

Research Article:

Phytochemical Profiling, Antioxidant Activity, and Chemotaxonomic Evaluation of Selected *Salvia* Species from the Kurdistan Region of Iraq

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Abstract

The genus *Salvia* L. (Lamiaceae) is famous for its remarkable phytochemical diversity and broad range of biological activities. Despite the taxonomic and medicinal importance of *Salvia* species from the Kurdistan Region of Iraq, comprehensive phytochemical investigations are still limited. Thus, the current study was aimed to characterize the phytochemical profile of seven *Salvia* species using a combination of gas chromatography-mass spectrometry (GC-MS) profiling, quantification of total phenolic content (TPC), total flavonoid content (TFC), DPPH inhibition and multivariate analyses to evaluate the phytochemical relationship among the species. The GC-MS analysis revealed 29–67 compounds in the studied species, giving rise to unique species-specific chemical fingerprints. The majority of metabolites identified were fatty acids, terpenoids, phenolic derivatives and norisoprenoids. Metabolite composition and phytochemical traits were considerably different between species. Among the studied taxa, the highest TPC (712.34 µg GAE/g), TFC (374.68 µg QE/g) and DPPH inhibition (12.4%) was found in *Salvia spinosa*. Hierarchical cluster analysis revealed two major clusters, comprising (1) *S. spinosa* and *S. bracteata* and (2) *S. indica*, *S. palaestina*, *S. trichoclada*, *S. multicaulis*, and *S. compressa*. The results indicate the phytochemical differences among the studied taxa and the efficiency of metabolite-based approaches for the elucidation of phytochemical relationships in the genus *Salvia*.

Keywords: Antioxidant capacity; bioactive compounds; Lamiaceae; *Salvia*; secondary metabolites.

1. Introduction

The genus *Salvia* L. is one of the most taxonomically complex genera in the Lamiaceae family with approximately 900 taxa distributed in different ecological zones of the world [1, 2]. The genus members are famous for their aromatic properties, medicinal significance and a rich diversity of bioactive secondary metabolites which have garnered considerable scientific attention from botanists, chemists and pharmacologists [3, 4]. Previous studies have demonstrated that *Salvia* extracts exhibit several therapeutic properties including reduction of hyperglycemia, increased

activity of antioxidant enzymes, enhancement of memory, anxiolytic effects, and potential use in treatment of central nervous system disorders [5, 6].

Salvia species, like other members of Lamiaceae, are characterized by herbaceous or shrubby growth, opposite leaves, quadrangular stems, and glandular trichomes, which are sites of biosynthesis for essential oils and phenolic compounds [7, 8]. However, the genus shows considerable morphological diversity, phenotypic plasticity and broad ecological range, which have made species delimitation considerably problematic, as overlapping morphological characteristics and environmental influences on diagnostic traits

often obscure species boundaries and complicate the identification of closely related taxa. The use of phytochemical profiling in combination with molecular markers has become increasingly common as complementary approaches to assist in species discrimination and taxonomic interpretation [9, 10].

The biological activities of *Salvia* species are usually related to secondary metabolites. Of these compounds, phenolic and flavonoid compounds are particularly interesting because they are major contributors to the antioxidant capacity and useful phytochemical markers. Antioxidants protect biological systems by preventing or slowing down oxidation processes induced by free radicals and reactive oxygen species that can otherwise damage cell membranes, induce lipid oxidation and lead to DNA damage [11]. These effects depend on the species, diversity, extraction method and growing-condition. Thus, understanding the species-specific differences in the composition of secondary metabolites is important not only for pharmacological evaluation but also for species discrimination and phytochemical characterization [12].

Comparative phytochemical approaches based on the investigation of patterns of metabolite distribution among related plant species provide valuable information for species discrimination and for the evaluation of phytochemical relationships. Advances in analytical techniques that can detect trace levels of metabolites [12, 13] have led to increasing applications of phytochemical profiling in systematic, ecological and biodiversity studies. Variations of terpenoids, phenolic compounds and other secondary metabolites could provide useful information on phytochemical relationships and ecological adaptations of the genus *Salvia*. These approaches are particularly useful in regions such as the Kurdistan Region of Iraq, where closely related species occur in different environmental conditions that may result in phytochemical differences among the taxa [14].

Iraq, in particular the Kurdistan Region, is a very important area for wild *Salvia* diversity with a rich collection of taxa representing the Middle Eastern flora [15, 16]. The mountainous topography of the region, together with its Mediterranean-like climate and heterogeneous edaphic conditions, offers a wide range of habitats for many *Salvia* taxa. In the north of Iraq there are *Salvia* species such as *Salvia bracteata* L., *S. compressa* Vent., *S. indica* L., *S. multicaulis* Vahl, *S. palaestina* Benth., *S. spinosa* L. and *S. trichoclada* Benth. that are widespread in the north of Iraq and are known to be part of the native flora [17]. These species are ethnobotanically important in the region, being traditionally used in the treatment of several diseases like infection, digestive disorders and inflammatory diseases and are related to their content of secondary metabolites [18].

Gas chromatography–mass spectrometry (GC–MS) is one of the most widely used techniques for detailed phytochemical analysis [19]. GC–MS provides qualitative characterization and relative quantification of volatile and semivolatile metabolites such as monoterpenes, sesquiterpenes, diterpenes, fatty acid derivatives, and phenolic compounds [20]. These classes of compounds are closely related to the antioxidant and antimicrobial activities attributed to *Salvia* [21]. Furthermore, the GC–MS profiling provides

reproducible chemical fingerprints for systematic comparisons among species from different geographical origins [22].

The phytochemical composition and antioxidant capacity of *Salvia* species have been investigated across several countries, including Italy [23], Turkey [24, 25], Iran [26], Tunisia [27], and the USA [28]. Most previous studies have focused on single-technique approaches, and few have combined plant chemical composition and antioxidant activities with multivariate clustering to distinguish *Salvia* species. On the other hand, examining plant species in common geographical areas with overlapping ecological conditions can lead to phytochemical divergence within species, which can be more confidently attributed to taxonomic/genetic factors. The genus *Salvia* has been studied extensively via phytochemical and gas chromatography–mass spectrometry (GC–MS) analyses; however, no exhaustive study has combined triplicate phytochemical assays and pooled gas chromatography–mass spectrometry (GC–MS) profiling of multiple taxa from the Kurdistan Region of Iraq. This integrative approach presents the first systematic description of volatile and semivolatile constituents in these taxa, which extends the phytochemical database of *Salvia* species in this underexplored region. To our knowledge, no comparative phytochemical investigation integrating GC–MS profiling, antioxidant-related parameters, and multivariate analysis has previously been conducted on *Salvia* species from the Kurdistan Region of Iraq. Therefore, the objectives of the present study were to (1) characterize the phytochemical profiles of seven native *Salvia* species in the Kurdistan Region of Iraq via gas chromatography–mass spectrometry (GC–MS) analysis; (2) evaluate their total phenolic content (TPC), total flavonoid content (TFC), and DPPH inhibition; and (3) perform hierarchical cluster analysis (HCA) and generate a heatmap to explore the phytochemical relationships among the investigated taxa on the basis of their phytochemical profiles.

2. Materials and methods

2.1. Chemicals

Folin-Ciocalteu reagent, methanol, sodium carbonate (Na_2CO_3), aluminum chloride solution (AlCl_3), potassium acetate (CH_3COOK), and 2,2-diphenyl-1-picrylhydrazyl (DPPH) were obtained from Merck (Darmstadt, Germany).

2.2. Sample Collection and Study Regions

From spring to autumn of 2025, seven samples of *Salvia* L. taxa were collected from their natural habitats across multiple districts in the Kurdistan Region (Iraq). The taxa examined are illustrated in Figure 1, including *S. bracteata*, *S. compressa*, *S. indica*, *S. multicaulis*, *S. palaestina*, *S. spinosa*, and *S. trichoclada*. Field surveys were conducted at representative sites of different altitudes, climates and ecological settings to provide adequate coverage of the natural distributions of the taxa. Healthy and mature aerial parts were randomly sampled from several individuals of each taxon to minimize the intraspecific variability. After

collection the plants were cleaned, transported to the laboratory and stored at 4 °C.

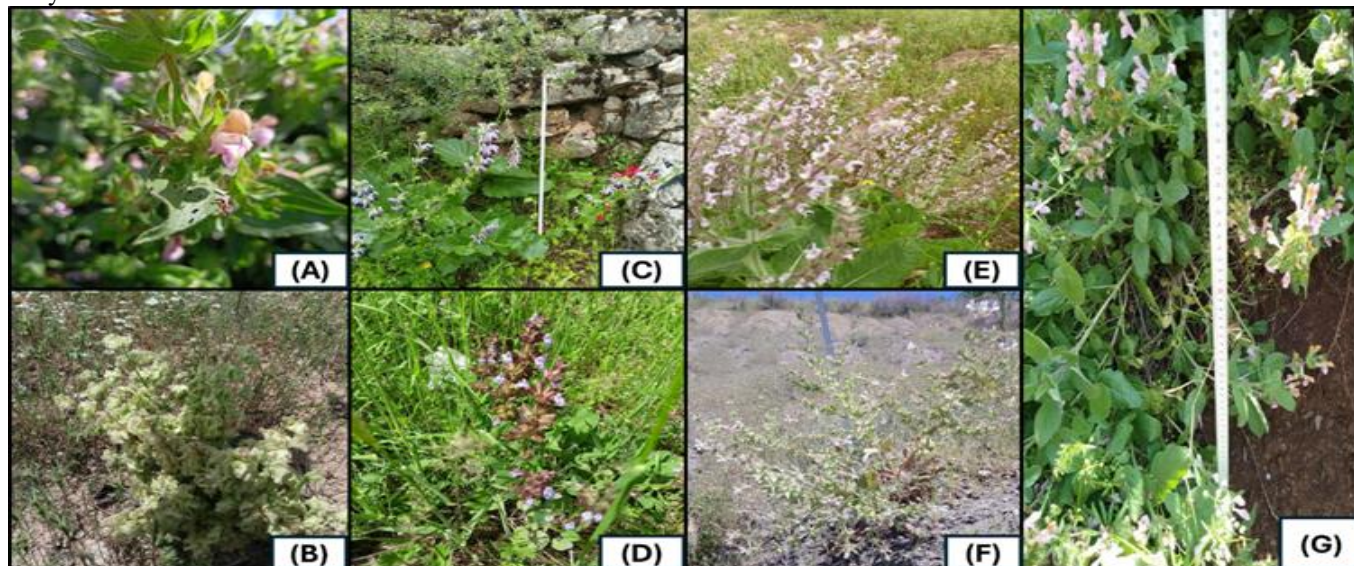


Figure 1: *Salvia* species investigated in this study, including *S. bracteata* (A), *S. compressa* (B), *S. indica* (C), *S. multicaulis* (D), *S. palaestina* (E), *S. spinosa* (F), and *S. trichoclada* (G).

The sampling was conducted in semimountainous and mountainous parts of Iraq at altitudes between 290 and 1985 m a.s.l. (Figure 2). The names of the plant taxa and voucher numbers as well as the altitudes of the sampling areas (Kirkuk (FKI), Rawanduz (MRO), Erbil (FAR), Sulaymaniyah (MSU) and Amadya (MAM)) are shown in Table 1. These areas are recognized as important centres of *Salvia* diversity

in northern Iraq. All taxa were identified by standard floristic keys and morphological characters. Voucher specimens were identified and deposited in the herbarium of the University of Sulaimani. Each species was given a voucher number (SUFA-67 to SUFA-73) to ensure traceability and reproducibility of the research.

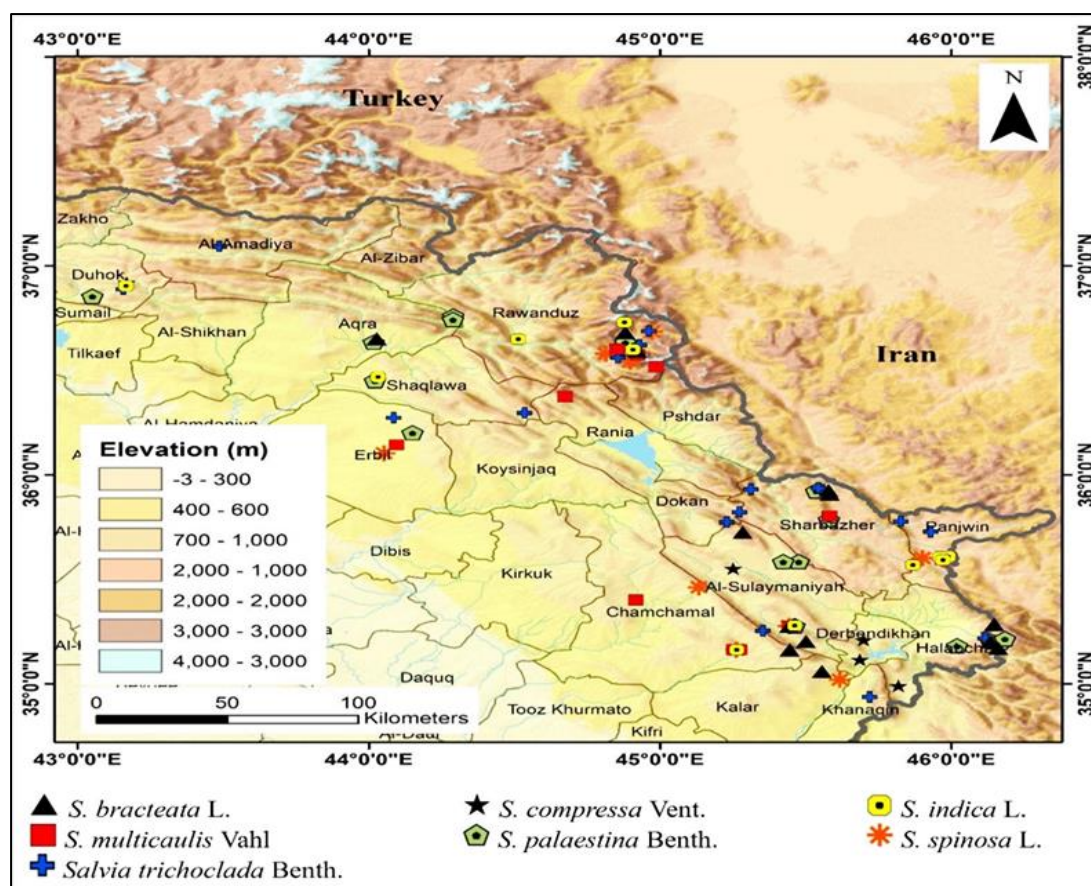


Figure 2: Geographical distribution of *Salvia* across northern Iraq.

Table 1: Distribution of *Salvia* taxa across districts of the Kurdistan Region of Iraq

Taxa name	Voucher number	Locations	Altitude (m)
<i>S. bracteata</i> L.	SUFA-67	MSU, FAR, MAM, and MRO	870-1985
<i>S. compressa</i> Vent.	SUFA-68	MSU and FKI	400-1070
<i>S. indica</i> L.	SUFA-69	MSU, MRO, and MAM	290-1680
<i>S. multicaulis</i> Vahl	SUFA-70	MSU, FAR, FKI, MAM, and MRO	680 -1350
<i>S. palaestina</i> Benth.	SUFA-71	MSU, FAR, FKI, MAM, and MRO	620-1700
<i>S. spinosa</i> L.	SUFA-72	MSU, FAR, FKI, and MRO	400-1160
<i>S. trichoclada</i> Benth.	SUFA-73	MSU, FAR, MAM, and MRO	865-1970

MSU = Sulaymaniyah district; FAR = Erbil district; MAM = Amadya district; MRO = Rawandwz district; FKI = Kirkuk district.

2.3. Preparation of Plant Extracts

In the first step, leaves from different *Salvia* L. species were frozen in liquid nitrogen and then thoroughly powdered. Then, methanol (1 mL) was added to 0.1 g of each sample, and the mixture was placed in a water bath at 45 °C for 3 h. Finally, the mixture was centrifuged at 4500 rpm for 20 min, and the supernatant was collected for subsequent analyses [29].

2.4. Gas Chromatography–Mass Spectrometry (GC–MS) Analysis

The leaf extracts of seven *Salvia* taxa were analyzed via GC–MS (Agilent 7890B–5977B) equipped with an HP-5MS UI capillary column (30 m × 0.25 mm × 0.25 µm; 5% phenyl methyl siloxane). The purge flow rate was 3 mL/min, and the column head pressure was 7.07 psi. The carrier gas was high-purity helium (99.99%) at a constant flow rate of 1.0 mL/min. The samples (1 µL) were injected in splitless mode at an injector temperature of 290 °C. The GC oven program was as follows: 40 °C (1 min hold) to 300 °C at a ramp rate of 10 °C/min. Mass spectra were recorded from *m/z* 35–650 via Agilent MassHunter software. The temperatures of the transfer line, ion source and quadrupole were maintained at 290 °C, 230 °C and 150 °C, respectively [30, 31].

Volatile and semivolatile compounds were identified by matching with the NIST 20 mass spectral library. The minimum criterion for spectral matching was a similarity index (SI) cutoff of ≥800 (out of 1000). Experimental retention indices (RIs) were calculated relative to a homologous series of *n*-alkanes (C8–C40, Sigma-Aldrich) under the same chromatographic conditions to increase identification accuracy. The experimental RIs were compared with literature values reported for nonpolar stationary phases (HP-5MS) with an acceptance window of ±15 RI units. Compounds passing both the spectral similarity threshold and the agreement of the RI were considered tentatively identified (Metabolomics Standards Initiative, MSI Level 2). Compounds whose mass spectra and retention times were specifically matched to those of authentic reference standards run under identical conditions were confirmed (MSI Level 1) [32].

2.5. Total Phenolic Content (TPC) of Plant Extracts

The TPC of the plant leaf extracts was measured as described in previous studies [33]. First, 100 µL of the methanolic extract was mixed with Folin–Ciocalteu (2.1 mL) and 20% Na₂CO₃ (1.8 mL) and then kept in the dark at 25 °C for 1 h. Gallic acid solutions (0.1–1 mg/mL) were applied to generate a calibration curve, and TPC values were calculated from the linear regression equation. The absorbance was recorded at 765 nm via a UV–visible spectrophotometer (Thermo Electron, UK), and the data are expressed as µg of gallic acid equivalents per g of dry leaf weight (µg GAE/g DW).

2.6. Total Flavonoid Content (TFC) of Plant Extracts

Initially, the plant extract (0.5 mL) was added to methanol (1.5 mL), AlCl₃ (0.1 mL), 1 M CH₃COOK (0.1 mL), and distilled water (2.8 mL). In the next step, the solution was incubated at 25 °C for 45 min, and the absorbance was recorded at 415 nm via a spectrophotometer. Quercetin was used as a reference. The TFC was expressed as µg of quercetin equivalents per g of dry leaf weight (µg QE/g DW) [34].

2.7. DPPH Inhibition of Plant Extracts

The plant extract (30 µL) was poured into 1.7 mL of DPPH (0.15 mM methanolic solution), stirred (5 min), and then kept in a dark environment at 25 °C for 30 min. The control was methanol with DPPH. The absorbance was measured at 517 nm. DPPH inhibition (%) was calculated via the following equation (1) [35]:

$$\text{DPPH inhibition (\%)} = \frac{A_{\text{control}} - A_{\text{sample}}}{A_{\text{control}}} \times 100 \quad (1)$$

2.8. Statistical Analysis

All tests were conducted in triplicate for phytochemical evaluation. For GC–MS analysis, the replicates were pooled, and only one composite sample was tested (see supplementary files). The data were analyzed via IBM SPSS Statistics v27, one-way analysis of variance (ANOVA), and Duncan's multiple range test. Hierarchical cluster analysis (HCA) was performed via Ward's method on the basis of Euclidean distance matrices derived from standardized

phytochemical data. Heatmap visualization was generated via ClustVis. The significance level was considered $p \leq 0.05$.

3. Results and Discussion

An integrated assessment of phytochemical diversity across the examined *Salvia* species was conducted via GC–MS profiling combined with the determination of TPC, TFC, and DPPH inhibition. The GC–MS analysis identified species-specific metabolites and dominant chemical classes, thereby enabling species-level phytochemical differentiation. At the same time, the TPC, TFC, and DPPH inhibition results revealed variation in the antioxidant capacity among the species, suggesting biochemical diversity and potential ecological adaptability. The combined approach enabled the comparison of phytochemical composition and antioxidant-related traits among species.

3.1. GC–MS Profiling of *Salvia* species

GC–MS analysis of the *S. bracteata* extracts revealed 67 compounds (Table S1), of which the 25 most abundant

constituents are presented in Table 2. A diverse assemblage of fatty acid derivatives, monoterpenes, sesquiterpenes, and diterpenoid compounds characterized the chemical profile. The major constituents were α -linolenic acid (8.14%), α -pinene (7.13%), camphor (7.05%), palmitic acid (6.88%), camphene (6.44%), and 1,8-cineole (5.20%). Oxygenated monoterpenes, including borneol (2.25%) and bornyl acetate (1.49%), were also detected, suggesting that bioactive oxygenated terpenoids may be linked to the extract's biological properties. Other components identified in the chemical profile were sesquiterpenes: β -caryophyllene (2.14%), humulenol II (2.25%) and α -humulene (1.26%). Moreover, fatty acids and their methyl esters contained α -linolenic acid (8.14%), methyl oleate (7.65%), methyl stearate (1.98%) and stearic acid (1.46%). Ferruginol, a phenolic diterpenoid was detected at a relative abundance of 1.12 %. Linolenic acid is an important biological function of essential omega-3 fatty acids. It plays a role in cardiovascular health, reducing inflammation and as a precursor to longer-chain n-3 fatty acids. These beneficial effects are linked to enhanced lipid metabolism, immunomodulation, and protective effects against metabolic syndrome and cardiovascular injury [36].

Table 2: GC–MS profile of *Salvia bracteata* L.

	Compound of <i>S. bracteata</i>	Area (%)	RT
1	α -Linolenic acid	8.14	24.605
2	Methyl oleate	7.65	24.228
3	α -Pinene	7.13	8.871
4	Camphor	7.05	13.011
5	Palmitic acid	6.88	22.901
6	Camphene	6.44	9.185
7	1,8-Cineole	5.20	10.968
8	2,6-Phenanthrenediol, 1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-7-(1-methylethyl)-, [2S-(2.alpha.,4a.alpha.,10a.beta.)]-	2.73	28.368
9	Methyl palmitate	2.58	22.539
10	Humulenol II	2.25	19.68
11	Borneol	2.25	13.356
12	1H-Cyclopropa[a]naphthalene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, [1aR-(1a.alpha.,7.alpha.,7a.alpha.,7b.alpha.)]-	2.24	17.229
13	β -Caryophyllene	2.14	17.056
14	Methyl stearate	1.98	24.44
15	2,5-Methano-2H-thieno[3,2-b]thiopyran-8-ol, hexahydro-, acetate, (2.alpha.,3a.beta.,5.alpha.,7a.beta.,8R*)-	1.83	27.111
16	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-1-Naphthalenepropanol,.alpha.-ethenyldecahydro-2-hydroxy-	1.79	17.747
17	.alpha.,2,5,5,8a-pentamethyl-, [1R-[1.alpha.pha.(R*),2.beta.,4a.beta.,8a.alpha.]]-	1.52	25.563
18	Bornyl acetate	1.49	15.147
19	Stearic acid	1.46	24.754
20	1(2H)-Naphthalenone, octahydro-4a,8a-dimethyl-7-(1-methylethyl)-, [4aR-(4a.alpha.,7.beta.,8a.alpha.)]-	1.42	20.175
21	2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane	1.39	24.904
22	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	1.29	18.305
23	Fumaric acid, 2-methylcyclohex-1-enylmethyl propyl ester	1.29	15.964
24	α -Humulene	1.26	17.496
25	Ferruginol	1.12	26.467

GC–MS profiling of *S. compressa* leaves identified 49 compounds (Table S2) of which 13 are shown in Figure 3. The major components were benzyl benzoate (17.06%), methyl elaidate (16.08%), α -linolenic acid (13.70%) and palmitic acid (11.55%). Other fatty acid methyl esters were methyl palmitate (5.72%) and methyl stearate (3.19%). Free fatty acids included stearic acid (2.80%). Phenolic constituents were also detected such as pyrogallol (2.28%), 2-methoxy-4-vinylphenol (0.60%) and 4-vinylphenol (0.58%), indicating the presence of compounds often associated with antioxidant activity. In addition, trace amounts of

sesquiterpene alcohols, aromatic alcohol derivatives, cyclohexanone-related compounds and oxygenated heterocycles were identified. *S. compressa* showed a phytochemical profile mainly constituted by aromatic esters and fatty acid derivatives, which clearly differentiated this species from the other *Salvia* species studied. Benzyl benzoate is most well known as a topical scabicide and pediculicide and is used extensively against *Sarcoptes scabiei* (scabies mites) and lice. It acts as a contact neurotoxin, penetrating the exoskeleton of the mite, causing paralysis and death [37].

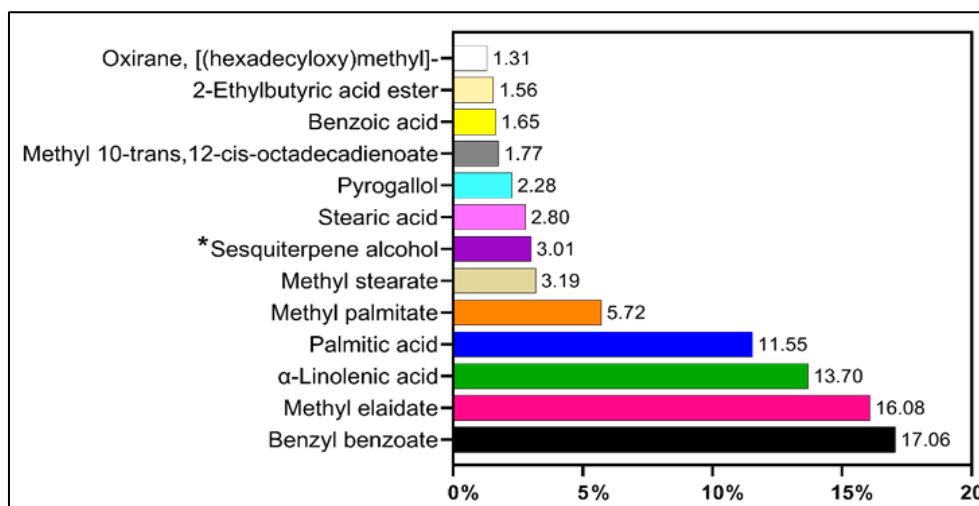


Figure 3: GC–MS profile of *Salvia compressa* Vent. *1-Naphthalenepropanol, α -ethenyldecahydro-2-hydroxy- α -phenyl, 2,5,5,8a-pentamethyl-, [1R-[1. α .(R*), 2. β ., 4a. β ., 8a. α].]-

Chemical profiling of *S. indica* leaves revealed a broad spectrum of 46 tentatively identified compounds (Table S3). The 10 major constituents are shown in Table 3. The chemical composition is dominated by sesquiterpene alcohols and fatty acid derivatives. The major component was a putatively identified naphthalenepropanol-type sesquiterpene alcohol (27.05%) followed by methyl elaidate (18.38%), spathulenol (7.29%), palmitic acid (6.36%) and methyl palmitate (5.88%). Other oxygenated sesquiterpenes included a dihydroxylated naphthalenepropanol derivative (3.57%) and a tricyclic hydroxylated sesquiterpene (1.07%). Prominent were also the constituents of fatty acids, especially elaidic acid (3.55%), methyl stearate (3.38%) and

methyl octadecadienoate isomer (1.26%). The presence of elaidic acid and its methyl ester (methyl elaidate) may be a partial methylation occurring during extraction or the natural state of lipid metabolism in this species. *S. indica* phytochemical profile was characterized by the predominance of sesquiterpene alcohols and the abundance of the fatty acids and their methyl esters. Methyl elaidate is the methyl ester of elaidic acid, a major trans fatty acid found in hydrogenated oils, and has biological activity mainly through its conversion to elaidic acid in cells. It affects lipid metabolism, cholesterol synthesis, inflammation and epigenetic regulation, important for cardiovascular disease, obesity and cancer risk [38].

Table 3: GC–MS profile of *Salvia indica* L.

	Compound of <i>Salvia indica</i>	Area (%)	RT
1	1-Naphthalenepropanol, α -ethenyldecahydro-2-hydroxy- α -phenyl, 2,5,5,8a-pentamethyl-, [1R-[1. α .(R*), 2. β ., 4a. β ., 8a. α].]-	27.05	25.571
2	Methyl elaidate	18.38	24.228
3	Spathulenol	7.29	19.036
4	Palmitic acid	6.36	22.885
5	Methyl palmitate	5.88	22.539
6	1-Naphthalenepropanol, α -ethenyldecahydro-2,4-dihydroxy- α -phenyl, 2,5,5,8a-pentamethyl-, [1R-(1. α .(R*), 2. β ., 4. α ., 4a. β ., 8a. α .)]-	3.57	27.268
7	Elaidic acid	3.55	24.566
8	Methyl stearate	3.38	24.44
9	Methyl 9-cis,11-trans-octadecadienoate	1.26	24.998
10	5. α -Hydroxy-4. α ., 8,10,11-tetramethyltricyclo[6.3.0.0(2,4)]undec-10-ene	1.07	20.866

The phytochemical compositions of *S. multicaulis* are presented in Figure 4 and Table S4.

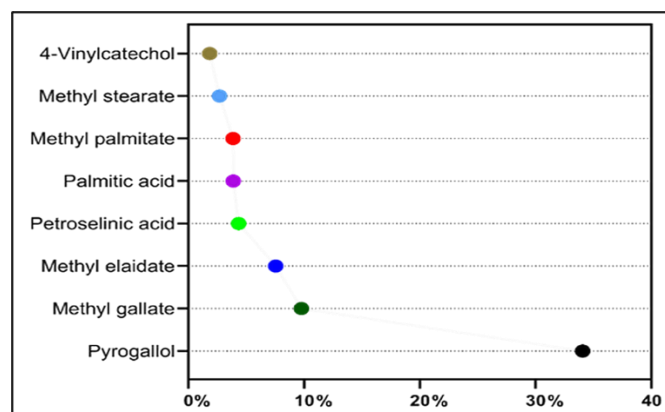


Figure 4: GC-MS profile of *Salvia multicaulis* Vahl.

The profile was dominated by phenolic metabolites, with pyrogallol representing the most abundant constituent (34.1%), followed by methyl gallate (9.8%) and 4-vinylcatechol (1.7%). Fatty acid derivatives, including methyl elaidate (8.9%), petroselinic acid (4.2%), palmitic acid (3.2%), methyl palmitate (3.1%), and methyl stearate (2.1%), were also abundant. Minor constituents detected at early retention times included low-molecular-weight polar metabolites such as pyranone derivatives, thymine, and N-hydroxymethylacetamide, as well as trace amounts of

sugar-derived compounds. Minor terpenoid-related compounds were also identified. *S. multicaulis* presented a phenolic-rich phytochemical profile complemented by lipid-derived constituents.

GC-MS analysis of *S. palaestina* revealed 45 fatty acids, fatty acid methyl esters, terpenoid derivatives, glycerolipids, and minor aromatic metabolites (Table S5), 12 of which are listed in Table 4. The chemical profile was dominated by fatty acid methyl esters, particularly methyl oleate (23.60%), followed by naphthalenepropanol-type sesquiterpene alcohol (13.08%), methyl palmitate (8.74%), palmitic acid (7.36%), methyl stearate (7.16%), and α -linolenic acid (6.45%). The additional fatty acid constituents included stearic acid (3.08%) and a methyl octadecadienoate isomer (1.48%). Glycerol tricaprylate (3.04%), a triglyceride, was also detected among the major constituents. Other notable compounds included loliolide (1.90%), a carotenoid-derived norisoprenoid lactone, a hydroxylated naphthalenepropanol sesquiterpene alcohol (1.51%), and a benzopyran derivative (1.28%). Overall, *S. palaestina* presented a phytochemical profile characterized by the codominance of fatty acid methyl esters and oxygenated sesquiterpenes. Methyl oleate shows notable biological activity, primarily as an antimicrobial agent against multidrug-resistant bacteria, while also serving as a precursor to oleic acid, which regulates lipid metabolism, energy storage, and signaling pathways [39]

Table 4: GC-MS profile of *Salvia palaestina* Benth.

	Compound of <i>S. palaestina</i>	Area (%)	RT
1	Methyl oleate	23.60	24.228
2	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-2-hydroxy-.alpha.-pha.,2,5,5,8a-pentamethyl-, [1R-[1.alpha.(R*),2.beta.,4a.beta.,8a.alpha.]]-pha.]]-	13.08	25.564
3	Methyl palmitate	8.74	22.539
4	Palmitic acid	7.36	22.885
5	Methyl stearate	7.16	24.44
6	α -Linolenic acid	6.45	24.59
7	Stearic acid	3.08	24.747
8	Glycerol tricaprylate	3.04	30.772
9	Loliolide	1.90	21.165
10	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-4-hydroxy-.alpha.-pha.,5,5,8a-tetramethyl-2-methylene-, [1S-[1.alpha.pha.(R*),4.beta.,4a.beta.,8a.alpha.]]-	1.51	25.697
11	Methyl 9-cis,11-trans-octadecadienoate	1.48	24.998
12	4,2,8-Ethanylylidene-2H-1-benzopyran, octahydro-4-methyl-	1.28	25.179

Figure 5 illustrates the major composition of *S. spinosa* and all 64 detected chemicals are summarized in Table S6. The predominant chemical classes were phenolic and aromatic compounds, particularly hydroxyquinol (20.73%) and benzoic acid (15.02%) indicating the predominance of phenolic and aromatic metabolites. The profile was further enriched with other aromatic constituents such as methyl benzoate (1.08%). Furan derivatives were also present in high amounts, especially 2-allylfuran (8.74%) and 2,4-dihydroxy-2,5-dimethyl-3(H)-furan-3-one (1.23%). Fatty acids

and methyl esters were found to contribute significantly to middle and late retention regions such as oleic acid (3.97%), methyl palmitate (3.05%), palmitic acid (2.92%) and 13-octadecenoic acid methyl ester (3.48%). The sugar-derived compounds were methyl β -D-glucopyranoside (1.36%) and the minor constituents were γ -sitosterol (1.04%), a phytosterol. Characteristic profiles of phenolic and aromatic phytochemicals in *S. spinosa* were supplemented with furan derivatives, fatty acids and carbohydrate-derived compounds.

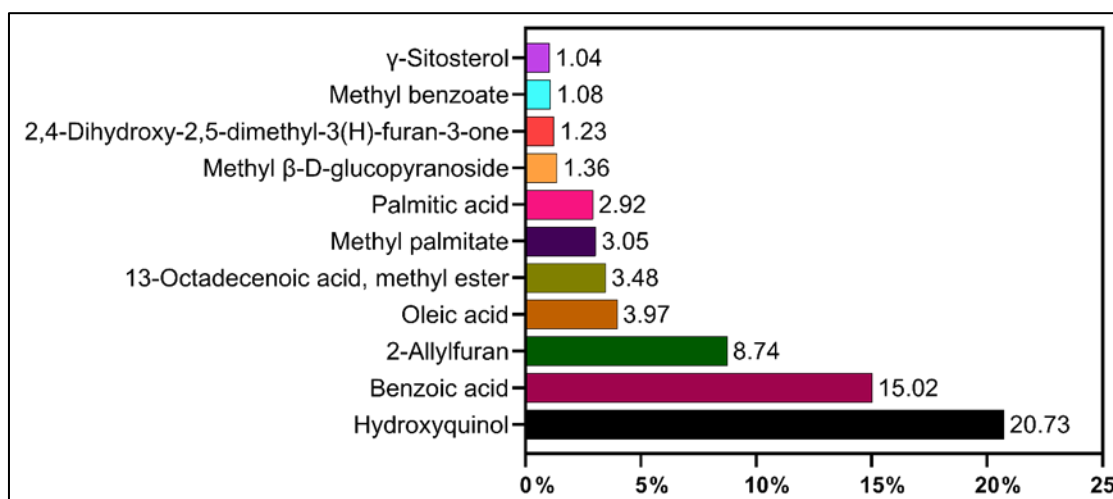


Figure 5: GC-MS profile of *Salvia spinosa* L.

The 10 main chemical compositions of *S. trichoclada* are presented in Table 5 and all 46 detected chemicals are listed in Table S7. The results showed a chemically heterogeneous profile, mainly composed of lipid-derived components, with terpenoid and aromatic compounds in minor amounts. The chemical composition was characterized by a high abundance of fatty acids and their methyl esters, especially α -linolenic acid (22.14%), methyl elaidate (17.62%), palmitic acid (14.66%), methyl palmitate (6.20%) and methyl stearate (4.91%) which represented about 65% of the total chromatographic area. The naphthalenepropanol-type sesquiterpene alcohol was also abundant (7.54 %), indicating that the oxygenated sesquiterpenes contributed to the profile. The minor components were a methyl

octadecadienoate isomer (1.29%), an acyclic sesquiterpene hydrocarbon of the farnesene type (1.33%), camphor (1.15%), an oxygenated monoterpene also found in *S. bracteata*, and a benzopyran derivative (1.09%) previously reported from *S. palaestina*. The predominant phytochemical profile of *S. trichoclada* consists of saturated and unsaturated fatty acids and fatty acid methyl esters. α -Linolenic acid (ALA) is an essential omega-3 fatty acid with strong biological activity: it improves cardiovascular health, reduces inflammation through oxylipin metabolites, and supports metabolic balance, although its

conversion to EPA/DHA is limited. Recent studies highlight its role in lowering triglycerides, C-reactive protein, and cardiovascular risk [40].

Table 5: GC-MS profile of *Salvia trichoclada* Benth.

	Compound of <i>S. trichoclada</i>	Area (%)	RT
1	α -Linolenic acid	22.14	24.613
2	Methyl elaidate	17.62	24.228
3	Palmitic acid	14.66	22.901
4	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-2-hydroxy-.alpha.-pha.,2,5,5,8a-pentamethyl-, [1R-[1.alpha.(R*),2.beta.,4a.beta.,8a.alpha.]]-	7.54	25.564
5	Methyl palmitate	6.20	22.539
6	Methyl stearate	4.91	24.44
7	(2Z,4E)-3,7,11-Trimethyl-2,4,10-dodecatriene	1.33	25.697
8	Methyl 9-cis,11-trans-octadecadienoate	1.29	24.998
9	Camphor	1.15	13.027
10	4,2,8-Ethanylylidene-2H-1-benzopyran, octahydro-4-methyl-	1.09	25.179

Ertas *et al.* (2021) investigated five *Salvia* taxa (*S. cerinopruinosa*, *S. cerinopruinosa*, *S. pseudeuphratica*, *S. rosifolia*, and *S. kurdica*) in Turkey. They reported that the main components of their essential oils were camphor (55.80%) and germacrene-D (41.79%) and that oleic acid (72.65%) was the major fatty acid component [41]. In another study, *Salvia* species were found to contain diterpenes ($n = 19$), flavonoids ($n = 18$), phenolic and organic acids ($n = 15$), sesterpenes ($n = 5$), and triterpenes ($n = 2$) [42]. Researchers in the USA reported that the primary constituents

of 3 *Salvia* species are oxygenated monoterpenoids [28]. Other authors in South Africa noted a clear difference between *S. stenophylla* and *S. runcinate* [43]. A study conducted in Iran identified five primary fatty acids in *Salvia* seed oils: α -linolenic acid, linoleic acid, oleic acid, palmitic acid, and stearic acid [44]. In Greece, the authors reported that 1,8-cineole was the main volatile in *S. fruticosa*, accounting for 34.8–39.0%, whereas *S. pomifera* contained relatively high levels of α -thujone (19.7–41.0%) [45]. The main compounds in the oils were (E)-nerolidol in *S.*

runcinata and *S. stenophylla* and ledol in *S. repens* [46]. Another researcher reported that the main constituents included α -pinene in *S. albigata* (12%), camphor in *S. blepharochlaena* (29%), borneol in *S. virgata* (20%), 1,8-cineole in *S. absconditiflora* (30%), and linalool in *S. palaestina* (27%) [47]. Demirpolat (2024) reported that the primary compounds in the 6 *Salvia* taxa examined were 1,8-cineol, caryophyllene oxide, spathulenol, and borneol [48]. In another study, the main component of *S. hispanica* was rosmarinic acid (0.92 mg/g) [49]. Panțuroiu *et al.* (2026) reported that *S. sclarea* has relatively high contents of rosmarinic and protocatechuic acids, whereas *S. pratensis* contains relatively high contents of hydroxycinnamic acids [50]. *S. clandestina* contains a high level of danshensu (4.8 mg/g), whereas *S. sclarea* is rich in rosmarinic acid (15.6 mg/g) [24]. These findings suggest that genetic factors mainly determine the ability to modify volatile compound production. When a chemotype of *S. lavandulifolia* was exposed to relatively high temperatures, it presented increased expression of β -caryophyllene, caryophyllene oxide, and manool [51].

3.2. TPC, TFC, and DPPH Inhibition

The TPC, TFC, and DPPH inhibition of *Salvia* species are shown in Figure 6. There were significant differences in the TPC, TFC, and DPPH inhibition values among the species ($p < 0.05$). Among the investigated taxa, *S. spinosa* presented the highest TPC ($712.3 \pm 2.46 \mu\text{g GAE/g}$), TFC ($374.7 \pm 2.91 \mu\text{g QE/g}$), and DPPH inhibition ($12.4 \pm 0.03\%$), indicating strong antioxidant potential. *S. bracteata* ranked second in terms of phytochemical content (TPC = $661.4 \pm 4.02 \mu\text{g GAE/g}$, TFC = $348.8 \pm 5.11 \mu\text{g QE/g}$, and DPPH inhibition = $11.6 \pm 0.02\%$). In contrast, *S. compressa* presented the lowest TPC value ($444.2 \pm 9.15 \mu\text{g GAE/g}$), whereas *S. multicaulis* presented the lowest TFC ($234.6 \pm 2.58 \mu\text{g QE/g}$) and DPPH inhibition ($9.09 \pm 0.03\%$). The antioxidant capacity of plants is influenced primarily by their phenolic and flavonoid contents, which enable them to efficiently neutralize free radicals via hydrogen or electron donation [52, 53].

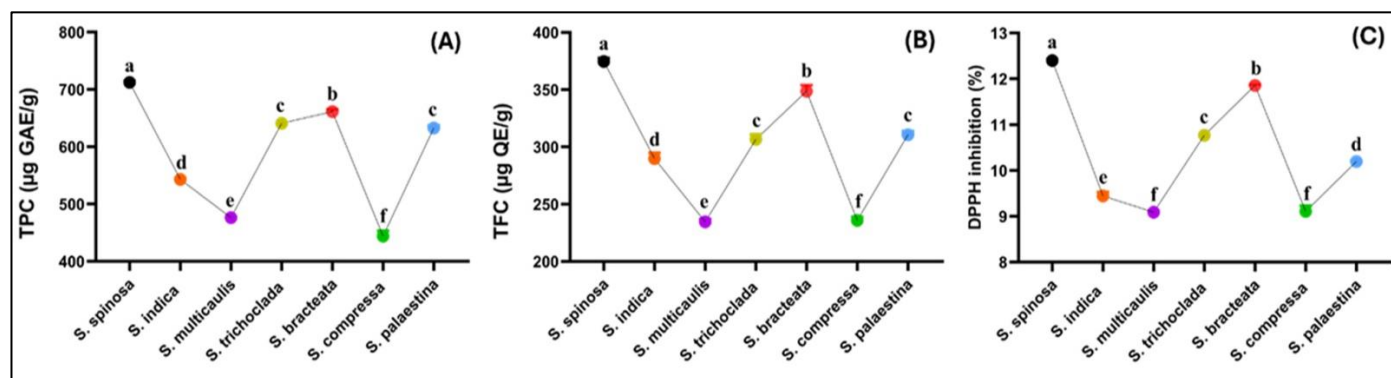


Figure 6: TPC (A), TFC (B), and DPPH inhibition (C) of different *Salvia* species. Different small letters in each chart indicate statistically significant differences ($p < 0.05$) among *Salvia* species.

The findings of this study align with previous reports on *Salvia* species from the Mediterranean and Asian regions, which documented high TPC and strong antioxidant capacity in selected taxa [54, 55]. Authors in Iran investigated the antioxidant capacity of 20 distinct *Salvia* species and reported significant variation in the TFC of the species studied ($p < 0.05$). In line with our results, *S. spinosa* presented the greatest accumulation at $374.68 \mu\text{g QE/g DW}$, whereas *S. multicaulis* presented the lowest accumulation [10]. The authors of Türkiye reported that the TFC, TPC, and DPPH inhibition of *S. absconditiflora* were $412.4 \text{ mg QE/100 g}$, 184.8 mg GAE/g , and $185.1 \mu\text{mol TE/g}$, respectively [56]. A previous study on *Salvia* species from Eastern Europe revealed that the order of antioxidant activity potency among species is as follows: *S. officinalis* > *S. verticillata* > *S. sclarea* > *S. kopetdaghensis* > *S. aethiopis* > *S. tesquicola* [41]. Another study examined four *Salvia* hybrids and reported that the TPC (mg GAE/g) values for *S. fruticosa* $\times$ *S. officinalis*, *S. aramiensis* $\times$ *S. officinalis*, *S. aramiensis* $\times$ *S. officinalis*, and *S. fruticosa* $\times$ *S. officinalis* were 92.10, 90.99, 91.00, and 87.99, respectively, whereas the TFC (mg RE/g) values were 50.85, 34.60, 34.86, and 41.63, respectively [57]. In *S. modesta*, the TPC (mg

GAE/g) was greater in the aqueous decoction extract (78.63) than in the methanolic extract (60.50) and the dichloromethane extract (24.18). DPPH inhibition (mg TE/g) was highest in the methanol extract (97.76), followed by the aqueous decoction extract (89.52) and the dichloromethane extract (14.43). These data support the importance of extraction solvent polarity in determining the recovery of phenolic and flavonoid compounds [58]. A study reported that *S. verticillata* is rich in phenolics, with a mean of $359.6 \pm 11.7 \text{ mg GAE/g}$ and a DPPH inhibition IC_{50} of $15.8 \mu\text{g/mL}$ [59]. Another study reported that the TPC and DPPH inhibition of *S. hispanica* were $1.64 \pm 0.21 \text{ mg GAE/g}$ and 68.83%, respectively [49]. In another study, the TPC of *S. pratensis* was 79.22 mg GAE/g , whereas that of *S. sclarea* was 52.50 mg GAE/g . Additionally, the DPPH IC_{50} values were $6.67 \mu\text{g/mL}$ for *S. sclarea* and $3.16 \mu\text{g/mL}$ for *S. pratensis* [50]. The observed discrepancies in the TPC, TFC, and DPPH inhibition values in the current study, compared with those reported in the literature, may be affected by factors such as species-dependent regulation of phenolic biosynthesis, geographical origin, climate conditions, extraction solvent concentration, and plant developmental stages at the time of sampling [10]. Phenolic compounds are

among the most important classes of plant secondary metabolites, serving as antioxidants, UV protectants, and defense molecules against herbivores and pathogens [60].

3.3. Multivariate analysis

The overlap of phenotypic features among *Salvia* species complicates traditional morphological classification. Currently, integrating GC and antioxidant data may help with species delimitation [61,62]. As illustrated in Figure 7, hierarchical cluster analysis (HCA) of the compounds

identified via GC–MS classified the seven *Salvia* species into two main clusters at the chosen dissimilarity level. The first cluster included *S. spinosa* and *S. bracteata*, indicating a potential phytochemical relationship among these species. The second major cluster included *S. indica*, *S. palaestina*, *S. trichoclada*, *S. multicaulis*, and *S. compressa*. In the second cluster, *S. palaestina* and *S. trichoclada* were closely related, whereas *S. multicaulis* and *S. compressa* constituted a separate subgroup. The clustering pattern revealed significant chemical diversity among the *Salvia* species studied, highlighting unique metabolite signatures for each species.

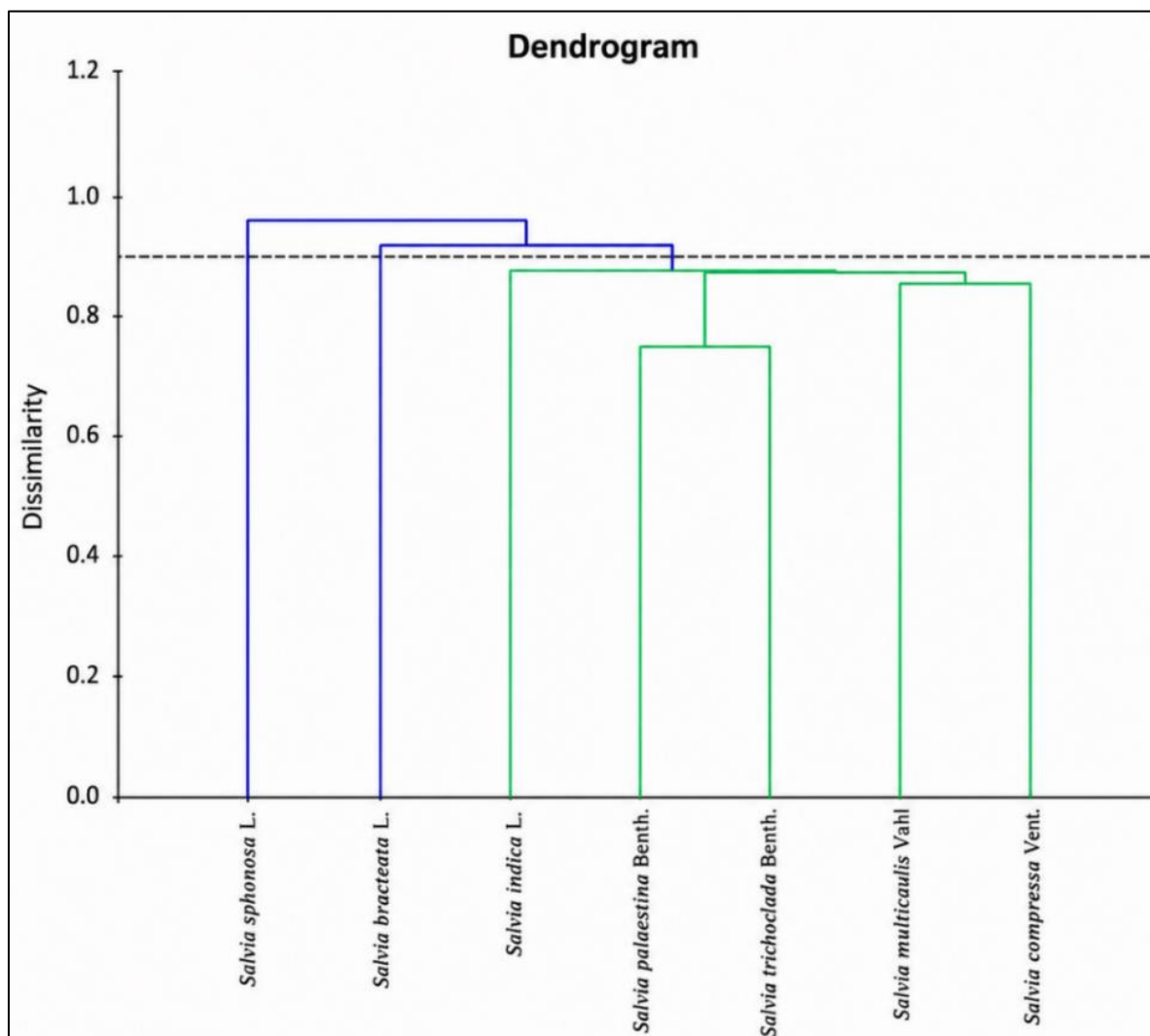


Figure 7 Dendrogram of hierarchical cluster analysis (HCA) illustrating the grouping of the investigated *Salvia* species on the basis of their GC–MS-identified chemical compounds.

Figure 8 displays the heatmap and hierarchical clustering (UPGMA) based on the TPC, TFC, and DPPH inhibition for the seven *Salvia* species. The heatmap shows the phytochemical variation among *Salvia* species by visualizing the TPC, TFC, and DPPH inhibition. Warmer colors indicate higher values and are associated mainly with *S. spinosa* and *S. bracteata*, whereas cooler colors are typical of *S. multicaulis* and *S. compressa*. The similar distribution

patterns among TPC, TFC, and DPPH inhibition might indicate an identical buildup of these secondary metabolites across taxa. The UPGMA clustering was consistent with the hierarchical clustering, separating species with higher phytochemical contents from those with lower contents. These results suggest that traits related to phenolics and flavonoids can be used to distinguish between species.

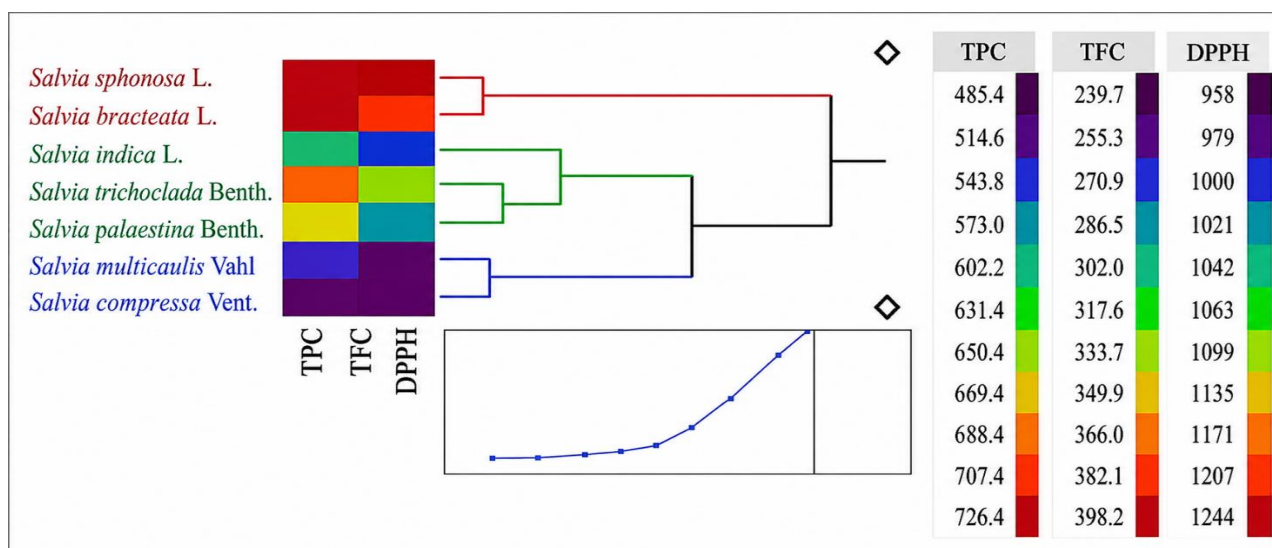


Figure 8 Heatmap and hierarchical cluster analysis (UPGMA) of *Salvia* species based on TPC, TFC, and DPPH inhibition. The color gradients represent variations in phytochemical content among the studied taxa.

The authors in Iran concluded that flavonoids are effective markers for understanding the taxonomic relationships among *Salvia* species. They reported that *S. spinosa* was discrete from *S. reuterana* on the basis of cluster analysis. Although *S. nemorosa* and *S. virgata* share remarkable morphological similarities, they are clearly distinct species. Additionally, *S. spinosa* and *S. macrosiphon* clustered together, whereas *S. ceratophylla* and *S. multicaulis* formed distinct groups [63]. Luca *et al.* reported that *S. austriaca*, *S. nutans*, and *S. officinalis* each formed distinct clusters. In contrast, the other species, including *S. sclarea*, *S. tesquicola*, *S. aethiopis*, *S. verticillata*, *S. nemorosa*, and *S. pratensis*, presented similar compositions [42]. In one study, the UPGMA dendrogram divided *Salvia* species into two clusters. Caprylic, behenic, and lignoceric acids were the main features for grouping species within the genus. *S. chloroleuca* and *S. atropatana* were placed in cluster I and distinguished from other species on the basis of their shoot fatty acid profiles [64]. It was also reported that the aerial parts are more identical to each other than the roots are. The chemical variations were driven primarily by sugiol in *S. yangii* leaves and by carnosic acid quinone in *S. abrotanoides*. In the roots, the differences were supported by the presence of 5 norditerpenoids in *S. yangii* and 2 flavonoids plus 1 norditerpenoid in *S. abrotanoides* [65]. Saleh analyzed the chemical composition of ten *Salvia* species via FTIR spectroscopy, and cluster analysis revealed that *S. syriaca* and *S. spinosa* are the closest species [66]. Authors in Italy reported similarities between the profiles of *S. fruticosa* and *S. officinalis*, whereas *S. clandestina* and *S. sclarea* had distinct compositions [23]. Foutami *et al.* examined herbarium samples from four *Salvia* species obtained over 150 years in the Mediterranean and compared them with modern plants. They reported that neither the collection year nor the altitude affected the chemical composition of these species, which was determined primarily by species and geographic factors [67, 68]. Furthermore, another study

revealed that the diversity of *Salvia* compounds is influenced by environmental factors [69].

Since secondary metabolite profiles of plants can be influenced by factors such as environmental conditions and plant growth stage, which are independent of genetics, the clustering patterns presented in this study must be combined with molecular markers and morphological examinations. Therefore, our results rely on phytochemical compositions and do not definitively determine phylogenetic or taxonomic relationships.

4. Conclusion

In the present study, GC–MS profiling, TPC, TFC, and DPPH inhibition were performed for seven *Salvia* species. Furthermore, the chemotaxonomic affinities of the species were assessed via multivariate analyses. There are considerable differences in phytochemical traits and specific chemical signatures among *Salvia* taxa. GC–MS analysis revealed distinct classes of bioactive compounds, including fatty acids, terpenoids, norisoprenoids, and aromatic metabolites. *S. spinosa* presented the highest TPC, TFC, and DPPH inhibition values. Hierarchical clustering and heatmap analyses revealed distinct phytochemical relationships among species, identifying two major clusters. One of the most important limitations of our study was financial constraints, which prevented us from including molecular markers and phylogenetic analyses. The results not only enrich the chemical characterization of *Salvia* species but also provide a methodological framework for future phytochemical surveys in the region. This work contributes to the scientific knowledge of *Salvia* chemistry, reports new compounds, defines methodological standards and provides the basis for further pharmacological and conservation studies. Future studies should integrate molecular phylogenetics and biological activity assays to clarify the evolutionary relationships and taxonomic boundaries within this diverse genus in Iraq.

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Author contributions

Lanja Hewa Khal: Formal analysis, Investigation, Methodology. Shamiran Salih Abdulrahman: Methodology, Writing - Review & Editing, Data interpretation. Ali Mala Khedir Galalae and Djshwar Dhahir Lateef: Methodology, Writing - Review & Editing, Data interpretation. Jotyar Jassim Muhammed: Writing – original draft, Investigation, Formal analysis. Hawar Halshoy: Formal analysis, Investigation, Methodology, Writing – original draft, Writing - Review & Editing. Lanja Hewa Khal and Kamaran Salh Rasul: Supervision, project administration, conceptualization, writing, review, and editing.

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Data availability statement

The datasets generated during and/or analyzed during the current study are available from the corresponding author upon reasonable request.

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Not applicable

Conflicts of interest

The authors declare that they have no conflicts of interest.

Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the author(s) used AI tools to improve language and readability. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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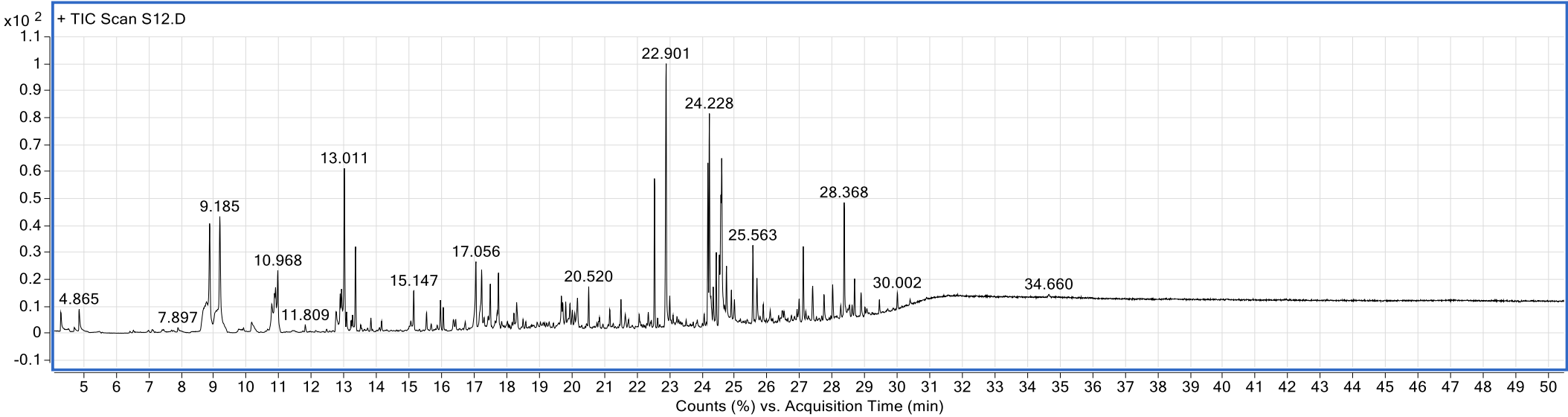
Supplementary Tables

Table S1: *Salvia bracteata* L

Peak	R.T.	Area	Pct Total	Area Pct	Library/ID	Ref	CAS	Qual
1	4.299	607096	0.84	0.8397	3-Methoxy-2,2-dimethyloxirane	4872	026196-04-3	40
2	4.716	147913	0.205	0.2046	2-Propenoic acid, methyl ester	1896	000096-33-3	25
3	4.865	639438	0.884	0.8845	Methanamine, N-hydroxy-N-methyl-	363	005725-96-2	5
4	5.485	173031	0.239	0.2393	Butanoic acid, 2-methyl-, methyl ester	9322	000868-57-5	78
5	6.53	211056	0.292	0.2919	4-(Methylthio)-1-butene	4899	020582-83-6	9
6	7.111	95410	0.132	0.132	2-Furanmethanol	3475	000098-00-0	55
7	7.457	147491	0.204	0.204	Butanoic acid, 2-methylene-, methyl ester	8286	002177-67-5	60
8	7.708	74239	0.103	0.1027	N-Methyl-N-(2-hydroxyethyl)carbamic acid, methyl ester	16780	056475-94-6	38
9	7.897	217058	0.3	0.3002	Sulfide, 2-hydroxybutyl 2-hydroxypropyl	40127	1010159-77-2	25
10	8.871	5154689	7.13	7.13	(1S)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	18189	007785-26-4	97
11	9.185	4655108	6.439	6.439	Camphene	17993	000079-92-5	96
12	9.916	369461	0.511	0.511	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one	23815	010230-62-3	49
13	10.167	502242	0.695	0.6947	Decane	22067	000124-18-5	55
14	10.968	3755939	5.195	5.1953	Eucalyptol	30918	000470-82-6	93
15	11.463	125436	0.174	0.1735	6-Thiabicyclo[3.2.1]octane	14169	000279-91-4	43
16	11.809	157098	0.217	0.2173	D-Alanine, N-propargyloxycarbonyl-, tridecyl ester	262604	1000347-74-4	64
17	12.469	71575	0.099	0.099	Maltol	12679	000118-71-8	64
18	13.011	5097414	7.051	7.0508	(+)-2-Bornanone	29115	000464-49-3	98
19	13.356	1628146	2.252	2.2521	endo-Borneol	30950	000507-70-0	97
20	13.513	144735	0.2	0.2002	Terpinen-4-ol	30971	000562-74-3	91
21	13.718	109689	0.152	0.1517	Cyclohexene, 1-methyl-4-(1-methylethylidene)-	18196	000586-62-9	80
22	13.828	227486	0.315	0.3147	Bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-	29367	000515-00-4	97
23	14.158	286526	0.396	0.3963	Ethanol, 2-phenoxy-	19879	000122-99-6	97
24	15.147	1079822	1.494	1.4936	Bornyl acetate	71351	000076-49-3	99
25	15.54	326239	0.451	0.4513	2-Methoxy-4-vinylphenol	28303	007786-61-0	95
26	15.682	180693	0.25	0.2499	Sabinyol stearate	312695	1000465-84-3	27
27	15.964	932639	1.29	1.29	Fumaric acid, 2-methylcyclohex-1-enylmethyl propyl ester	155412	1000345-15-4	35
28	16.436	471031	0.652	0.6515	.alpha.-Cubebene	80165	017699-14-8	95

29	16.726	184446	0.255	0.2551	1-Fluoro-1-hex-1-ynyl-2,2-dimethyl-cyclopropane	43318	1000300-49-2	46
30	17.056	1544934	2.137	2.137	Caryophyllene	80121	000087-44-5	99
31	17.229	1621583	2.243	2.243	1H-Cyclopropa[a]naphthalene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, [1aR-(1a.alpha.,7.alpha.,7a.alpha.,7b.alpha.)]-	80556	017334-55-3	99
32	17.496	907340	1.255	1.255	1,4,7,-Cycloundecatriene, 1,5,9,9-tetramethyl-, Z,Z,Z-	80275	1000062-61-9	98
33	17.747	1294281	1.79	1.7903	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	78053	000644-30-4	99
34	18.305	933441	1.291	1.2911	Naphthalene, 1,2,3,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S-cis)-	80407	000483-76-1	96
35	18.502	347311	0.48	0.4804	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	54796	017092-92-1	86
36	18.769	133543	0.185	0.1847	2,3,5,6-Tetrafluoroanisole	55332	002324-98-3	83
37	18.934	115923	0.16	0.1603	o-Cymene	16996	000527-84-4	60
38	19.68	1630121	2.255	2.2548	Humulenol-II	99145	019888-00-7	99
39	20.175	1026794	1.42	1.4203	1(2H)-Naphthalenone, octahydro-4a,8a-dimethyl-7-(1-methylethyl)-, [4aR-(4a.alpha.,7.beta.,8a.alpha.)]-	102095	001803-39-0	99
40	20.52	626142	0.866	0.8661	Caryophyllene	80121	000087-44-5	81
41	20.85	390048	0.54	0.5395	Phenol, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, (R)-	96787	030199-26-9	50
42	21.165	477849	0.661	0.661	Loliolide	71178	005989-02-6	99
43	21.51	457278	0.633	0.6325	Caryophyllene	80124	000087-44-5	68
44	21.644	450094	0.623	0.6226	Isospathulenol	99149	088395-46-4	81
45	22.068	405627	0.561	0.5611	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	170894	000084-69-5	90
46	22.351	436382	0.604	0.6036	(3S,3aS,6R,7R,9aS)-1,1,7-Trimethyldecahydro-3a,7-methanocyclopenta[8]annulene-3,6-diol	121146	002649-64-1	99
47	22.539	1867628	2.583	2.5833	Hexadecanoic acid, methyl ester	161211	000112-39-0	99
48	22.901	4975760	6.883	6.8825	n-Hexadecanoic acid	143511	000057-10-3	99
49	23.733	180362	0.249	0.2495	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3.alpha.,4a.beta.,6a.alpha.,10a.beta.,10b.alpha.)]-	187057	000596-84-9	83
50	23.859	228653	0.316	0.3163	2,6,10-Dodecatriene-1,12-diol, 6-(hydroxymethyl)-10-methyl-2-(4-methyl-3-penten-1-yl)-, 1-acetate	273672	1083197-50-5	58
51	24.228	5527949	7.646	7.6463	9-Octadecenoic acid (Z)-, methyl ester	194438	000112-62-9	99
52	24.44	1431411	1.98	1.9799	Methyl stearate	197277	000112-61-8	99
53	24.605	5886985	8.143	8.143	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	171208	000463-40-1	99
54	24.754	1055488	1.46	1.46	Octadecanoic acid	179093	000057-11-4	99
55	24.904	1004806	1.39	1.3899	2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane	102038	1000144-10-2	58
56	25.563	1100028	1.522	1.5216	1-Naphthalenepropanol, .alpha.-ethenyldodecahydro-2-hydroxy-.alpha.,2,5,5,8a-pentamethyl-, [1R-[1.alpha.(R*),2.beta.,4a.beta.,8a.alpha.]]-	209676	000515-03-7	93
57	25.697	717043	0.992	0.9918	4,6-Bis(1,1'-dimethylethyl)-2',5'-dimethoxy-1,1'-biphenyl-2-ol	251487	1000326-27-3	38
58	26.098	329562	0.456	0.4559	1,4-Dimethyl-8-isopropylidenetricyclo[5.3.0.0(4,10)]decane	80299	1010140-07-7	55

59	26.467	808580	1.118	1.1184	Ferruginol	181930	000514-62-5	91
60	26.985	548265	0.758	0.7584	4-(3-Methyl-2-oxobutoxy)-7H-furo[3,2-g][1]benzopyran-7-one	181183	005058-15-1	53
61	27.111	1320705	1.827	1.8268	2,5-Methano-2H-thieno[3,2-b]thiopyran-8-ol, hexahydro-, acetate, (2.alpha.,3a.beta.,5.alpha.,7a.beta.,8R*)-	110794	035636-01-2	90
62	27.402	568364	0.786	0.7862	3-Chloro-8-methylthio-11H-indolo[3,2-c]quinoline	196451	155249-85-7	49
63	27.747	476783	0.659	0.6595	3-(4-Methoxyphenyl)benzo[f]quinazoline	181815	068725-85-9	60
64	28.014	706811	0.978	0.9777	Phthalic acid, di(2-propylpentyl) ester	295658	1000377-93-5	81
65	28.368	1975003	2.732	2.7319	2,6-Phenanthrenediol, 1,2,3,4,4a,9,10,10a-octahydro-1,1,4a-trimethyl-7-(1-methylethyl)-, [2S-(2.alpha.,4a.alpha.,10a.beta.)]-	202381	000564-73-8	49
66	28.69	631819	0.874	0.8739	3-Methylseleno-2-(1,3-dioxolan-2-yl)benzo[b]thiophene	198667	071740-02-8	98
67	28.886	381544	0.528	0.5278	9,10-Anthracenedione, 1,3,5-trihydroxy-7-propyl-	196670	055670-30-9	78



Suppliment

Table S2: Salvia compressa Vent

Peak	R.T.	Area	Pct Total	Area Pct	Library/ID	Ref	CAS	Qual
1	4.307	364094	1.06	1.0603	3-Methoxy-2,2-dimethyloxirane	4872	026196-04-3	39
2	4.724	80088	0.233	0.2332	1-Butanamine, N-methyl-	2149	000110-68-9	12

3	4.904	310564	0.904	0.9044	O-Butylisourea	9051	057536-14-8	9
4	5.446	114590	0.334	0.3337	Butanoic acid, 2-methyl-, methyl ester	9322	000868-57-5	78
5	6.538	102444	0.298	0.2983	Propanamide, 2-hydroxy-	2441	002043-43-8	5
6	6.962	67381	0.196	0.1962	10-Oxatetracyclo[5.5.2.0(1,5).0(8,12)]tetradecane-9,11,14-trione, 4-[(2-methoxyethoxy)methoxy]-5-methyl-	261337	1000154-01-5	38
7	7.104	66263	0.193	0.193	Ethanethioamide, N,N-dimethyl-	5172	000631-67-4	38
8	7.402	133929	0.39	0.39	3-Methylbenzyl alcohol, TBDMS derivative	118517	1000364-16-7	59
9	7.826	180276	0.525	0.525	Benzyl alcohol, TBDMS derivative	101600	053172-91-1	64
10	7.976	106131	0.309	0.3091	Tellurium, bis[(.eta.-5-cyclopentadienyl)-nickel-(triethylphosphine)]	346989	1000161-69-8	36
11	8.816	102298	0.298	0.2979	1,3-Cyclopentanedione	3488	003859-41-4	80
12	9.955	205461	0.598	0.5983	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one	23814	010230-62-3	58
13	10.191	448302	1.306	1.3055	Oxirane, [(hexadecyloxy)methyl]-	197326	015965-99-8	72
14	11.055	93231	0.272	0.2715	Benzyl alcohol	6064	000100-51-6	95
15	11.817	133486	0.389	0.3887	1,3,5-Triazine-2,4,6-triamine	12521	000108-78-1	80
16	12.147	90684	0.264	0.2641	Benzoic acid, methyl ester	18735	000093-58-3	83
17	12.634	78157	0.228	0.2276	Cyclohexanone, 2-ethyl-	13010	004423-94-3	52
18	12.956	110925	0.323	0.323	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	23823	028564-83-2	83
19	13.262	565622	1.647	1.6472	Benzoic acid	11265	000065-85-0	94
20	14.095	199558	0.581	0.5811	4-Vinylphenol	10651	002628-17-3	95
21	15.532	205297	0.598	0.5979	2-Methoxy-4-vinylphenol	28303	007786-61-0	94
22	16.365	782824	2.28	2.2797	1,2,3-Benzenetriol	12695	000087-66-1	95
23	16.978	146506	0.427	0.4267	Pyrazole-5-carboxylic acid, 3-methyl-	12628	000696-22-0	53
24	17.19	171012	0.498	0.498	4-Vinylbenzene-1,2-diol	18699	006053-02-7	87
25	17.763	140134	0.408	0.4081	Cycloheptasiloxane, tetradecamethyl-	340530	000107-50-6	87
26	18.062	136113	0.396	0.3964	Phenol, 3,5-bis(1,1-dimethylethyl)-	82765	001138-52-9	91
27	18.502	83104	0.242	0.242	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-, (R)-	54797	017092-92-1	91
28	18.902	205903	0.6	0.5996	Benzoic acid, hexyl ester	82480	006789-88-4	96
29	19.177	134856	0.393	0.3927	2-((2R)-2-Hydroxycyclohexyl)acetic acid, methyl ether, methyl ester	60519	1000501-25-2	27
30	20.191	182865	0.533	0.5325	Benzoic acid, 2-methylpropyl ester	52603	000120-50-3	53
31	20.819	189754	0.553	0.5526	Tetradecanoic acid	109279	000544-63-8	92
32	21.102	5857637	17.059	17.0585	Benzyl Benzoate	89937	000120-51-4	97
33	22.068	268206	0.781	0.7811	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	170894	000084-69-5	86
34	22.539	1964376	5.721	5.7206	Hexadecanoic acid, methyl ester	161211	000112-39-0	98

35	22.893	3965169	11.547	11.5473	n-Hexadecanoic acid	143511	000057-10-3	99
36	23.513	179660	0.523	0.5232	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3.alpha.,4a.beta.,6a.alpha.,10a.beta.,10b.alpha.)]-	187053	000596-84-9	91
37	23.733	175164	0.51	0.5101	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3.alpha.,4a.beta.,6a.alpha.,10a.beta.,10b.alpha.)]-	187053	000596-84-9	91
38	24.228	5522170	16.082	16.0816	9-Octadecenoic acid, methyl ester, (E)-	194450	001937-62-8	99
39	24.432	1094118	3.186	3.1863	Methyl stearate	197276	000112-61-8	99
40	24.605	4702510	13.695	13.6946	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	171210	000463-40-1	99
41	24.747	959996	2.796	2.7957	Octadecanoic acid	179093	000057-11-4	99
42	24.998	606628	1.767	1.7666	Methyl 10-trans,12-cis-octadecadienoate	191901	1000336-44-2	99
43	25.564	1033564	3.01	3.0099	1-Naphthalenepropanol, .alpha.-ethenyldodecahydro-2-hydroxy-.alpha.,2,5,5,8a-pentamethyl-, [1R-[1.alpha.(R*),2.beta.,4a.beta.,8a.alpha.]]-	209676	000515-03-7	93
44	26.538	279304	0.813	0.8134	8-Methyl-6-nonenamide	44363	1000293-20-9	42
45	27.229	61320	0.179	0.1786	Arsenous acid, tris(trimethylsilyl) ester	251605	055429-29-3	38
46	27.512	109692	0.319	0.3194	Benz[b]-1,4-oxazepine-4(5H)-thione, 2,3-dihydro-2,8-dimethyl-	83671	1000258-63-4	38
47	28.015	750129	2.185	2.1845	Bis(2-ethylhexyl) phthalate	295611	000117-81-7	90
48	29.004	534481	1.557	1.5565	2-Ethylbutyric acid, 2,7-dimethyloct-5-yn-7-en-4-yl ester	135998	1000371-19-7	38
49	30.002	342494	0.997	0.9974	2'-Hydroxy-5'-methylacetophenone, TMS derivative	101296	097389-69-0	43

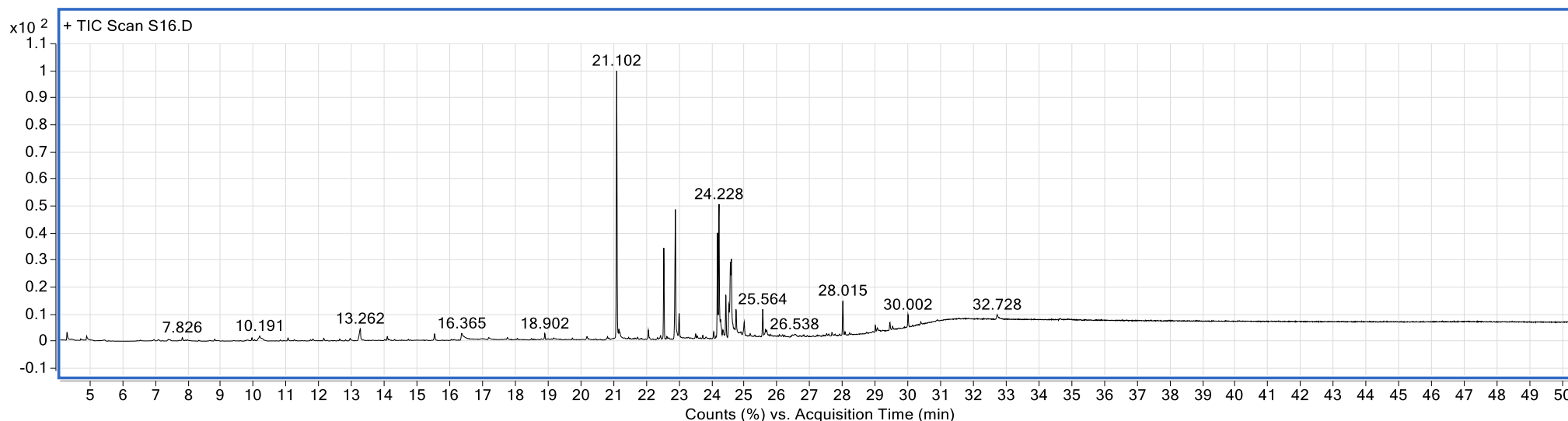


Table S3: *Salvia indica* L

Peak	R.T.	Area	Pct Total	Area Pct	Library/ID	Ref	CAS	Qual
1	4.323	168360	0.593	0.5925	L-Cysteine, S-methyl-N-trifluoroacetyl-, methyl ester	129759	1000452-89-7	38
2	4.896	328401	1.156	1.1558	4-(Methylthio)-1-butene	4899	020582-83-6	9
3	5.485	141000	0.496	0.4963	Butanoic acid, 2-methyl-, methyl ester	9324	000868-57-5	78
4	7.001	113472	0.399	0.3994	Tricyclo[5.2.2.0(2,6)]undecan-11-one-8,9-dicarboxylic anhydride, 3-[(2-methoxyethoxy)methoxy]-2-methyl-	261336	1000155-17-7	38
5	7.465	126629	0.446	0.4457	Methyl tiglate	8109	006622-76-0	76
6	8.871	148294	0.522	0.5219	Tricyclo[2.2.1.0(2,6)]heptane, 1,7,7-trimethyl-	18211	000508-32-7	87
7	9.766	227278	0.8	0.7999	Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-	18259	018172-67-3	95
8	10.191	366493	1.29	1.2899	Decane	22068	000124-18-5	91
9	10.835	120814	0.425	0.4252	Eucalyptol	30926	000470-82-6	53
10	11	187176	0.659	0.6588	Eucalyptol	30928	000470-82-6	95
11	12.924	187474	0.66	0.6598	Bicyclo[3.1.0]hexan-3-ol, 4-methylene-1-(1-methylethyl)-, [1S-(1.alpha.,3.beta.,5.alpha.)]-	29445	000471-16-9	43
12	13.364	121435	0.427	0.4274	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1S-endo)-	31308	000464-45-9	90
13	13.836	93153	0.328	0.3279	(-)-Myrtenol	29076	019894-97-4	94
14	15.147	83871	0.295	0.2952	Bornyl acetate	71351	000076-49-3	95
15	15.54	97017	0.341	0.3415	2-Methoxy-4-vinylphenol	28303	007786-61-0	83
16	16.443	87075	0.306	0.3065	4-Butylbenzoic acid, 4-methylpentyl ester	150908	1000293-52-5	37
17	16.577	132802	0.467	0.4674	(-)-.beta.-Bourbonene	80215	005208-59-3	95
18	17.056	98875	0.348	0.348	Caryophyllene	80127	000087-44-5	98
19	17.205	171099	0.602	0.6022	4-Vinylbenzene-1,2-diol	18699	006053-02-7	76
20	17.834	122525	0.431	0.4312	Germacrene D	80116	023986-74-5	78
21	18.737	212274	0.747	0.7471	2(1H)-Naphthalenone, 3,4,4a,5,8,8a-hexahydro-4a-methyl-, trans-	39742	055283-48-2	46
22	19.036	2071588	7.291	7.291	1H-Cycloprop[e]azulen-7-ol, decahydro-1,1,7-trimethyl-4-methylene-, [1ar-(1a.alpha.,4a.alpha.,7.beta.,7a.beta.,7b.alpha.)]-	99377	006750-60-3	99
23	19.428	85621	0.301	0.3013	Naphthalene, decahydro-	19425	000091-17-8	80
24	19.727	173302	0.61	0.6099	10,10-Dimethyl-2,6-dimethylenebicyclo[7.2.0]undecan-5.beta.-ol	99291	019431-80-2	72
25	20.088	273469	0.962	0.9625	Alloaromadendrene oxide-(1)	99226	1000156-12-8	62
26	20.277	140367	0.494	0.494	4-Isopropenyl-4,7-dimethyl-1-oxaspiro[2.5]octane	54912	1000187-81-7	56
27	20.583	212757	0.749	0.7488	1-((1S,3aR,4R,7S,7aS)-4-Hydroxy-7-isopropyl-4-methyloctahydro-1H-inden-1-yl)ethanone	121144	001911-78-0	47
28	20.866	302621	1.065	1.0651	5.alpha.-Hydroxy-4.alpha.,8,10,11-tetramethyltricyclo[6.3.0.0(2,4)]undec-10-ene	99343	141922-47-6	56
29	21.165	188320	0.663	0.6628	Loliolide	71178	005989-02-6	98

30	21.636	167121	0.588	0.5882	1,4-Methanoazulen-7(1H)-one, octahydro-4,8,8,9-tetramethyl-, (+)-	99296	018319-28-3	60
31	21.934	112931	0.397	0.3975	2,4,5,5,8a-Pentamethyl-6,7,8,8a-tetrahydro-5H-chromene	82809	1000195-40-9	50
32	22.068	223161	0.785	0.7854	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	170894	000084-69-5	90
33	22.359	200531	0.706	0.7058	Decahydro-1,1,4a,5,6-pentamethylnaphthalene	85375	080655-44-3	64
34	22.539	1670217	5.878	5.8783	Hexadecanoic acid, methyl ester	161203	000112-39-0	99
35	22.885	1805547	6.355	6.3546	n-Hexadecanoic acid	143511	000057-10-3	99
36	23.285	250602	0.882	0.882	cis-13-Octadecenoic acid	176218	013126-39-1	70
37	24.228	5221170	18.376	18.3759	9-Octadecenoic acid, methyl ester, (E)-	194450	001937-62-8	99
38	24.44	958822	3.375	3.3746	Methyl stearate	197277	000112-61-8	99
39	24.566	1009831	3.554	3.5541	9-Octadecenoic acid, (E)-	176223	000112-79-8	98
40	24.998	358497	1.262	1.2617	Methyl 9-cis,11-trans-octadecadienoate	191892	013058-52-1	99
41	25.571	7686209	27.052	27.0516	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-2-hydroxy-.alpha.,2,5,5,8a-pentamethyl-, [1R-[1.alpha.(R*),2.beta.,4a.beta.,8a.alpha.]]-	209676	000515-03-7	91
42	26.475	195675	0.689	0.6887	1-Pyrrolidinocarbonylmethyl piperazine	72419	039890-45-4	52
43	27.111	83690	0.295	0.2945	Benzo[h]quinoline, 2,4-dimethyl-	84038	000605-67-4	38
44	27.268	1013867	3.568	3.5683	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-2,4-dihydroxy-.alpha.,2,5,5,8a-pentamethyl-, [1R-(1.alpha.(R*),2.beta.,4.alpha.,4a.beta.,8a.alpha.)]-	229496	109189-32-4	86
45	28.014	310238	1.092	1.0919	Bis(2-ethylhexyl) phthalate	295608	000117-81-7	81
46	29.012	361417	1.272	1.272	Arsenous acid, tris(trimethylsilyl) ester	251605	055429-29-3	38

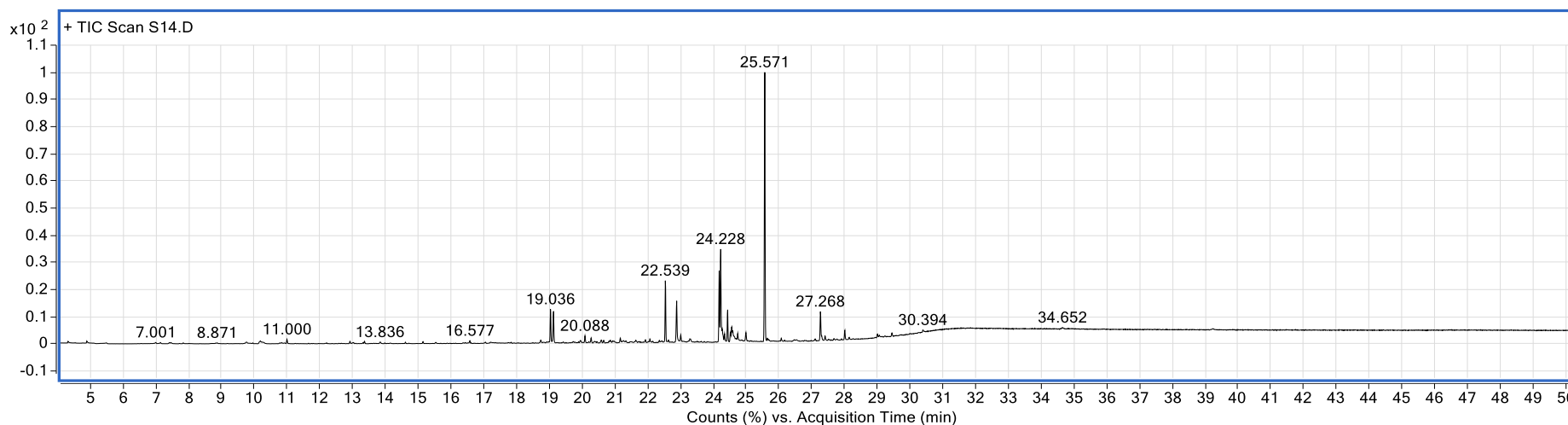
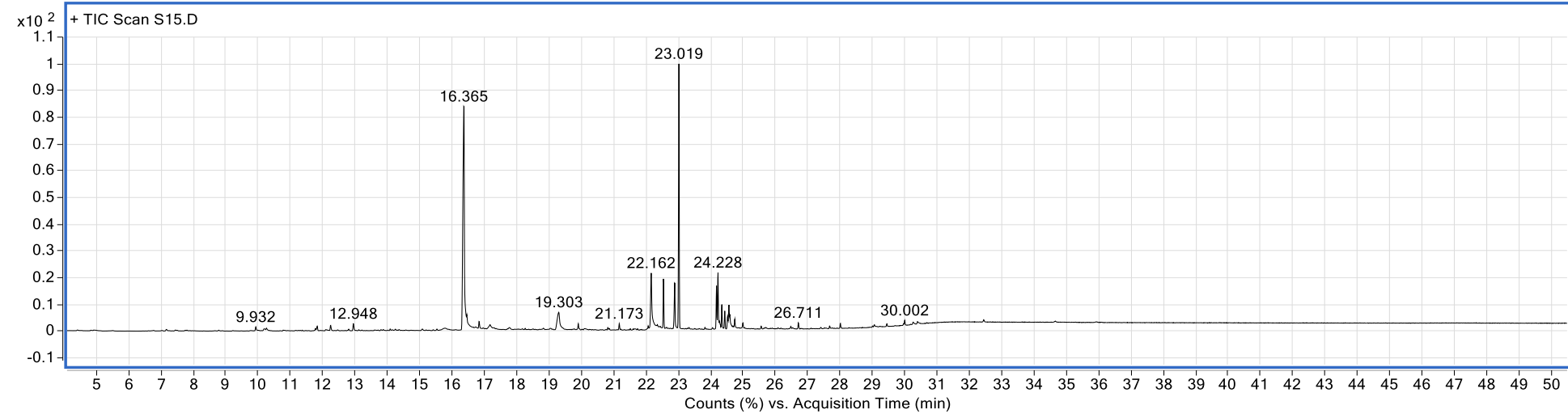


Table S4: *Salvia multicaulis* Vahl

Peak	R.T.	Area	Pct Total	Area Pct	Library/ID	Ref	CAS	Qual
1	4.92	388782	0.538	0.5382	N-Hydroxymethylacetamide	2442	000625-51-4	10
2	9.932	360330	0.499	0.4988	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	23823	028564-83-2	78
3	10.261	643880	0.891	0.8913	2H-Pyran-2,6(3H)-dione	7060	005926-95-4	64
4	11.833	571139	0.791	0.7906	Thymine	12602	000065-71-4	64
5	12.249	570942	0.79	0.7903	Thymine	12602	000065-71-4	38
6	12.948	482592	0.668	0.668	4H-Pyran-4-one, 2,3-dihydro-3,5-dihydroxy-6-methyl-	23823	028564-83-2	94
7	15.784	783323	1.084	1.0843	2(5H)-Thiophenone	4051	003354-32-3	43
8	16.365	24602797	34.057	34.0568	1,2,3-Benzenetriol	12701	000087-66-1	95
9	17.174	1323993	1.833	1.8328	4-Vinylbenzene-1,2-diol	18699	006053-02-7	42
10	17.779	310908	0.43	0.4304	.beta.-D-Glucopyranose, 1,6-anhydro-	38156	000498-07-7	38
11	19.303	3152654	4.364	4.3641	Butyric acid, p-fluorophenyl ester	56396	000587-89-3	35
12	19.908	348908	0.483	0.483	4,4,5,8-Tetramethylchroman-2-ol	82514	082391-05-7	42
13	20.819	299028	0.414	0.4139	Tetradecanoic acid	109284	000544-63-8	99
14	21.172	398909	0.552	0.5522	Loliolide	71178	005989-02-6	99
15	21.738	293919	0.407	0.4069	Cyclododecanone	56827	000830-13-7	42
16	22.162	7059048	9.772	9.7716	Benzoic acid, 3,4,5-trihydroxy-, methyl ester	59464	000099-24-1	96
17	22.539	2785654	3.856	3.8561	Hexadecanoic acid, methyl ester	161211	000112-39-0	98
18	22.885	2799541	3.875	3.8753	n-Hexadecanoic acid	143511	000057-10-3	99
19	23.019	11880568	16.446	16.4459	Dibutyl phthalate	170759	000084-74-2	96
20	24.228	5452914	7.548	7.5483	9-Octadecenoic acid, methyl ester, (E)-	194450	001937-62-8	99
21	24.432	1947876	2.696	2.6964	Methyl stearate	197276	000112-61-8	99
22	24.566	3131157	4.334	4.3344	6-Octadecenoic acid	176211	1000336-66-8	99
23	24.998	544309	0.753	0.7535	9,11-Octadecadienoic acid, methyl ester, (E,E)-	191928	013038-47-6	99
24	25.564	402845	0.558	0.5576	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-2-hydroxy-.alpha.,2,5,5,8a-pentamethyl-, [1R-[1.alpha.(R*),2.beta.,4a.beta.,8a.alpha.]]-	209676	000515-03-7	86
25	26.483	296544	0.41	0.4105	4,8,12,16-Tetramethylheptadecan-4-olide	229563	096168-15-9	95
26	26.711	385176	0.533	0.5332	2,6,10,14-Hexadecatetraen-1-ol, 3,7,11,15-tetramethyl-, acetate, (E,E,E)-	239663	061691-98-3	68
27	28.014	280200	0.388	0.3879	Bis(2-ethylhexyl) phthalate	295611	000117-81-7	70
28	29.067	382183	0.529	0.529	Ethoxy(phenyl)silanediol, 2TMS	233553	1000496-86-0	49
29	30.002	360364	0.499	0.4988	1-Dimethyl(phenyl)silyloxypentane	101603	1000280-41-7	27

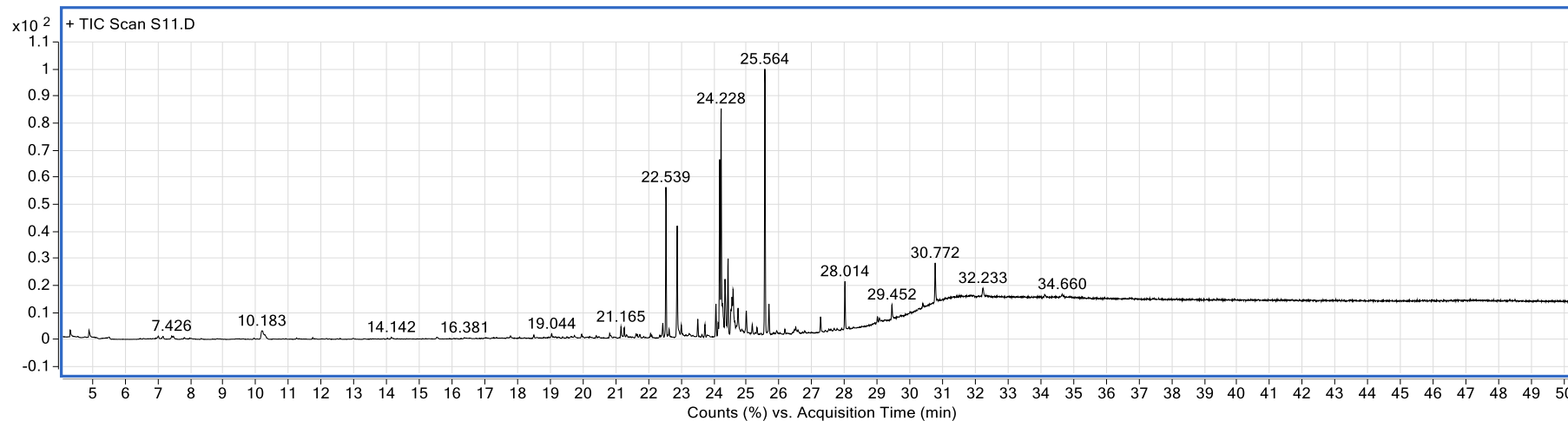


Suppliment

Table S5: Salvia palaestina Benth

Peak	R.T.	Area	Pct Total	Area Pct	Library/ID	Ref	CAS	Qual
1	4.323	227161	1.031	1.031	sec-Butyl nitrite	5120	000924-43-6	9
2	4.763	59380	0.269	0.2695	2,2-Dimethoxybutane	10029	003453-99-4	45
3	4.896	275954	1.252	1.2524	O-Butylisourea	9051	057536-14-8	38
4	5.509	128243	0.582	0.582	Butanoic acid, 2-methyl-, methyl ester	9316	000868-57-5	78
5	6.577	72773	0.33	0.3303	3-Methyl-2-butenic acid, hexadecyl ester	229565	060129-26-2	9
6	7.017	85679	0.389	0.3889	2-Cyclopentene, 1,4-bis(methoxyethoxymethoxy)-, cis-	168087	1000156-00-3	40
7	7.166	56375	0.256	0.2559	Ethanethioamide, N,N-dimethyl-	5172	000631-67-4	47
8	7.426	137037	0.622	0.6219	Benzaldehyde, 3-pentafluorophenoxymethyl-4-methoxy-	238718	329222-68-6	35
9	7.811	64928	0.295	0.2947	3-Methylthiophenyl isocyanate	40780	028479-19-8	38
10	7.983	55867	0.254	0.2536	Dimethylhydroxymethylphosphine	2731	033796-25-7	46
11	8.816	53950	0.245	0.2449	2-Cyclopenten-1-one, 2-hydroxy-	3508	010493-98-8	50
12	10.183	408867	1.856	1.8557	Decane	22066	000124-18-5	94
13	11.243	76295	0.346	0.3463	Indole-2-one, 2,3-dihydro-N-hydroxy-4-methoxy-3,3-dimethyl-	83645	1010129-52-1	43
14	14.142	60644	0.275	0.2752	Cyclotetrasiloxane, octamethyl-	194656	000556-67-2	78
15	16.381	102076	0.463	0.4633	Pyrrolidin-1-propionic acid	23334	076234-38-3	64

16	17.355	57422	0.261	0.2606	Furan, 2,5-dihydro-3-methyl-	1628	001708-31-2	25
17	17.787	110153	0.5	0.4999	4-(2,6,6-Trimethylcyclohexa-1,3-dienyl)but-3-en-2-one	64838	001203-08-3	42
18	18.502	104612	0.475	0.4748	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	54783	015356-74-8	94
19	19.044	128770	0.584	0.5844	2-Furanmethanol	3472	000098-00-0	43
20	19.743	88832	0.403	0.4032	Ethanol, 2-(3-methylphenoxy)-	30198	013605-19-1	46
21	19.963	81062	0.368	0.3679	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-	106667	072777-88-9	72
22	20.206	62498	0.284	0.2836	Chloromethyl phenyl sulfide	35062	007205-91-6	53
23	20.411	102541	0.465	0.4654	2-Cyclohexen-1-one, 4-(3-hydroxybutyl)-3,5,5-trimethyl-	87398	036151-02-7	90
24	20.819	158320	0.719	0.7185	Tetradecanoic acid	109281	000544-63-8	98
25	21.165	418334	1.899	1.8986	Loliolide	71178	005989-02-6	99
26	21.628	154045	0.699	0.6991	1-Oxaspiro[4.5]decan-2-one, 6-isopropenyl-9-methyl-	85102	1010157-58-3	38
27	22.068	100919	0.458	0.458	Phthalic acid, isobutyl nonyl ester	257769	1000309-04-4	90
28	22.539	1925558	8.739	8.7392	Hexadecanoic acid, methyl ester	161211	000112-39-0	99
29	22.885	1622311	7.363	7.3629	n-Hexadecanoic acid	143511	000057-10-3	99
30	23.513	191634	0.87	0.8697	1H-Naphtho[2,1-b]pyran, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3.alpha.,4a.beta.,6a.alpha.,10a.beta.,10b.alpha.)]-	187057	000596-84-9	95
31	23.733	203484	0.924	0.9235	1H-Naphtho[2,1-b]pyran, 3-ethenyldecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3.alpha.,4a.beta.,6a.alpha.,10a.beta.,10b.alpha.)]-	187057	000596-84-9	91
32	24.228	5200917	23.604	23.6045	9-Octadecenoic acid (Z)-, methyl ester	194438	000112-62-9	99
33	24.44	1577500	7.16	7.1595	Methyl stearate	197276	000112-61-8	99
34	24.59	1420001	6.445	6.4447	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	171210	000463-40-1	98
35	24.747	677541	3.075	3.075	Octadecanoic acid	179093	000057-11-4	99
36	24.998	326223	1.481	1.4806	Methyl 9-cis,11-trans-octadecadienoate	191892	013058-52-1	99
37	25.179	282068	1.28	1.2802	4,2,8-Ethanylylidene-2H-1-benzopyran, octahydro-4-methyl-	52934	078596-05-1	50
38	25.564	2881818	13.079	13.0792	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-2-hydroxy-.alpha.,2,5,5,8a-pentamethyl-, [1R-[1.alpha.(R*),2.beta.,4a.beta.,8a.alpha.]]-	209676	000515-03-7	93
39	25.697	331557	1.505	1.5048	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-4-hydroxy-.alpha.,5,5,8a-tetramethyl-2-methylene-, [1S-[1.alpha.(R*),4.beta.,4a.beta.,8a.alpha.]]-	207402	001438-66-0	68
40	25.925	138002	0.626	0.6263	2-(2-Methylpropyl)oxybenzylidene acetophenone	173646	1000395-75-7	30
41	26.176	99524	0.452	0.4517	Methyl 18-methylnonadecanoate	232223	1000424-52-4	83
42	26.506	314334	1.427	1.4266	Quinoline, 6-bromo-	84252	005332-25-2	38
43	27.268	215546	0.978	0.9783	1-Naphthalenepropanol, .alpha.-ethenyldecahydro-2,4-dihydroxy-.alpha.,2,5,5,8a-pentamethyl-, [1R-(1.alpha.(R*),2.beta.,4.alpha.,4a.beta.,8a.alpha.)]-	229496	109189-32-4	30
44	28.014	523962	2.378	2.378	Bis(2-ethylhexyl) phthalate	295608	000117-81-7	81
45	30.772	668900	3.036	3.0358	Glycerol tricaprylate	331809	000538-23-8	46



Suppliment

Table S6: Salvia spinosa L

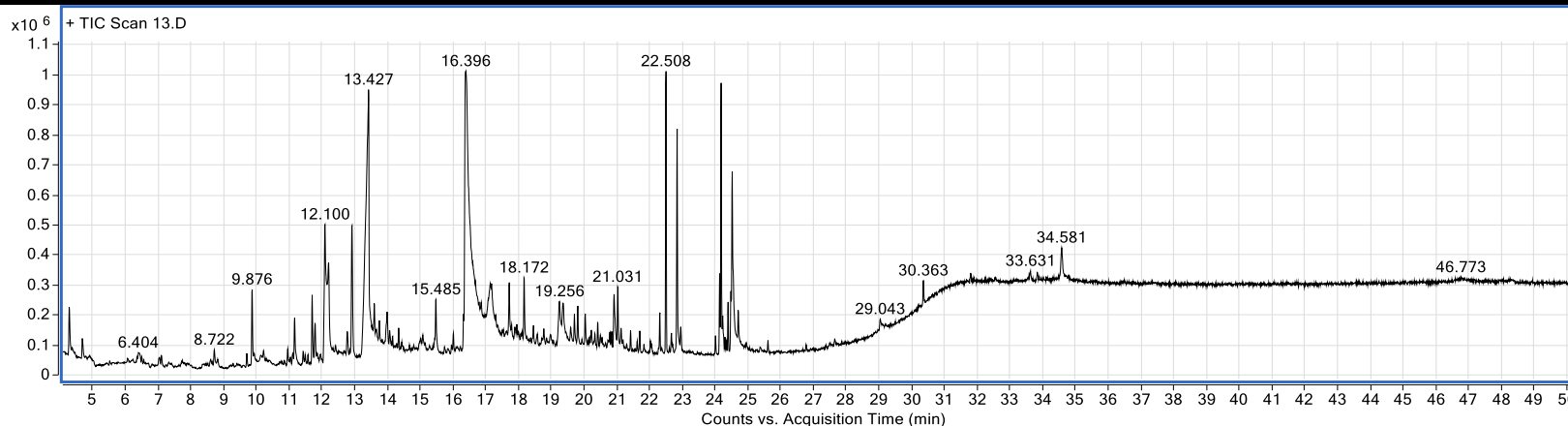
Peak	RT	Name	Formula	Precursor	Score (Lib)	Area	Base Peak	CAS ID	Area %	Library
1	4.294	Propane, 2-fluoro-2-methyl-	C4H9F	61	51.97	300939	61	353-61-7	0.711766	NIST20.L
2	4.38	Propane, 2-fluoro-2-methyl-	C4H9F	61	51.07	112453	61	353-61-7	0.265968	NIST20.L
3	4.693	2-Propenoic acid, ethenyl ester	C5H6O2	55.02	72.44	234068	55.02	2177-18-6	0.553606	NIST20.L
4	7.047	Propanedioic acid, dimethyl ester	C5H8O4	102.98	57.39	117677	102.98	108-59-8	0.278324	NIST20.L
5	7.106	1H-Imidazole-4-methanol	C4H6N2O	98.02	79.41	93225	98.02	822-55-9	0.220491	NIST20.L
6	7.745	1-(2,2,2-Trifluoroethyl)-1H-pyrazol-3-amine	C5H6F3N3	96.01	49.83	100905	96.01	947179-47-7	0.238655	NIST20.L
7	8.719	Diethylcyanamide	C5H10N2	98.02	70.25	173632	98.02	617-83-4	0.410666	NIST20.L
8	9.873	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furan-3-one	C6H8O4	100.99	80.72	521663	100.99	10230-62-3	1.233811	NIST20.L
9	10.153	Propanoic acid, anhydride	C6H10O3	57.03	48.53	282651	57.03	123-62-6	0.668512	NIST20.L
10	10.224	2H-Pyran-2,6(3H)-dione	C5H4O3	84.02	73.72	124681	84.02	5926-95-4	0.294889	NIST20.L
11	10.395	Pinocampyl tiglate, iso-	C15H24O2	83.06	65.07	92014	83.06	1000383-57-6	0.217627	NIST20.L
12	10.96	Propanoic acid, 3-chloro-, 4-formylphenyl ester	C10H9ClO3	122	70.09	100012	122	1010142-41-5	0.236543	NIST20.L
13	11.111	4-sec-Butylmorpholine	C8H17NO	114	65.23	113778	114	67061-36-3	0.269102	NIST20.L
14	11.17	Benzaldehyde, 2-hydroxy-	C7H6O2	122	89.59	271595	122	90-02-8	0.642363	NIST20.L

15	11.435	2,4,5-Trihydroxypyrimidine	C4H4N2O3	128.01	80.91	102410	128.01	496-76-4	0.242215	NIST20.L
16	11.706	1-Ethyl-2-pyrrolidinone	C6H11NO	113.02	77.13	369076	113.02	2687-91-4	0.87292	NIST20.L
17	11.797	Thymine	C5H6N2O2	126	84.81	318396	126	65-71-4	0.753054	NIST20.L
18	12.095	Benzoic acid, methyl ester	C8H8O2	105	91.89	454722	105	93-58-3	1.075486	NIST20.L
19	12.207	2-Propenoic acid, oxiranylmethyl ester	C6H8O3	55.02	58.63	2457233	55.02	106-90-1	5.811724	NIST20.L
20	12.781	l-Alanine, N-methoxycarbonyl-, tridecyl ester	C18H35NO4	101.99	64.36	216282	101.99	1010313-38-1	0.511539	NIST20.L
21	12.921	1-Methyl-5-fluorouracil	C5H5FN2O2	144	78.21	1019942	144	1000427-92-0	2.412316	NIST20.L
22	13.428	Benzoic acid	C7H6O2	105	95.01	6351812	105	65-85-0	15.02299	NIST20.L
23	13.603	5-Methoxypyrrolidin-2-one	C5H9NO2	84.02	69.39	160440	84.02	63853-74-7	0.379465	NIST20.L
24	13.757	Methyl salicylate	C8H8O3	120.03	85.09	102414	120.03	119-36-8	0.242224	NIST20.L
25	13.971	Heptane, 1,1'-oxybis-	C14H30O	69.03	61.06	216142	69.03	629-64-1	0.511208	NIST20.L
26	13.999	Methyl morpholine-3-carboxylate	C6H11NO3	86	74.54	217636	86	126264-49-1	0.514742	NIST20.L
27	14.347	4-Methoxycarbonyl-4-butanolide	C6H8O4	85.02	89.33	123105	85.02	3885-29-8	0.291162	NIST20.L
28	14.441	Ketone, methyl 2-methyl-1,3-oxothiolan-2-yl	C6H10O2S	102.98	54.44	90374	102.98	33266-06-7	0.213748	NIST20.L
29	15.02	1H-Imidazole-4-carboxamide, 5-amino-	C4H6N4O	55.02	43.51	231862	55.02	360-97-4	0.548388	NIST20.L
30	15.085	1-(Methylthio)-3-pentanone	C6H12OS	86	54.41	117092	86	66735-69-1	0.27694	NIST20.L
31	15.501	Phenol, 5-ethenyl-2-methoxy-	C9H10O2	150	71.27	90347	150	621-58-9	0.213684	NIST20.L
32	16.327	N-Ethyl-2-carbomethoxyazetidine	C7H13NO2	84.02	75.87	259372	84.02	54773-04-5	0.613454	NIST20.L
33	16.385	Furan, 2-(2-propenyl)-	C7H8O	107.99	60.55	3696644	107.99	75135-41-0	8.743117	NIST20.L
34	16.393	1,2,4-Benzenetriol	C6H6O3	126	72.13	8766660	126	533-73-3	20.73446	NIST20.L
35	16.423	N-Ethyl-2-carbomethoxyazetidine	C7H13NO2	84.02	78.74	529866	84.02	54773-04-5	1.253212	NIST20.L
36	17.148	1,3-Propanediol, 2-ethyl-2-(hydroxymethyl)-	C6H14O3	57.03	62.71	1102942	57.03	77-99-6	2.608623	NIST20.L
37	17.192	Ethanone, 1-(2-hydroxyphenyl)-	C8H8O2	136.03	68.85	133188	136.03	118-93-4	0.31501	NIST20.L
38	18.176	2-Hydroxy-1-(1'-pyrrolidiyl)-1-buten-3-one	C8H13NO2	112.04	78.83	416296	112.04	184427-18-7	0.984602	NIST20.L
39	19.251	Carbonic acid, bis(2-ethylhexyl) ester	C17H34O3	59.98	58.1	516248	59.98	14858-73-2	1.221004	NIST20.L
40	19.37	.beta.-D-Glucopyranoside, methyl	C7H14O6	59.98	69.37	573288	59.98	709-50-2	1.355912	NIST20.L
41	19.813	Imidazolo[1,2-a]pyrimidine-2,5(1H,3H)-dione, 3,7-dimethyl-	C8H9N3O2	150	68.34	183193	150	53854-19-6	0.433279	NIST20.L
42	20.041	6-Methoxychromanone	C10H10O3	150	76.96	171720	150	5802-17-5	0.406144	NIST20.L
43	20.421	4-(7-Methyloctyl)phenol	C15H24O	135.02	61.68	116697	135.02	24518-48-7	0.276006	NIST20.L
44	20.92	6-Trifluoromethyl-2H,4H-[1,2,4]triazine-3,5-dione	C4H2F3N3O2	110.04	55.04	459334	110.04	1000295-93-2	1.086394	NIST20.L
45	21.034	l-Proline, N-allyloxycarbonyl-, heptyl ester	C16H27NO4	154.06	65.04	326899	154.06	1000313-65-3	0.773165	NIST20.L
46	22.316	9-Hexadecenoic acid, methyl ester, (Z)-	C17H32O2	55.02	80.75	205271	55.02	1120-25-8	0.485497	NIST20.L

47	22.504	Hexadecanoic acid, methyl ester	C17H34O2	74.04	83.77	1287705	74.04	112-39-0	3.045615	NIST20.L
48	22.671	1-Nonylcycloheptane	C16H32	55.02	69.4	88062	55.02	1000371-47-7	0.20828	NIST20.L
49	22.844	n-Hexadecanoic acid	C16H32O2	73.03	88.87	1235180	73.03	57-10-3	2.921386	NIST20.L
50	24.142	Methyl 9-cis,11-trans-octadecadienoate	C19H34O2	67.01	77.2	307411	67.01	13058-52-1	0.727073	NIST20.L
51	24.187	13-Octadecenoic acid, methyl ester	C19H36O2	55.02	92.73	1471323	55.02	56554-47-3	3.479899	NIST20.L
52	24.4	Methyl stearate	C19H38O2	74.04	85.76	201598	74.04	112-61-8	0.476809	NIST20.L
53	24.486	3-Cyclohexene-1-acetic acid, .alpha.-oxo-, methyl ester	C9H12O3	67.01	46.07	128482	67.01	77846-83-4	0.303879	NIST20.L
54	24.525	Oleic Acid	C18H34O2	55.02	87.49	1679880	55.02	112-80-1	3.973168	NIST20.L
55	24.553	2-Indanone, 4,5,6,7-tetrahydro-	C9H12O	79	50.6	192738	79	20990-33-4	0.455854	NIST20.L
56	24.711	Octadecanoic acid	C18H36O2	73.03	72.66	225545	73.03	57-11-4	0.533448	NIST20.L
57	24.965	Isobutylheptyloctylamine	C19H41N	67.01	36.47	107638	67.01	1000310-32-1	0.25458	NIST20.L
58	29.043	Dodecadienyl tiglate, 2E, 4E-	C17H28O2	69.03	54.38	155537	69.03	1000383-65-5	0.367868	NIST20.L
59	30.359	Tridecanol, 2-ethyl-2-methyl-	C16H34O	57.03	74.6	153277	57.03	1010115-66-1	0.362523	NIST20.L
60	31.055	2-Fluoro-3-trifluoromethylbenzoic acid, 2-nitro-5-fluorophenyl ester	C14H6F5NO4	191	48.61	370370	191	1000357-65-0	0.875981	NIST20.L
61	31.804	Eicosane, 1-iodo-	C20H41I	281.02	39.65	1116222	281.02	1000406-31-8	2.640032	NIST20.L
62	32.901	Beryllium, hexakis[.mu.-(3-butenato-O:O')]-.mu.4-oxotetra-	C24H30Be4O13	161.98	36.09	93764	161.98	56377-88-9	0.221766	NIST20.L
63	34.583	.gamma.-Sitosterol	C29H50O	414.21	55.17	440900	414.21	83-47-6	1.042795	NIST20.L
64	35.485	2-Amino-4-hydroxy-6-phenethyl pteridine	C14H13N5O	267	43.45	288791	267	3/6/4215	0.683034	NIST20.L

42280619

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Suppliment

Table S7: *Salvia trichoclada* Benth

Peak	R.T.	Area	Pct Total	Area Pct	Library/ID	Ref	CAS	Qual
1	4.307	466312	1.394	1.3938	sec-Butyl nitrite	5120	000924-43-6	5
2	4.865	449876	1.345	1.3447	O-Butylisourea	9051	057536-14-8	40
3	5.493	198807	0.594	0.5942	Butanoic acid, 2-methyl-, methyl ester	9324	000868-57-5	78
4	6.546	95536	0.286	0.2856	1-Diisopropylsilyloxy-3-methylbut-2-ene	75606	1000299-57-8	38
5	7.002	79433	0.237	0.2374	10-Oxatetracyclo[5.5.2.0(1,5).0(8,12)]tetradecane-9,11,14-trione, 4-[(2-methoxyethoxy)methoxy]-5-methyl-	261337	1000154-01-5	64
6	7.457	127523	0.381	0.3812	2-Butenoic acid, 2-methyl-, methyl ester, (Z)-	8287	005953-76-4	81
7	7.952	137105	0.41	0.4098	Dimethyl sulfide	391	000075-18-3	9
8	8.793	134260	0.401	0.4013	Cyclopentanone, 2-methyl-	3625	001120-72-5	80
9	10.183	414886	1.24	1.2401	Decane	22067	000124-18-5	74
10	11.778	122103	0.365	0.365	2-Isopropylpyrrolidine	7899	1010424-35-0	58
11	13.027	383738	1.147	1.147	(+)-2-Bornanone	29115	000464-49-3	98
12	13.357	122310	0.366	0.3656	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1S-endo)-	31314	000464-45-9	90
13	14.166	117916	0.352	0.3525	Ethanol, 2-phenoxy-	19881	000122-99-6	87
14	15.148	74251	0.222	0.2219	Isobornyl acetate	71374	000125-12-2	83
15	16.365	133188	0.398	0.3981	N-Ethyl-2-carbomethoxyazetidine	23343	054773-04-5	80
16	17.056	89896	0.269	0.2687	(1R,9R,E)-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-4-ene	80324	068832-35-9	70
17	17.229	104652	0.313	0.3128	1H-Cyclopropa[a]naphthalene, 1a,2,3,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, [1aR-(1a.alpha.,7.alpha.,7a.alpha.,7b.alpha.)]-	80557	017334-55-3	46
18	17.748	98108	0.293	0.2932	Benzene, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	78053	000644-30-4	55
19	18.502	123641	0.37	0.3696	2(4H)-Benzofuranone, 5,6,7,7a-tetrahydro-4,4,7a-trimethyl-	54783	015356-74-8	90
20	19.028	179718	0.537	0.5372	Undecane	33080	001120-21-4	60
21	19.672	150862	0.451	0.4509	.alpha.-D-Mannofuranoside, 1-nonyl-	206489	1000160-13-8	27
22	19.955	112174	0.335	0.3353	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-	106667	072777-88-9	80
23	20.167	169163	0.506	0.5056	2-Furanmethanol	3472	000098-00-0	25
24	20.819	166711	0.498	0.4983	Tetradecanoic acid	109279	000544-63-8	93
25	21.165	304663	0.911	0.9106	Loliolide	71178	005989-02-6	99
26	21.66	163933	0.49	0.49	Neophytadiene	171299	000504-96-1	91
27	22.068	165857	0.496	0.4958	1,2-Benzenedicarboxylic acid, butyl octyl ester	241876	000084-78-6	83
28	22.539	2073156	6.197	6.1967	Hexadecanoic acid, methyl ester	161211	000112-39-0	99
29	22.901	4904384	14.659	14.6594	n-Hexadecanoic acid	143511	000057-10-3	99

30	23.513	240490	0.719	0.7188	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3.alpha.,4a.beta.,6a.alpha.,10a.beta.,10b.alpha.)]-	187053	000596-84-9	95
31	23.733	215782	0.645	0.645	1H-Naphtho[2,1-b]pyran, 3-ethenyldodecahydro-3,4a,7,7,10a-pentamethyl-, [3R-(3.alpha.,4a.beta.,6a.alpha.,10a.beta.,10b.alpha.)]-	187057	000596-84-9	91
32	24.228	5893601	17.616	17.6162	9-Octadecenoic acid, methyl ester, (E)-	194450	001937-62-8	99
33	24.44	1643415	4.912	4.9122	Methyl stearate	197276	000112-61-8	99
34	24.613	7407255	22.141	22.1406	9,12,15-Octadecatrienoic acid, (Z,Z,Z)-	171210	000463-40-1	99
35	24.998	430321	1.286	1.2862	Methyl 9-cis,11-trans-octadecadienoate	191892	013058-52-1	99
36	25.179	364842	1.091	1.0905	4,2,8-Ethanylylidene-2H-1-benzopyran, octahydro-4-methyl-	52934	078596-05-1	70
37	25.564	2523216	7.542	7.542	1-Naphthalenepropanol, .alpha.-ethenyldodecahydro-2-hydroxy-.alpha.,2,5,5,8a-pentamethyl-, [1R-[1.alpha.(R*),2.beta.,4a.beta.,8a.alpha.]]-(2Z,4E)-3,7,11-Trimethyl-2,4,10-dodecatriene	209676	000515-03-7	93
38	25.697	444043	1.327	1.3273		82901	172549-29-0	80
39	26.074	280758	0.839	0.8392	pyrido[1,2-a]indole-7-carbonitrile, 6,10-dihydro-8-(4-methoxyphenyl)-10,10-dimethyl-6-oxo-	251463	1000398-23-2	81
40	26.53	183036	0.547	0.5471	2-Ethylacridine	84007	055751-83-2	42
41	27.111	181437	0.542	0.5423	2-Ethylacridine	84007	055751-83-2	35
42	27.268	134436	0.402	0.4018	1H-Indene, 5-butyl-6-hexyloctahydro-	153497	055044-36-5	41
43	27.41	265470	0.793	0.7935	4,4'-(Ethane-1,1-diyl)diphenol, TMS derivative	181666	1000488-41-7	64
44	28.015	632477	1.89	1.8905	Bis(2-ethylhexyl) phthalate	295608	000117-81-7	87
45	29.004	357456	1.068	1.0684	Di-n-decylsulfone	255613	111530-37-1	38
46	29.452	393389	1.176	1.1759	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	295779	006422-86-2	90

