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GC–MS analysis of volatile constituents of *Blumea axillaris* (Asteraceae)

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Abstract
Medicinal plants are important sources of biologically active compounds used in pharmaceutical and therapeutic applications. The present study investigates the phytochemical constituents and volatile compounds present in *Blumea axillaris*, a medicinal herb belonging to the family Asteraceae. The aerial parts of the plant were collected and essential oil was extracted through steam distillation using a Clevenger- type apparatus. Preliminary phytochemical screening was performed to detect major classes of secondary metabolites. Further analysis of the essential oil was carried out using Gas Chromatography–Mass Spectrometry (GC–MS) to identify volatile constituents. Phytochemical screening revealed the presence of flavonoids, phenols, tannins, sterols, and terpenoids. GC–MS chromatographic analysis indicated the presence of several compounds including linalool, copaene, caryophyllene, and other terpenoid derivatives. Many of these compounds are associated with antioxidant, antimicrobial, and anti-inflammatory properties. The findings suggest that *Blumea axillaris* may serve as a promising natural source of bioactive compounds with potential pharmaceutical applications.

Keywords: *Blumea axillaris*, GC–MS analysis, phytochemical screening, essential oil, medicinal plants

Introduction

Aromatic plants are frequently used in traditional medicine because of their essential oils and volatile constituents. In last few years, there has been an increase in the use of aromatic medicinal plants and their essential oils in scientific research and industrial applications including nutritional pharmaceutical and cosmetic uses. At present, approximately 3000 essential oils are known. 300 of which are commercially important especially for the pharmaceutical, agronomic, food, cosmetic, and perfume industry. As essential oils represent a source of antimicrobial, antioxidants and anticancer components, they are currently attracting increasing interest in the scientific community and there is much research being performed on their pharmacological activities, particularly their antimicrobial, antioxidant, anti- inflammatory, and anticancer properties, which are important in the prevention and treatment of diseases of microbial and oxidative stress origin, such as bacterial and viral infections, inflammations, cancers, and cardiovascular diseases, including atherosclerosis and thrombosis.Volatile oil, also known as essential oil, is a natural oil that is extracted from various parts of plants, including flowers, leaves, stems, roots, and fruits. The oil is called "volatile" because it quickly evaporates when exposed to air. Volatile oils are composed of complex mixtures of organic compounds, including terpenes, esters, alcohols, ketones, and phenols, among others. These compounds give volatile oils their characteristic fragrance and therapeutic properties. Volatile oils have been used for thousands of years for their medicinal, cosmetic, and aromatic properties. They have a wide range of applications, including in aromatherapy, massage therapy, skincare, and food flavoring. (Zhi-long Jiang and Ke Yuan 2014) [5]

Spectroscopic technique has become a powerful tool for the qualitative and quantitative analysis of biological and pharmaceutical materials. Gas chromatography-mass spectrometry (GC-MS) is used to gain qualitative results of detected metabolites for biological samples as it provides superior distinguish ability, detection sensitivity and integrated standard mass spectrometry library. (Juan Li *et al*., 2013).

The Asteraceae family is characterized by its composite flower head, which is made up of many individual flowers arranged in a head-like structure. Each flower head is composed of a central disk and surrounding ray flowers, or sometimes only disk flowers or ray flowers. The family is also known for its unique arrangement of the reproductive structures, with the stamens and pistils fused together to form a tube- like structure called the corolla. (Funk *et al*. 2009) [9]

In addition to their ornamental value, many Asteraceae plants have significant medicinal properties and are widely used in traditional medicine systems around the world. For example, plants such as Echinacea, Chamomile, and Feverfew have been used to treat various ailments such as inflammation, infections, and pain. Despite their importance, Asteraceae plants face several threats, including habitat loss, over- exploitation, and climate change. Therefore, there is an urgent need to study and conserve these plants, especially those with medicinal properties. (Yuxin Pang and an Wang 2014) [10]

Medicinal plants play a significant role in traditional and modern medicine due to the presence of biologically active compounds. Plants synthesize a wide range of secondary metabolites such as alkaloids, flavonoids, phenolic compounds, tannins, and terpenoids which contribute to their pharmacological properties.

The family Asteraceae is one of the largest families of flowering plants and includes many species with medicinal value. *Blumea axillaris* is an aromatic herb traditionally used for treating fever, inflammation, and respiratory disorders.

Gas Chromatography–Mass Spectrometry (GC–MS) is widely used for identification of volatile compounds present in plant extracts. This technique allows separation and

characterization of chemical constituents based on their retention time and mass spectral patterns.
The objective of the present study was to investigate the phytochemical composition and volatile constituents of *Blumea axillaris* using GC–MS analysis.

Materials and Methods

1. Collection of Plant Material

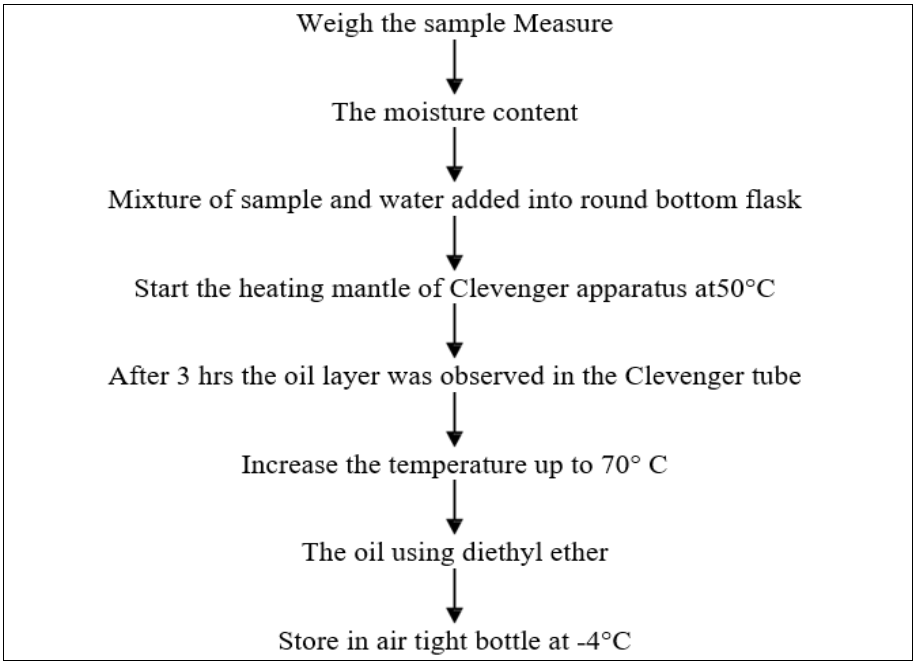
Fresh aerial parts of *Blumea axillaris* were collected from the campus area of Sant Gadge Baba Amravati University, Amravati, Maharashtra. The plant was authenticated in the Department of Botany.

2. Preparation of Plant Material

The collected plant material was washed thoroughly with distilled water and shade dried for several days. The dried material was stored in clean containers until further analysis.

3. Extraction of Essential Oil

Essential oil was extracted by steam distillation using a Clevenger-type apparatus. The plant material was placed in a round-bottom flask containing distilled water and heated. The steam carrying volatile oil was condensed and collected. The separated oil was stored at low temperature for further analysis.



4. Phytochemical Screening

Table 1: Qualitative phytochemical tests were carried out to detect the presence of major secondary metabolites

Phytochemical	Test Used	Observation
Alkaloids	Mayer's reagent	White precipitate
Flavonoids	Lead acetate test	Yellow precipitate
Phenols	Ferric chloride test	Blue coloration
Tannins	Gelatin test	Brown coloration
Sterols/Terpenoids	Salkowski test	Red coloration

5. GC–MS Analysis

GC–MS analysis was carried out to identify volatile constituents present in the essential oil. The sample was injected into a GC–MS instrument equipped with a capillary column using helium as the carrier gas.
The compounds were identified by comparing the obtained mass spectra with the NIST spectral library database.

Table 2: Components identified in essential oil of Blumea axillaries

Peak no.	Retention Time	Compound Name	Molecular Formula	Molecular Weight	Area %
1	5.332	Benzenemethanol, 4-methyl-	$C_8H_{10}O$	122	0.79
2	5.721	Cycloheptane	C_7H_{14}	98	0.99
3	8.123	3-Octen-5-yne, 2,7-dimethyl-, (E)-	$C_{10}H_{16}$	136	0.91
4	9.310	Eucalyptol	$C_{10}H_{18}O$	154	0.73
5	9.463	Cyclopentane, 1-methyl-1-(2-methyl-2-	$C_{10}H_{16}$	136	1.46
6	9.852	Cyclohexene, 1-methyl-4-(1-methyleth	$C_9H_3O_{12}$	296	0.93
7	9.970	1,3-Benzenedimethanol, 2-hydroxy-5-	$C_{15}H_{24}$	204	1.15
8	10.880	8,11,14-Eicosatrienoic acid, (Z,Z,Z)-	$C_{12}H_{15}N$	173	4.23
9	11.005	3,5-Heptadienal, 2-ethylidene-6-methyl	$C_{15}H_{24}$	204	1.74
10	11.695	cis-Chrysanthenol	$C_{15}H_{24}$	204	1.28
11	11.860	D-Verbenone	$C_{15}H_{24}$	204	1.55
12	12.010	Bicyclo[3.1.0]hexan-2-one, 4-methyl-1	$C_{15}H_{24}$	204	3.49

13	12.172	2-Isopropylidene-3-methylhexa-3,5-die	S_6	192	1.20
14	12.408	5-Caranol, (1S,3R,5S,6R)-(-) -	$C_{16}H_{34}$	226	3.39
15	12.655	5-Caranol, trans,trans-(+)-	$C_{20}H_{42}$	282	2.56
16	13.658	2-Allyl-4-methylphenol	$C_{17}H_{34}O_2$	270	2.91
17	13.875	Cyclohexanol, 2-methyl-5-(1-methyleth	$C_9H_9NOS_2$	211	0.75
18	14.015	(1S,3S,4S,5R)-1-Isopropyl-4-methylbi	$C_{29}H_{60}$	408	1.94
19	14.184	(E)-2,6-Dimethylocta-2,5,7-trien-4-one	$C_{20}H_{32}$	272	1.11
20	14.518	(1S-(1Alpha,2alpha,4beta))-1-isoprope	$C_{20}H_{30}$	270	2.59
21	15.010	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-tr	$C_{27}H_{56}$	380	1.65
22	17.767	.alpha.-ylangene	$C_{15}H_{24}$	204	1.55
23	18.938	Longifolene			3.83
24	19.140	Bicyclo[7.2.0]undec-4-ene, 4,11,11-tri	$C_{15}H_{24}$	204	1.86
25	19.598	Caryophyllene	$C_{15}H_{24}$	204	2.00
26	21.153	Tau-Cadinol acetate	$C_{15}H_{24}$	204	6.48
27	21.455	1H-Cycloprop[e]azulen-7-ol, decahydr	$C_{17}H_{28}O_2$	264	0.87
28	21.545	Kessane	$C_{15}H_{24}O$	220	1.49
29	21.753	2H-3,9a-Methano-1-benzoxepin, octah	$C_{15}H_{26}O$	222	2.77
30	22.335	2-Isopropyl-5-methylphenyl 2-methylb	$C_{15}H_{26}O$	222	3.83
31	22.573	D-Limonene	$C_{15}H_{22}O_2$	234	1.42
32	22.630	.beta.-Guaiene	$C_{10}H_{16}$	136	1.20
33	22.803	(1R,7S,E)-7-Isopropyl-4,10-dimethyle	$C_{15}H_{24}$	204	2.22
34	23.001	Lanceol, cis	$C_{15}H_{24}O$	220	1.60
35	23.165	Santalol, cis,.alpha.-	$C_{15}H_{22}O$	220	1.36
36	23.308	1H-Cycloprop[e]azulene, 1a,2,3,5,6,7,	$C_{15}H_{22}O$	220	2.29
37	23.708	Junenol	$C_{15}H_{24}$	204	2.75
38	24.555	Naphthalene, decahydro-4a-methyl-1-m	$C_{15}H_{26}O$	222	3.35
39	26.565	cis-p-mentha-1(7),8-dien-2-ol	$C_{15}H_{24}$	204	0.86
40	26.685	6-Methoxythymyl 2-methylbutyrate	$C_{10}H_{16}O$	152	1.59
41	27.335	((4aS,8S,8aR)-8-Isopropyl-5-methyl-3,	$C_{16}H_{24}O_3$	264	1.12
42	27.723	Spiro[4.5]decan-7-one, 1,8-dimethyl-8,	$C_{15}H_{24}O$	220	1.49
43	27.821	2,6-Dimethyl-1,3,5,7-octatetraene, E,E	$C_{15}H_{24}O_2$	236	1.80
44	28.010	2-Pentadecanone, 6,10,14-trimethyl-	$C_{10}H_{14}$	134	0.78
45	28.180	Spiro[4.5]decan-7-one, 1,8-dimethyl-8,	$C_{18}H_{36}O$	268	2.35
46	28.728	(3R,3aR,4aS,5R,9aS)-3,5,8-Trimethyl-	$C_{15}H_{24}O_2$	236	1.92
47	29.643	l-(+)-Ascorbic acid 2,6-dihexadecanoat	$C_{15}H_{22}O_2$	234	4.21
48	32.292	(7-Methylcyclopenta[c]pyran-4-yl)met	$C_{38}H_{68}O_8$	652	3.83

Results and Discussion

Preliminary phytochemical screening revealed the presence of several classes of secondary metabolites including flavonoids, phenolic compounds, tannins, sterols, and terpenoids. These compounds are widely reported to possess biological activities such as antioxidant, antimicrobial, and anti-inflammatory effects, which may contribute to the medicinal value of the plant.

GC–MS analysis of the essential oil extracted from the aerial parts of *Blumea axillaris* revealed the presence of numerous volatile constituents. The chromatogram displayed multiple peaks corresponding to different chemical compounds identified through comparison with the NIST spectral library database. Major constituents detected included terpenoid derivatives such as caryophyllene, copaene, limonene, and other oxygenated terpenes. Many of these compounds have been reported in previous studies to exhibit antimicrobial and pharmacological properties.

The presence of these bioactive compounds suggests that *Blumea axillaris* may serve as a potential natural source of therapeutic agents and supports its traditional medicinal use.

1. Phytochemical Screening

Preliminary phytochemical screening confirmed the presence of several secondary metabolites including flavonoids, phenols, tannins, sterols, and terpenoids. These compounds are known to possess biological activities such as antioxidant and antimicrobial properties.

2. GC–MS Analysis

GC–MS chromatographic analysis revealed several peaks corresponding to volatile chemical constituents.

Table 3: Compounds Identified by GC–MS

Peak	Retention Time (min)	Compound Identified	Nature
1	~7	Linalool	Monoterpene alcohol
2	~9	Copaene	Sesquiterpene
3	~10	Caryophyllene	Sesquiterpene
4	~12	Caryophyllene oxide	Oxygenated terpene
5	~15	Lycopene derivative	Carotenoid
6	~18	Ascorbic acid derivative	Antioxidant compound

These compounds are reported to possess antimicrobial, antioxidant, and anti- inflammatory properties.

Fig 1: Clevenger apparatus used for extraction of essential oil

Fig 2: Extracted essential oil samples using Clevenger apparatus

Fig 3 : Qualitative phytochemical tests

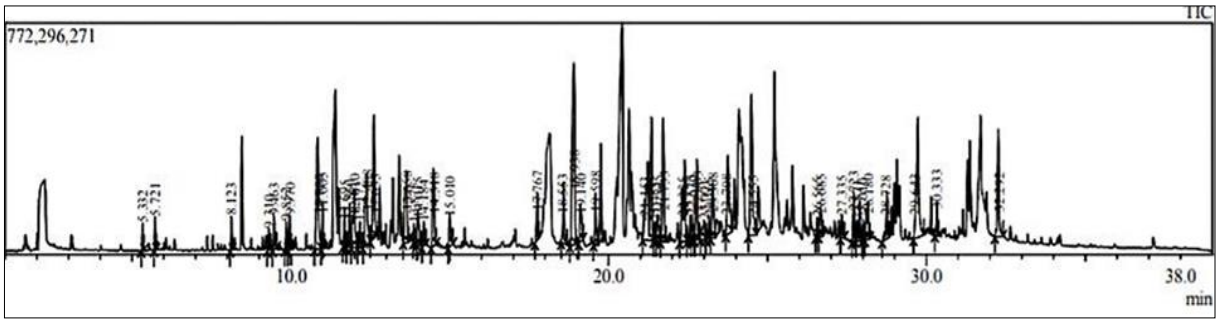
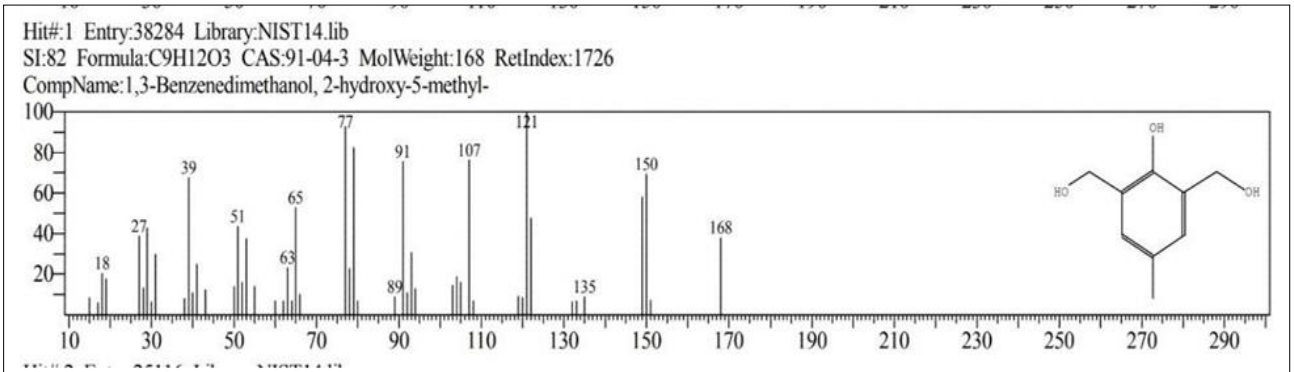


Fig 4: GC–MS chromatogram showing separation of volatile compounds in *Blumea axillaris* extract.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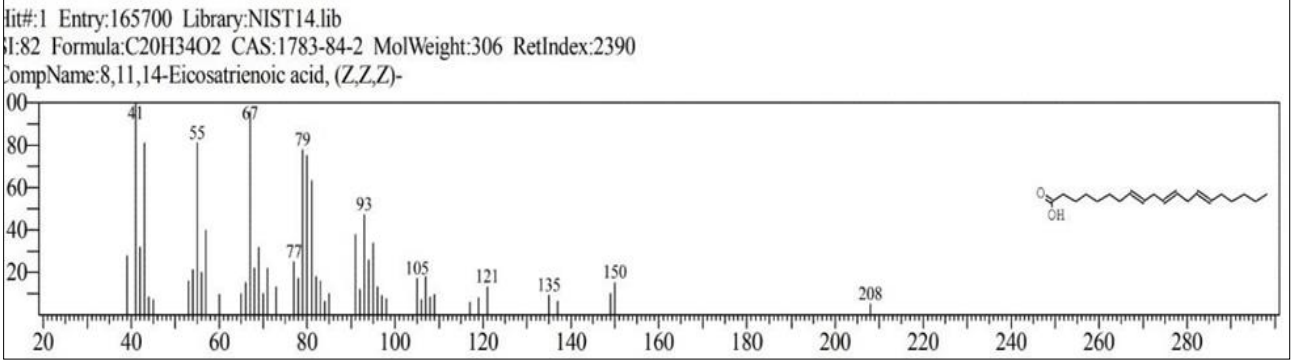
CompName:1,3-Benzenedimethanol, 2-hydroxy-5-methyl-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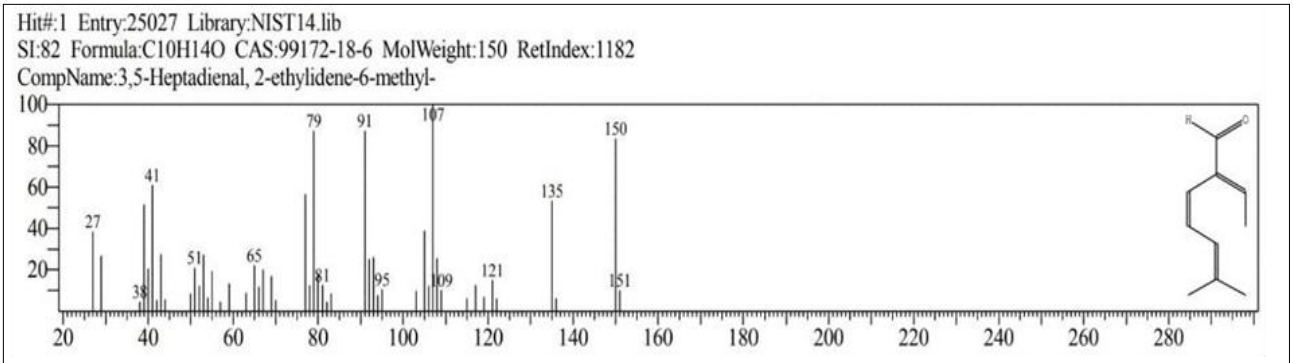
CompName:8,11,14-Eicosatrienoic acid, (Z,Z,Z)-


Hit#:1 Entry:25027 Library:NIST14.lib
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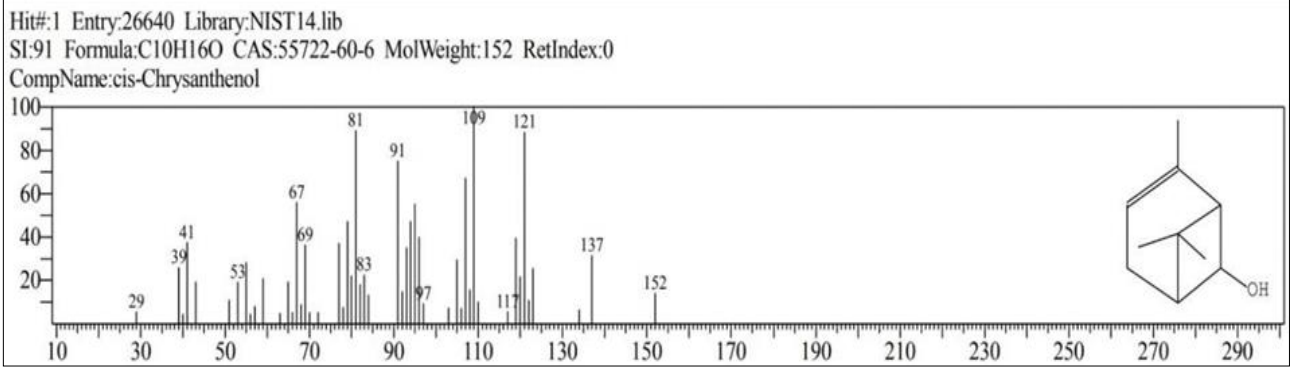
CompName:3,5-Heptadienal, 2-ethylidene-6-methyl-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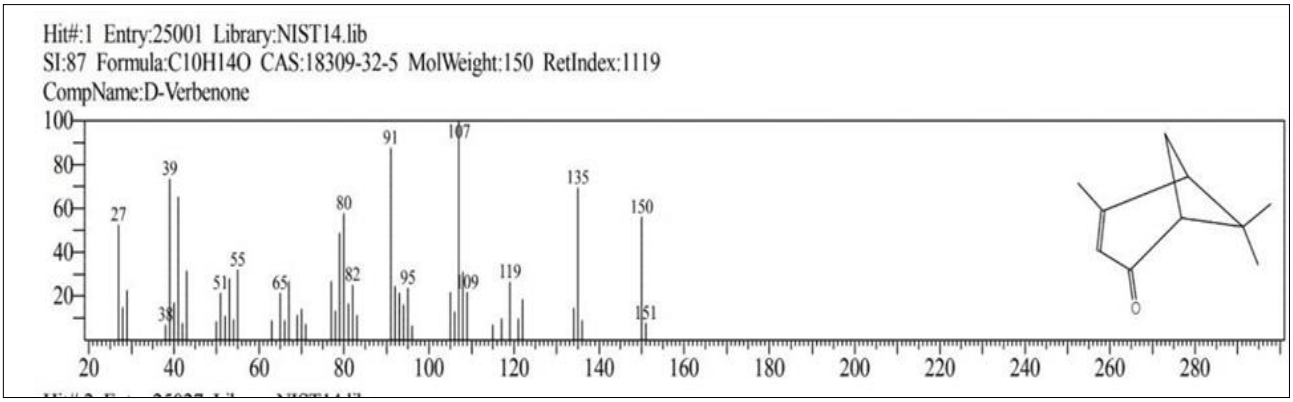
CompName:cis-Chrysanthenol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CompName:D-Verbenone

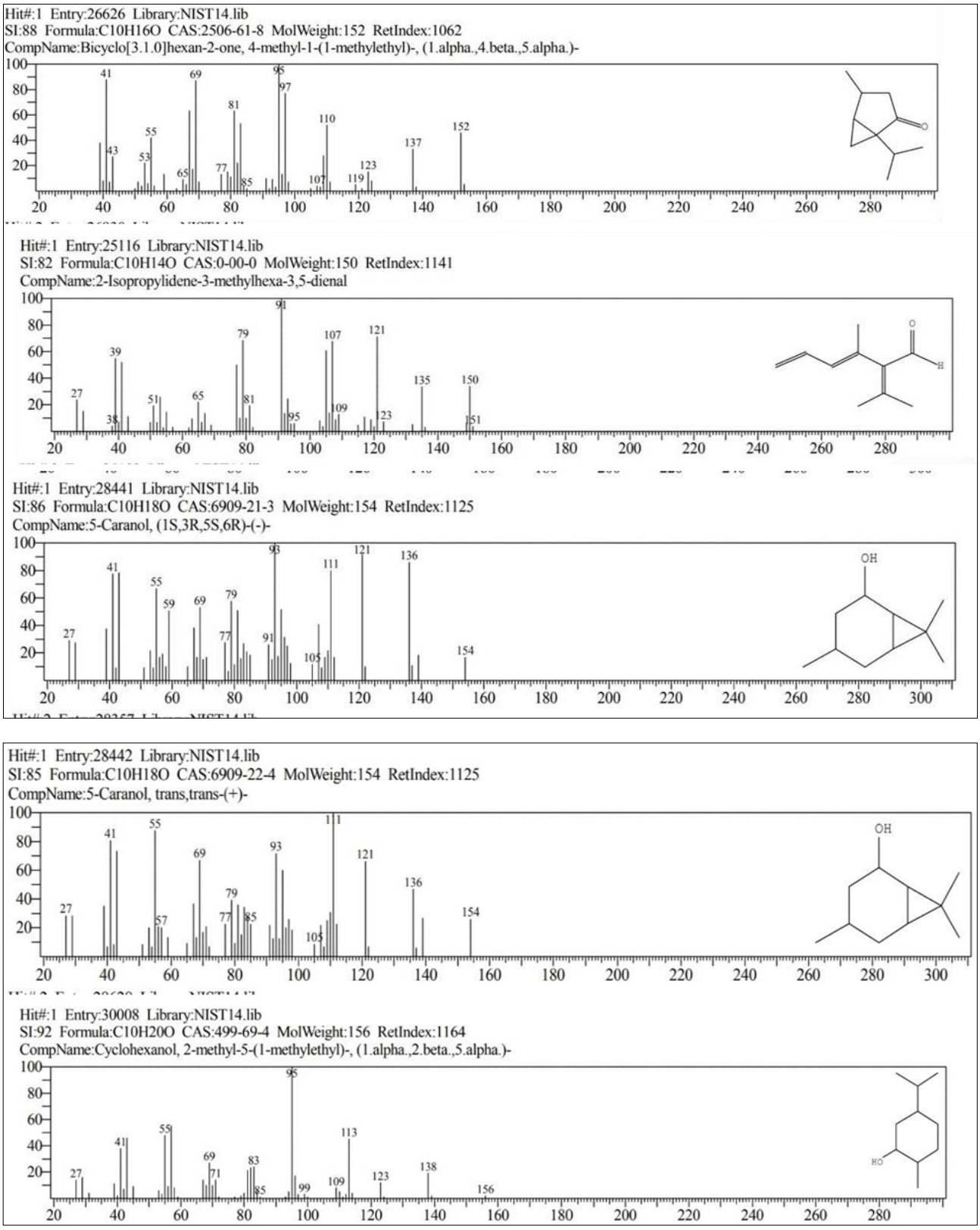

Fig 5: Mass spectra of major compounds identified through GC–MS analysis

Conclusion

The present study investigated the phytochemical composition and volatile constituents of *Blumea axillaris*. Preliminary phytochemical screening confirmed the presence of several important secondary metabolites. GC–MS analysis revealed multiple volatile compounds including terpenoid derivatives.

The results highlight the medicinal potential of *Blumea axillaris* as a natural source of bioactive compounds. Further research is required to isolate and evaluate the pharmacological activities of individual compounds.

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