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GC-MS Profiling And Identification Of Bioactive Volatile Compounds In *Valeriana Wallichii* DC Root And Rhizome Extracts

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Abstract
Valeriana wallichii DC, a highly polymorphic perennial herb from the Valerianaceae family, holds a prominent place in traditional Indian, Tibetan, and Chinese medicine for treating neurological, dermatological, gastrointestinal, and cardiovascular ailments. This study employed Gas Chromatography-Mass Spectrometry (GC-MS) to investigate the phytochemical composition of V. wallichii root and rhizome extracts prepared using Soxhlet extraction with methanol and n-hexane. The GC-MS analysis revealed a diverse array of volatile constituents: 43 compounds in the methanolic extract, with major components including 9,12-octadecadienoic acid (18.48%), palmitic acid (17.90%), and linolenic acid (14.74%); and 38 compounds in the hexane extract, with veridiflorol (23.65%), α-cadinol (13.87%), and verrucarol (8.04%) as dominant constituents. Several of these compounds are known for their therapeutic, nutritional, and industrial applications. The results demonstrate the efficacy of GC-MS in the comprehensive profiling of phytoconstituents, supporting the standardization, quality control, and pharmacological exploration of herbal medicines. The findings reinforce the therapeutic potential of Valeriana wallichii and highlight the need for further investigation of its bioactive and yet unidentified compounds.

Keywords: *Valeriana wallichii DC, GC-MS, Soxhlet extraction, phytochemistry, volatile compounds, herbal medicine.*

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I. Introduction

Valeriana wallichii DC is a perennial herbaceous plant belonging to the family Valerianaceae. It has been traditionally utilized in Indian, Tibetan, and Chinese medicinal systems for centuries, especially in the treatment of neurological, dermatological, and gastrointestinal disorders[1]. This species is highly polymorphic and known by various vernacular names across different Indian languages—such as Mushkbala (Hindi), Tagar (Marathi), and Tagarai (Tamil)—highlighting its broad ethnobotanical recognition.

Valerians are recognized as reservoirs of complex essential oil mixtures, predominantly composed of volatile compounds, including lipids, terpenoids, ketones, phenols, and various oxygenated derivatives[2,3]. These constituents are known for their Anxiolytic, stress and Antidepressant Effects[4,5,6.] Additional properties include sleep improvement[7], antimicrobial properties[8], insecticidal, cognitive performance[9], hepatoprotective activity[10], gastrointestinal and cardiovascular disease[11] and antioxidant properties[12].

The identification and characterization of such phytoconstituents is a cornerstone of modern pharmacognosy and phytochemistry. Among the analytical techniques available, Gas Chromatography-Mass Spectrometry (GC-MS) has emerged as a powerful and widely adopted tool for analyzing complex mixtures of volatile and semi-volatile organic compounds derived from plant materials. GC-MS combines the high-resolution separation capability of gas chromatography with the precise detection and identification power of mass spectrometry[13].

This dual analytical strength makes GC-MS indispensable for the chemical profiling of medicinal plants, aiding not only in the standardization and quality control of herbal formulations but also in identifying bioactive compounds for pharmacological evaluation. A study has used GCMS for metabolite analysis of the two varieties of *Indica* rice seed[14]. Ultimately, the application of GC-MS facilitates the development of evidence-based herbal medicines and supports the advancement of plant-derived therapeutic agents [15,16]. In this regard, GC-MS serves as an indispensable tool in the advancement of evidence-based herbal medicine.

II. Material And Methods

The roots and rhizomes of *Valeriana wallichii* DC were collected from herbal market of Mumbai, India. Specimen samples were authenticated at NBRI, Lucknow, India. Roots and rhizomes were shade dried and were subjected to coarse powdered form by mechanical grinder. The sample preparation and chromatographic conditions for GC-MS were adopted from our previous study with slight modification[17].

Rhizome Powder was passed through a 40-mesh sieve to get a uniform particle size and then used for extraction purpose. Selected roots and rhizomes of *Valeriana wallichii* DC were extracted using Soxhlet extraction. The powder drug was extracted in soxhlet apparatus with the Methanol and n- Hexane separately, at 50-60 0C in 1:6 ratios in several batches for 16 – 18 hours. Extracts were filtered and stored in cool and dry place.

Two types of extract were obtained; 1) Soxhlet Methanolic Extract (SME), 2) Soxhlet Hexane Extract (SHE), All extracts were collected & concentrated under vacuum in a rotary flash evaporator (Equitron). The residue was dried in the desiccator and stored in cool and dry place for further use.

Preparation of plant extracts for analysis:
10 mg of each plant extract (SME and SHE) was dissolved in 10 mL of their respective solvents (methanol or n-hexane). Samples were sonicated and filtered through a 20 µm filter before injection into the GC column.

Chromatographic conditions for GC/MS:
The GC-MS analysis was carried out using Simadzu GCMS model QP2010 ultra, equipped with flame ionized detector (FID) and capillary column Rtx- 5MS (30m×0.25mm) 0.25um thickness. Helium was used as carrier gas. GC oven temperature was variable programmed from 600C-2200C. The temperature was raised 220 ^{0}C at the rate of 70 ^{0}C/min and hold for 10 min. Both SME and SHE samples were injected at temperature 250 ^{0}C, column oven temperature was maintained at 600C, split ratio was 10, pressure was maintained at 173.7 kPa, column flow was 3 mL/min. The gas chromatography-mass spectrometry (GC-MS) analyses were performed on detector GCMS-QP2010 ion source temperature was maintained at 250°. Mass-spectra recording was done by electron impact ionization at 70eV with scanning mass range recorded from 35 to 450, Injection volume (sample) was 2µl, and total run time was 16 min. The identity of each compound was assigned by comparison of their retention index (RI), relative to a standard mixture of n-alkanes, as well as by comparison of their spectra with those available from MS libraries (NIST/Wiley/Adams) and with the literature values.0 Relative amounts of individual components were calculated based on GC peak area (FID response) without using any correction factor.

III. Results And Conclusions

Results
Valeriana Wallichii DC Hexane Extract (SHE) when subjected to GCMS a total of 38 compounds were identified. Detail of compounds identified given in Table-1, snd chromatogram of compounds given in figure-1. Major constituents included: Veridiflorol (23.65%), α-Cadinol (13.87%), Verrucarol (8.04%), Oleic Acid (7.70%), Hexadecanoic Acid (7.40%), Valerenic Acid (0.49%)

In Methanol Extract (SME) 43 compounds were identified as shown in Figure-2, and compounds identified given in Table-2, with major constituents including: Palmitic Acid (17.90%), 9,12-Octadecadienoic Acid (18.48%), Linolenic Acid (14.74%), Furfural (5.53%), Valeric Acid (3.60%), Menthone (3.52%), Valerenic Acid (0.55%), Eugenol (0.24%), Pulegone (1.12%), Valerenic Anhydride (1.40%).

These compounds are known for their biological activities and are widely used in the food, cosmetic, and pharmaceutical industries. Several other constituents remain unidentified and warrant further study.

Discussion
The chemical profile revealed by GC-MS confirms the therapeutic potential of *Valeriana wallichii* DC through the presence of multiple bioactive constituents. The variation in chemical composition between methanolic and hexane extracts demonstrates the influence of solvent polarity on extraction efficiency.

Notably, valerenic acid and its derivatives—associated with neuropharmacological effects—were detected in both extracts. The presence of essential fatty acids, phenolic compounds, and terpenoids further supports its ethnomedicinal claims.

Chemical Constituents in VWME (Table 1)

Sr. No.	Plant extract	Area%	Structural formula
1	4H-Pyran-4-one,	0.12	C6H6O4
2	Tetrahydrofuran-5-on-2-methanol	0.25	C11H16O7
3	Furfural	5.53	C6H6O3
4	1,2,3-Propanetriol	0.72	C5H10O4

5	Quinuclidine-3-ol	0.25	C7H13NO
6	Isovaleric acid, propyl ester	0.34	C8H16O2
7	Valeric anhydride	1.40	C10H18O3
8	Anicon	0.37	C10H11ClO3
9	3-methylvaleric acid	0.86	C6H12O2
10	Hexanoic acid, 4-octyl ester	0.77	C14H28O2
11	Methyl eugenol	0.24	C11H14O2
12	Ethanone, 1-(4,5-diethyl-2-methyl-1-cyclopenten-1-yl)-	1.18	C12H20O-
13	Pulegone	1.12	C10H16O
14	Isoaromadendrene epoxide	0.29	C15H24O
15	Coumarin, 6-methyl-	0.44	C10H8O2
16	Decanal	4.67	C10H20O
17	Menthone	3.52	C10H16O2
18	Patchouli alcohol	0.18	C15H26O
19	2,5,6-Trimethyl-4-hepten-3-one	0.12	C10H18O
20	Homovanillyl alcohol	0.26	C9H12O3
21	valerenone	0.73	C15H26O
22	valerenic acid	0.55	C15H22O2
23	2,6-Dimethyl-8-(tetrahydropyran-2-yloxy)-octa-2,6-dien-1-ol	0.55	C15H26O3
24	Pentadecanoic aci	0.97	C15H30O2
25	9,19-Cyclo-27-norlanostan-25-one	1.29	C32H52O3
26	2-Octanone, 1-nitro-	0.24	C8H15NO3
27	Hexadecanoic acid, methyl esteri	1.37	C17H34O2
28	Valeric acid, hexadecyl ester	3.60	C21H42O2
29	Palmitic acid	17.91	C16H32O2
30	Phytol	2.24	C20H40O
31	Oleic Acid	0.25	C18H34O2
32	Heptadecanoic acid	0.48	C17H34O2
33	3-t-Butyl-2-methyl-6-(tetrahydropyran-2-yloxy)-hept-4-en-3-ol	0.89	C17H32O3
34	Mononorvalerenone	0.22	C14H22O2
35	Linoleic acid, methyl ester	3.39	C19H34O2
36	9,12,15-Octadecatrien-1-ol, (Z,Z,Z)-	3.50	C18H32O
37	Margaric acid methyl ester	0.50	C18H36O2
38	9,12-octadecadienoate	18.48	C19H34O2
39	Linolenic acid, methyl ester	14.74	C19H32O2
40	Octadecanoic acid, methyl ester	2.43	C19H38O2
41	Benzene, [1-(1,2,2-trimethylpropyl)hexyl]-	1.51	C18H30
42	1-Heptadec-1-ynyl-cyclohexanol	0.28	C23H42O
43	Sulfurous acid, decyl hexyl ester	1.27	C16H34O3S

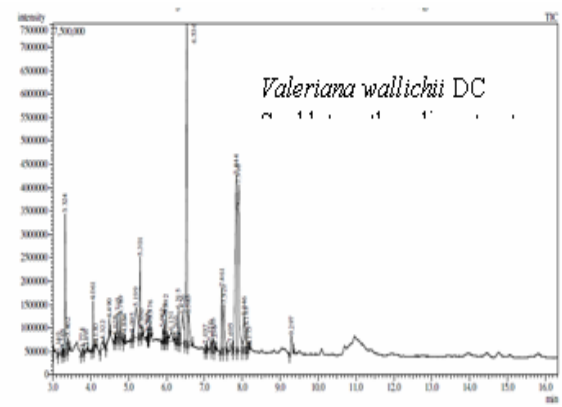

Figure 1. GCMS Chromatogram of VWSME

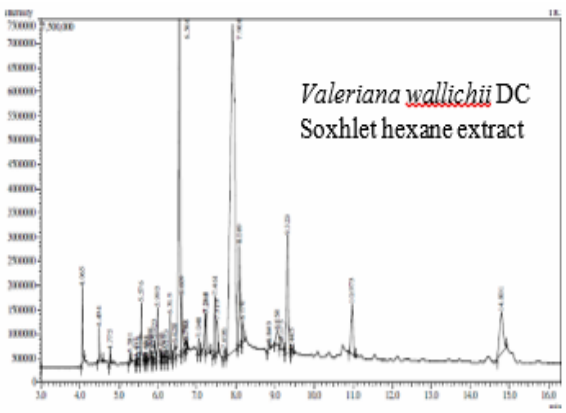

Figure 2. GCMS Chromatogram of VWSHE

Chemical Constituents in VWHE (Table-2)

Sr. No.	**Plant extract**	**Area%**	**Structural formula**
1	Isovaleric anhydride	1.36	C10H18O3
2	Valeric anhydride	0.70	C10H18O3
3	Cyclopentanecarboxylic acid, 2-acetyl-5-methyl-	0.25	C9H14O3
4	Sulfurous acid, dodecyl hexyl ester	0.20	C18H38O3S
5	Patchouli alcohol	0.05	C15H26O

6	Uric acid	0.16	C5H4N4O3
7	valerenone	1.55	C15H26O
8	Elemicin	0.11	C12H16O3
9	5-Decanone	0.10	C10H20O
10	Veridiflor	0.34	C15H26O
11	Isopulegol acetate	0.15	C12H20O2
12	9-Hexadecenoic acid	0.59	C16H30O2
13	Pentadecanoic acid	1.58	C15H30O2
14	1,2-Benzenedicar	0.17	C18H24O4
15	Globulol	0.18	C15H26O
16	Nerolidol isobutyrate	0.25	C19H32O2
17	Hexadecanoic acid, methyl ester	0.92	C17H34O2
18	6-Octadecenoic acid	0.63	C18H34O2
19	n-Hexadecanoic acid	23.65	C16H32O2
20	Tridecanedial	1.99	C13H24O2
21	Hexadecanoic acid, ethyl ester	0.29	C18H36O2
22	1,5,9-Cyclotetrad	0.21	C20H32
23	Oleic Acid	0.40	C18H34O2
24	trans-.beta.-Terpinyl pentanoate	1.56	C15H26O2
25	Fumaric acid, 2-methylallyl pentyl ester	1.21	C13H20O4
26	Linolenic acid	1.70	C18H32O2
27	Linolenic acid, methyl ester	1.40	C19H32O2
28	Kemester	0.24	C19H38O2
29	Grape seed oil	38.51	C18H32O2
30	Valeric acid, 2-tetradecyl ester	4.32	C19H38O2
31	1,7-Dodecadiene	0.95	C12H22
32	Valeric acid, hexadecyl ester	0.26	C21H42O2
33	Eicosane	0.98	C20H42
34	Tetracosane	0.68	C24H50
35	Undecane, 4,4-dimethyl-	5.59	C13H28
36	Valeric acid, 4-cyanophenyl ester	0.19	C12H13NO2
37	2,3-Octanedione	2.70	C8H14O2
38	S-Propyl 3-methylbutanethioate	3.89	C8H16OS

IV. Conclusion

GC-MS analysis of *Valeriana wallichii* DC roots and rhizomes revealed a complex and diverse phytochemical profile, reinforcing its pharmacological potential. The identification of volatile constituents such as Veridiflorol, α-Cadinol, and Valerenic acid underscores its relevance in traditional and modern phytotherapy. This study highlights the significance of advanced analytical tools like GC-MS in herbal drug development and the need for further pharmacological validation of lesser-known compounds.

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