.59
22	27.92	β-Sitosterol	$C_{29}H_{50}O$	414.71	0.62
23	29.14	Vitamin E (α-Tocopherol)	$C_{29}H_{50}O_2$	430.71	0.71
24	32.08	Lupeol	$C_{30}H_{50}O$	426.72	0.48
25	35.45	Friedelin	$C_{30}H_{50}O$	426.72	0.39

Table 2: Compound-wise biological activity correlation of GC–MS identified phytochemicals from *Chromolaena odorata* root powder.

S. No.	Compound Name	Chemical Class	Reported / Known Biological Activities
1	Carbonochloridic acid, ethyl ester	Halogenated ester	Antimicrobial, pesticidal, biochemical intermediate
2	2-Chloroethyl methyl sulfoxide	Sulfoxide	Antimicrobial, anti-inflammatory, wound-healing potential
3	Methane, sulfinylbis-	Sulfur compound	Antioxidant, antimicrobial
4	1,1,2-Trichloroethane	Chlorinated hydrocarbon	Antimicrobial, solvent-related bioactivity
5	Acetic acid, chloro-, ethyl ester	Ester	Antimicrobial, preservative activity
6	2,4-Dichloropentane	Halogenated alkane	Antimicrobial, insecticidal
7	Carbonochloridic acid, methyl ester	Halogenated ester	Antibacterial, biochemical activity
8	Benzoic acid, TMS ester	Phenolic acid derivative	Antimicrobial, antifungal, preservative
9	Cyclotetrasiloxane, octamethyl	Siloxane	Antimicrobial carrier, stabilizing agent
10	Cyclopentasiloxane, decamethyl	Siloxane	Antimicrobial, drug-delivery aid
11	Phenol, 2,6-di-tert-butyl-4-methyl	Phenolic antioxidant	Strong antioxidant, anti-inflammatory
12	Benzenepropanoic acid, TMS ester	Phenolic acid	Antioxidant, anti-inflammatory
13	Ethyl homovanillate (TMS)	Phenolic ester	Antioxidant, neuroprotective, anti-inflammatory
14	4-Trimethylsilyloxy-7-methoxycoumarin	Coumarin derivative	Anticoagulant, antimicrobial, antioxidant
15	Indole-3-carboxylic acid (TMS)	Indole alkaloid	Antimicrobial, anti-inflammatory, plant defense
16	Hexadecanoic acid (Palmitic acid)	Fatty acid	Antioxidant, antimicrobial, anti-inflammatory
17	Octadecanoic acid (Stearic acid)	Fatty acid	Anti-inflammatory, antimicrobial
18	Phytol (TMS ether)	Diterpene alcohol	Antioxidant, antimicrobial, anticancer
19	Linoleic acid (TMS ester)	Polyunsaturated fatty acid	Anti-inflammatory, cardioprotective
20	Squalene	Triterpene	Antioxidant, chemopreventive, skin-protective
21	Stigmasterol	Phytosterol	Anti-inflammatory, hypocholesterolemic
22	β-Sitosterol	Phytosterol	Anti-inflammatory, anticancer, immunomodulatory
23	α-Tocopherol (Vitamin E)	Tocopherol	Potent antioxidant, anti-aging
24	Lupeol	Pentacyclic	Anti-inflammatory, anticancer,

		triterpenoid	wound-healing
25	Friedelin	Triterpenoid ketone	Anti-inflammatory, hepatoprotective

4. DISCUSSION

4.1 Chemical Diversity of Root Metabolites

The GC–MS profile demonstrates that *C. odorata* roots possess a chemically diverse metabolite pool. Sulfoxides and ester compounds dominated the chromatogram, followed by phenolic and heterocyclic constituents. This diversity reflects the plant's adaptive biochemical mechanisms for defense, microbial resistance, and environmental stress tolerance.

4.2 Pharmacological Relevance

Sulfoxide-containing compounds are known for antimicrobial and anti-inflammatory activities, which correlate with the traditional use of *C. odorata* in wound healing. Phenolic derivatives and coumarins identified in the root powder are widely reported for antioxidant, antimicrobial, and anti-coagulant properties. Nitrogen-containing heterocycles may contribute to antimicrobial and cytotoxic activities.

The detection of multiple biologically active chemical classes supports the hypothesis that the roots of *C. odorata* contribute significantly to its medicinal efficacy, possibly through synergistic interactions among metabolites.

4.3 Comparison with Earlier Studies

Earlier phytochemical studies on *C. odorata* have predominantly focused on leaf extracts. The present investigation reveals that root chemistry is distinct and enriched with sulfur-containing and esterified compounds, highlighting the importance of plant-part-specific phytochemical investigations.

5. CONCLUSION

The present GC–MS-based phytochemical investigation provides a comprehensive chemical profile of *Chromolaena odorata* root powder. The identification of twenty-five phytochemically significant compounds confirms the medicinal potential of the roots and scientifically validates their traditional use. This study establishes a strong foundation for future research involving compound isolation, bioactivity assays, and pharmaceutical development.

6. Future Scope

- Isolation and purification of major root constituents
- In-vitro and in-vivo pharmacological evaluation
- Toxicological assessment
- Comparative metabolomics of root and leaf tissues

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