

**Date :** March 16, 2023

**CERTIFICATE OF ANALYSIS – GC PROFILING**

*SAMPLE IDENTIFICATION*

**Internal code :** 23C09-PTH02


**Customer identification :** Clary Sage ORGANIC - Spain - CC4105R

**Type :** Essential oil

**Source :** *Salvia sclarea*

**Customer :** Plant Therapy

*ANALYSIS*

**Method:** PC-MAT-014  - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Sylvain Mercier, M. Sc., Chimiste 2014-005

**Analysis date :** March 15, 2023

Checked and approved by :

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Alexis St-Gelais, Ph. D., Chimiste 2013-174

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Clear liquid

**Refractive index:**  $1.4600 \pm 0.0003$  (20 °C; method PC-MAT-016)

*CONCLUSION*

No adulterant, contaminant or diluent has been detected using this method.

## ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
Ethanol	0.01	Aliphatic alcohol
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Toluene	tr	Simple phenolic
Hexanal	tr	Aliphatic aldehyde
Octane	tr	Alkane
(2E)-Hexenal	0.04	Aliphatic aldehyde
(3Z)-Hexenol	0.11	Aliphatic alcohol
(2E)-Hexenol	0.14	Aliphatic alcohol
Hexanol	0.07	Aliphatic alcohol
3-Acetyl-3-methylcyclopentene	0.01	Aliphatic ketone
$\alpha$ -Thujene	0.01	Monoterpene
$\alpha$ -Pinene	0.24	Monoterpene
Camphene	0.04	Monoterpene
Benzaldehyde	0.01	Simple phenolic
$\beta$ -Pinene	0.17	Monoterpene
Sabinene	0.07	Monoterpene
Octen-3-ol	0.05	Aliphatic alcohol
Octan-3-one	0.01	Aliphatic ketone
Myrcene	0.77	Monoterpene
Octan-3-ol	0.01	Aliphatic alcohol
$\alpha$ -Phellandrene	0.01	Monoterpene
Pseudolimonene	0.01	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.04	Monoterpenic ether
$\alpha$ -Terpinene	0.01	Monoterpene
para-Cymene	0.05	Monoterpene
Limonene	0.41	Monoterpene
$\beta$ -Phellandrene	0.04	Monoterpene
(Z)- $\beta$ -Ocimene	0.31	Monoterpene
(E)- $\beta$ -Ocimene	0.51	Monoterpene
$\gamma$ -Terpinene	0.03	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
<i>trans</i> -Linalool oxide (fur.)	0.03	Monoterpenic alcohol
Terpinolene	0.13	Monoterpene
Linalool	21.24	Monoterpenic alcohol
Hotrienol	0.02	Monoterpenic alcohol
Dehydrosabinaketone	0.01	Normonoterpenic ketone
<i>cis</i> -para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
Unknown	tr	Unknown
allo-Ocimene	0.01	Monoterpene
<i>trans</i> -Pinocarveol	0.01	Monoterpenic alcohol

Camphor	0.04	Monoterpenic ketone
Nerol oxide	0.02	Aliphatic ether
Borneol	0.05	Monoterpenic alcohol
Terpinen-4-ol	0.05	Monoterpenic alcohol
para-Cymen-8-ol	0.02	Monoterpenic alcohol
$\alpha$ -Terpineol	3.00	Monoterpenic alcohol
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	0.01	Monoterpenic alcohol
Unknown	0.04	Unknown
Unknown	0.01	Unknown
Linalyl formate	0.23	Monoterpenic ester
Nerol	0.53	Monoterpenic alcohol
Unknown	tr	Monoterpenic ester
Neral	0.02	Monoterpenic aldehyde
Linalyl acetate	57.84	Monoterpenic ester
Geraniol	1.42	Monoterpenic alcohol
Geranial	0.04	Monoterpenic aldehyde
Unknown	0.01	Unknown
Neryl formate	0.04	Monoterpenic ester
Bornyl acetate	0.04	Monoterpenic ester
Thymol	0.01	Monoterpenic alcohol
Geranyl formate	0.10	Monoterpenic ester
Carvacrol	0.01	Monoterpenic alcohol
$\delta$ -Elemene	0.02	Sesquiterpene
Hodiendiol derivative	0.10	Oxygenated monoterpene
$\alpha$ -Cubebene	0.02	Sesquiterpene
$\alpha$ -Terpinyl acetate	0.06	Monoterpenic ester
Unknown	0.04	Monoterpenic ester
Unknown	0.04	Oxygenated monoterpene
Neryl acetate	0.76	Monoterpenic ester
$\alpha$ -Copaene	0.42	Sesquiterpene
$\beta$ -Bourbonene	0.11	Sesquiterpene
1,5-diepi- $\beta$ -Bourbonene	0.01	Sesquiterpene
$\beta$ -Cubebene	0.13	Sesquiterpene
Geranyl acetate	1.40	Monoterpenic ester
$\beta$ -Elemene	0.11	Sesquiterpene
$\gamma$ -4-Dimethylbenzenebutyral	0.03	Simple phenolic
$\alpha$ -Gurjunene	0.02	Sesquiterpene
$\beta$ -Caryophyllene	1.16	Sesquiterpene
$\beta$ -Copaene	0.03	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	0.01	Sesquiterpene
$\alpha$ -Humulene	0.07	Sesquiterpene
( <i>E</i> )- $\beta$ -Farnesene	0.02	Sesquiterpene
9-epi- $\beta$ -Caryophyllene	0.02	Sesquiterpene
Germacrene D	2.55	Sesquiterpene
$\beta$ -Selinene	0.02	Sesquiterpene
Hodiendiol derivative IV	0.19	Oxygenated monoterpene
$\alpha$ -Selinene	0.07	Sesquiterpene
Bicyclogermacrene	0.24	Sesquiterpene
$\alpha$ -Muurolene	0.06	Sesquiterpene
Germacrene A	0.06	Sesquiterpene
Hodiendiol derivative II	0.02	Oxygenated monoterpene
( <i>Z</i> )- $\alpha$ -Bisabolene	tr	Sesquiterpene

β-Bisabolene	0.04	Sesquiterpene
γ-Cadinene	0.07	Sesquiterpene
Cubebol	0.01	Sesquiterpenic alcohol
(3E,6E)-α-Farnesene	0.07	Sesquiterpene
(Z)-γ-Bisabolene	0.01	Sesquiterpene
trans-Calamenene	0.02	Sesquiterpene
δ-Cadinene	0.09	Sesquiterpene
α-Elemol	0.01	Sesquiterpenic alcohol
1,5-Epoxy-salvial-4(14)-ene	0.02	Sesquiterpenic ether
Spathulenol	0.17	Sesquiterpenic alcohol
Caryophyllene oxide	0.13	Sesquiterpenic ether
Salvial-4(14)-en-1-one	0.03	Aliphatic alcohol
Unknown	0.09	Oxygenated sesquiterpene
Torilenol	0.06	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.07	Unknown
Unknown	0.01	Unknown
τ-Cadinol	0.02	Sesquiterpenic alcohol
β-Eudesmol	0.07	Sesquiterpenic alcohol
α-Eudesmol	0.02	Sesquiterpenic alcohol
α-Cadinol	0.03	Sesquiterpenic alcohol
Unknown	0.03	Unknown
Bulnesol	0.01	Sesquiterpenic alcohol
(1βH)-Guai-9-en-11-ol?	0.01	Sesquiterpenic alcohol
Eudesma-4(15),7-dien-1β-ol	0.02	Sesquiterpenic alcohol
Unknown	0.03	Unknown
Phytone	0.03	Terpenic ketone
Sclareoloxide	0.02	Terpenic ether
Unknown	0.06	Unknown
Geranyl-para-cymene	0.04	Diterpene
Manoyl oxide	0.01	Diterpenic ether
Manool	0.03	Diterpenic alcohol
Sclareol	1.37	Diterpenic alcohol
<b>Consolidated total</b>	<b>98.81%</b>	

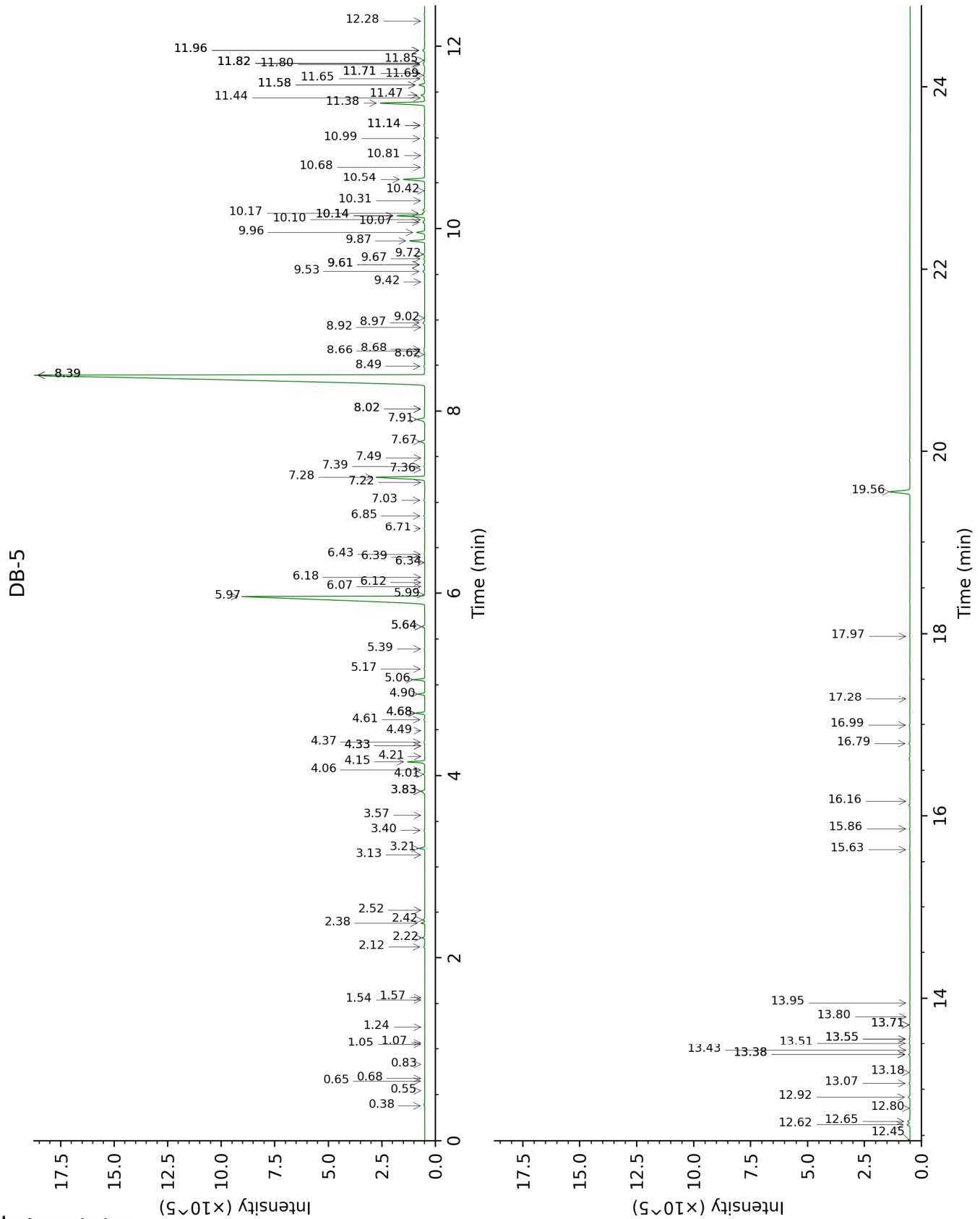
tr: The compound has been detected below 0.005% of total signal.

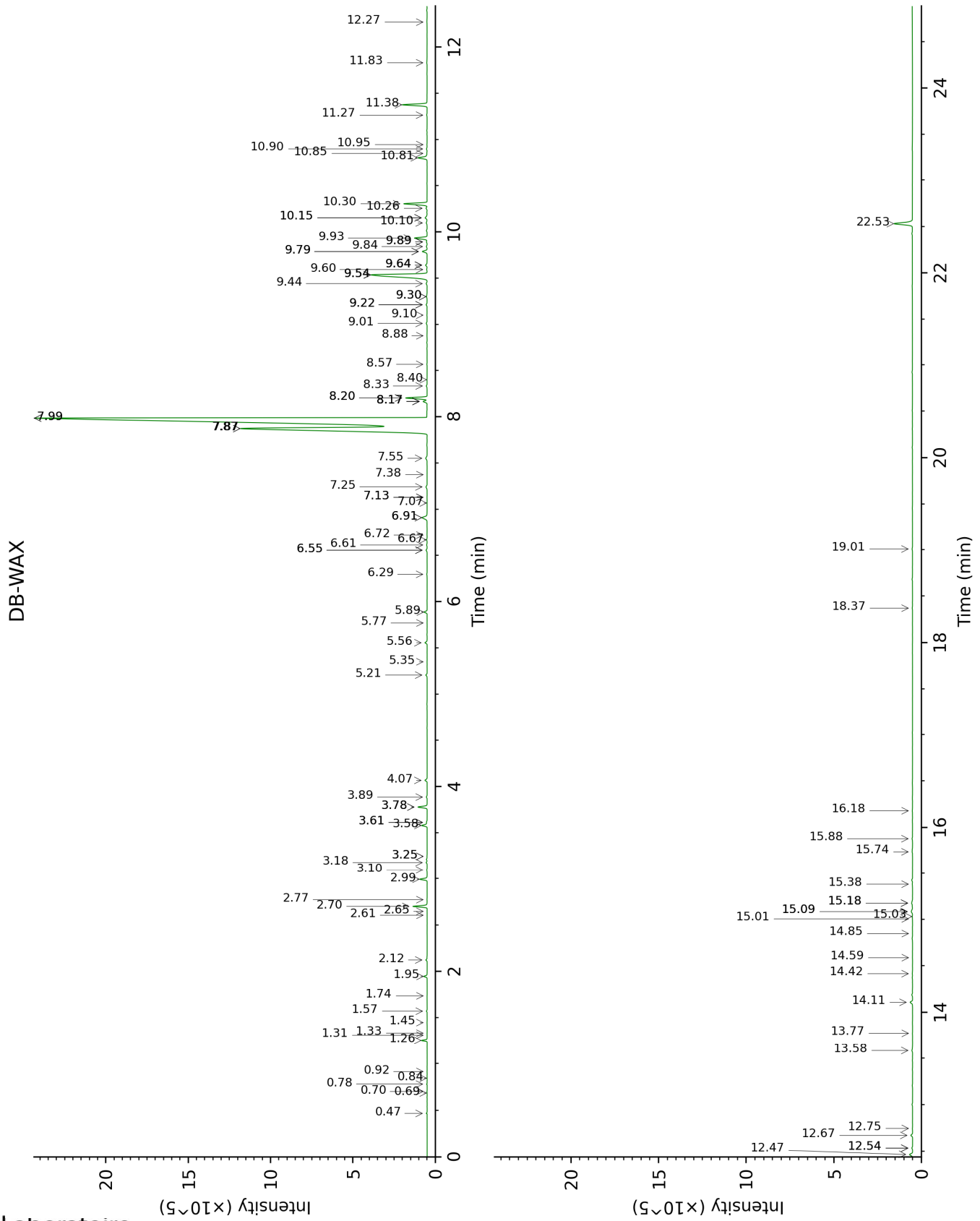
Note: no correction factor was applied

**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm is set to prioritize data from the most standard DB-5 column, and smallest values so as to avoid overestimating individual content. This process is semi-automatic. Advanced users are invited to consult the "Full analysis data" table after the chromatograms in this report to access the full untreated data and perform their own calculations if needed.

**Unknowns:** Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

This page was intentionally left blank. The following pages present the complete data of the analysis.







FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Ethanol	0.38	499	0.01	0.78	908	0.01
2-Methyl-3-buten-2-ol	0.54	606	tr	1.45	1014	0.01
Isovaleral	0.65	641	0.01	0.70	888	0.01
2-Methylbutyral	0.68	651	tr	0.69	881	tr
2-Ethylfuran	0.83	701	tr	0.84	919	tr
Isoamyl alcohol	1.05	733	0.01	3.25*	1179	0.01
2-Methylbutanol	1.07	736	tr	3.25*	1179	[0.01]
Toluene	1.24	759	tr	1.33	1002	tr
Hexanal	1.54	800	tr	1.74	1043	tr
Octane	1.57	803	tr	0.47	784	0.02
(2E)-Hexenal	2.12	849	0.04	3.18	1174	0.06
(3Z)-Hexenol	2.22	857	0.11	5.56	1348	0.13
(2E)-Hexenol	2.38	870	0.14	5.89	1372	0.17
Hexanol	2.42	873	0.07	5.21	1323	0.08
3-Acetyl-3-methylcyclopentene	2.52	882	0.01	0.92	931	tr
$\alpha$ -Thujene	3.14	926	0.01	1.31	999	tr
$\alpha$ -Pinene	3.21	931	0.24	1.26	991	0.23
Camphene	3.40	944	0.04	1.57	1026	0.03
Benzaldehyde	3.57	955	0.01	7.07	1460	0.01
$\beta$ -Pinene	3.83*	972	0.24	1.95	1065	0.17
Sabinene	3.83*	972	[0.24]	2.12	1084	0.07
Octen-3-ol	4.02	984	0.05	6.56*	1422	0.07
Octan-3-one	4.06	987	0.01	3.78*	1222	0.52
Myrcene	4.15	993	0.77	2.70	1134	0.74
Octan-3-ol	4.21	997	0.01	5.77	1364	0.01
$\alpha$ -Phellandrene	4.33*	1004	0.01	2.61	1126	0.01
Pseudolimonene	4.33*	1004	[0.01]	2.65	1130	0.01
<i>cis</i> -Dehydroxylinalool oxide	4.37	1007	0.04	3.61*	1209	0.04
$\alpha$ -Terpinene	4.49	1015	0.01	2.77	1140	0.01
para-Cymene	4.61	1022	0.05	3.89	1230	0.05
Limonene	4.68*	1027	0.43	2.99	1158	0.41
$\beta$ -Phellandrene	4.68*	1027	[0.43]	3.10	1167	0.04
(Z)- $\beta$ -Ocimene	4.90	1040	0.31	3.58	1206	0.32
(E)- $\beta$ -Ocimene	5.06	1050	0.51	3.78*	1222	[0.52]
$\gamma$ -Terpinene	5.17	1057	0.03	3.61*	1209	[0.04]
<i>cis</i> -Linalool oxide (fur.)	5.39	1071	0.02	6.30	1402	0.03
<i>trans</i> -Linalool oxide (fur.)	5.64*	1086	0.15	6.67	1430	0.03
Terpinolene	5.64*	1086	[0.15]	4.07	1244	0.13
Linalool	5.97	1107	21.24	7.87*†	1521	79.13
Hotrienol	5.99	1108	0.02	8.57	1575	0.01
Dehydrosabinaketone	6.07	1114	0.01	8.40	1562	0.01
<i>cis</i> -para-Menth-2-en-1-ol	6.12	1117	0.01	7.87*†	1521	[79.13]
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	6.18	1120	tr	9.30*	1635	0.06
allo-Ocimene	6.34	1131	0.01	5.35	1333	0.01

<i>trans</i> -Pinocarveol	6.39	1134	0.01	8.88	1600	0.01
Camphor	6.43	1136	0.04	6.91*	1448	0.44
Nerol oxide	6.71	1154	0.02	6.61	1426	0.03
Borneol	6.85	1163	0.05	9.54*	1654	5.71
Terpinen-4-ol	7.03	1174	0.05	8.33	1557	0.05
para-Cymen-8-ol	7.22	1187	0.02	11.27	1799	0.03
$\alpha$ -Terpineol	7.28	1190	3.00	9.54*	1654	[5.71]
Hodiendiol (2,6-dimethylocta-3,7-diene-2,6-diol)	7.36	1196	0.01	12.54*	1913	0.04
Unknown [m/z 43, 71 (80), 67 (55), 59 (51), 68 (44), 41 (43)...]	7.39	1198	0.04			
Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.49	1204	0.01	10.85	1764	0.02
Linalyl formate	7.67	1216	0.23	8.17*†	1544	1.43
Nerol	7.91	1232	0.53	10.81	1760	0.59
Unknown [m/z 121, 43 (93), 41 (37), 107 (35), 67 (33), 136 (32)... 154 (1)]	8.02*	1239	0.03	7.13*	1465	0.01
Neral	8.02*	1239	[0.03]	9.22*	1627	0.06
Linalyl acetate	8.39*	1264	59.59	7.99*†	1530	[79.13]
Geraniol	8.39*	1264	[59.59]	11.38	1809	1.42
Geranial	8.49	1271	0.04	9.84	1679	0.05
Unknown [m/z 121, 43 (75), 95 (57), 41 (34), 93 (33), 69 (28)...]	8.62	1279	0.01			
Neryl formate	8.66	1282	0.04	9.22*	1627	[0.06]
Bornyl acetate	8.68	1284	0.04	7.99*†	1530	[79.13]
Thymol	8.92	1299	0.01	14.85	2134	0.01
Geranyl formate	8.97	1303	0.10	9.64*	1662	0.11
Carvacrol	9.02	1306	0.01	15.09*	2158	0.13
$\delta$ -Elemene	9.42	1334	0.02	6.72	1434	0.01
Hodiendiol derivative	9.53	1342	0.10	12.67	1926	0.11
$\alpha$ -Cubebene	9.61*	1348	0.08	6.56*	1422	[0.07]
$\alpha$ -Terpinyl acetate	9.61*	1348	[0.08]	9.44	1646	0.06
Unknown [m/z 43, 121 (52), 93 (48), 79 (33), 41 (30), 136 (26), 81 (25)...]	9.67	1352	0.04			
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.72	1355	0.04	10.90	1768	0.04
Neryl acetate	9.87	1366	0.76	9.93	1686	0.75
$\alpha$ -Copaene	9.96	1372	0.42	6.91*	1448	[0.44]
$\beta$ -Bourbonene	10.07	1380	0.11	7.24	1473	0.10
1,5-diepi- $\beta$ -Bourbonene	10.10	1382	0.01	7.13*	1465	[0.01]
$\beta$ -Cubebene	10.14*	1385	1.41	7.55	1496	0.13
Geranyl acetate	10.14*	1385	[1.41]	10.30	1717	1.40
$\beta$ -Elemene	10.17	1387	0.11	8.17*†	1544	[1.43]
$\gamma$ -4-Dimethylbenzenebutyral	10.31	1397	0.03			

α-Gurjunene	10.42	1404	0.02	7.38	1483	0.01
β-Caryophyllene	10.54	1414	1.16	8.20*†	1547	[1.43]
β-Copaene	10.68	1424	0.03	8.17*†	1544	[1.43]
<i>trans</i> -α-Bergamotene	10.81	1434	0.01	8.20*†	1547	[1.43]
α-Humulene	10.99	1447	0.07	9.01	1611	0.06
( <i>E</i> )-β-Farnesene	11.14*	1458	0.04	9.30*	1635	[0.06]
9-epi-β-Caryophyllene	11.14*	1458	[0.04]	9.10	1618	0.02
Germacrene D	11.38	1476	2.55	9.54*	1654	[5.71]
β-Selinene	11.44	1480	0.02	9.60	1658	0.03
Hodiendiol derivative IV	11.47	1482	0.19			
α-Selinene	11.58*	1491	0.31	9.64*	1662	[0.11]
Bicyclogermacrene	11.58*	1491	[0.31]	9.79*	1674	0.30
α-Muurolene	11.65	1496	0.06	9.79*	1674	[0.30]
Germacrene A	11.68	1499	0.06	10.15*	1704	0.15
Hodiendiol derivative II	11.71*	1500	0.03	12.54*	1913	[0.04]
( <i>Z</i> )-α-Bisabolene	11.71*	1500	[0.03]	9.89*	1683	0.04
β-Bisabolene	11.80	1508	0.04	9.89*	1683	[0.04]
γ-Cadinene	11.82*	1509	0.10	10.10	1700	0.07
Cubebol	11.82*	1509	[0.10]	12.27	1888	0.01
(3 <i>E</i> ,6 <i>E</i> )-α-Farnesene	11.82*	1509	[0.10]	10.26	1713	0.07
( <i>Z</i> )-γ-Bisabolene	11.85	1511	0.01	9.64*	1662	[0.11]
<i>trans</i> -Calamenene	11.96*	1520	0.12	10.95	1772	0.02
δ-Cadinene	11.96*	1520	[0.12]	10.15*	1704	[0.15]
α-Elemol	12.28	1545	0.01	13.77	2029	0.01
1,5-Epoxy-salvial-4(14)-ene	12.45	1559	0.02	11.83	1850	0.03
Spathulenol	12.62	1572	0.17	14.11	2061	0.17
Caryophyllene oxide	12.65	1574	0.13	12.47	1907	0.20
Salvial-4(14)-en-1-one	12.80	1586	0.03	12.75	1933	0.02
Unknown [m/z 91, 119 (91), 79 (86), 93 (85), 41 (74), 107 (68), 105 (67), 134 (65)... 220 (1)]	12.92	1595	0.09			
Torilenol	13.07	1607	0.06	15.18*	2168	0.10
Unknown [m/z 135, 93 (66), 79 (58), 107 (54), 41 (42), 81 (41), 67 (41)... 220 (2)]	13.18	1617	0.03			
Unknown [m/z 43, 93 (89), 91 (88), 79 (87), 123 (76), 81 (75)...]	13.38*	1633	0.07	13.58	2011	0.07
Unknown [m/z 135, 93 (29), 79 (29), 41 (26), 107 (22), 67 (21), 69 (20)...]	13.38*	1633	[0.07]			
τ-Cadinol	13.43	1636	0.02	14.59	2108	0.02
β-Eudesmol	13.51	1643	0.07	15.09*	2158	[0.13]
α-Eudesmol	13.56*	1647	0.05	15.03	2153	0.02
α-Cadinol	13.56*	1647	[0.05]	15.18*	2168	[0.10]
Unknown [m/z 81, 41 (46), 79 (46), 93 (39), 91 (33), 107 (33)... 206 (8)]	13.71*	1660	0.04			
Bulnesol	13.71*	1660	[0.04]	15.01	2150	0.01

(1βH)-Guai-9-en-11-ol?	13.80	1667	0.01	15.38	2188	0.02
Eudesma-4(15),7-dien-1β-ol	13.95	1680	0.02	15.74	2225	0.03
Unknown [m/z 123, 191 (88), 81 (86), 41 (86), 151 (80), 91 (76)...]	15.63	1825	0.03	18.37	2512	0.02
Phytone	15.86	1846	0.03	14.42	2091	0.03
Sclareoloxide	16.16	1873	0.02			
Unknown [m/z 109, 132 (88), 157 (76), 119 (66), 91 (57), 105 (55)...]	16.79	1932	0.06			
Geranyl-para-cymene	16.99	1951	0.04	15.88	2240	0.04
Manoyl oxide	17.28	1978	0.01	16.18	2271	0.02
Manool	17.97	2045	0.03	19.01	2586	0.03
Sclareol	19.56	2207	1.37	22.53	3031	1.37
<b>Total identified</b>		<b>98.59%</b>			<b>98.25%</b>	
<b>Total reported</b>		<b>98.95%</b>			<b>98.40%</b>	

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

†: Peaks apexes were resolved, but peaks overlapped and were summed for analysis

tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index