

**Date :** December 21, 2022

**CERTIFICATE OF ANALYSIS – GC PROFILING**

*SAMPLE IDENTIFICATION*

**Internal code :** 22L15-PTH02

**Customer identification :** Clary Sage - Austria - CF0116R

**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 :** Amélie Simard, Analyste

**Analysis date :** December 19, 2022

Checked and approved by :

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

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Faintly yellow liquid

**Refractive index:**  $1.4583 \pm 0.0003$  (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
2-Pentanone	tr	Aliphatic ketone
2-Ethylfuran	tr	Furan
Hexanal	0.01	Aliphatic aldehyde
(2E)-Hexenal	0.03	Aliphatic aldehyde
(3Z)-Hexenol	0.13	Aliphatic alcohol
(2E)-Hexenol	0.08	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
$\alpha$ -Pinene	0.71	Monoterpene
Camphene	0.03	Monoterpene
Benzaldehyde	0.04	Simple phenolic
$\beta$ -Pinene	0.43	Monoterpene
Sabinene	0.01	Monoterpene
Octen-3-ol	0.04	Aliphatic alcohol
Octan-3-one	0.01	Aliphatic ketone
Myrcene	0.37	Monoterpene
Octanal	0.03	Aliphatic aldehyde
$\alpha$ -Phellandrene	0.02	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.03	Monoterpenic ether
<i>para</i> -Cymene	0.01	Monoterpene
Limonene	0.42	Monoterpene
$\beta$ -Phellandrene	0.01	Monoterpene
1,8-Cineole	0.01	Monoterpenic ether
(Z)- $\beta$ -Ocimene	0.19	Monoterpene
(E)- $\beta$ -Ocimene	0.60	Monoterpene
$\gamma$ -Terpinene	0.02	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.03	Monoterpenic alcohol
Terpinolene	0.01	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.09	Monoterpenic alcohol
Linalool	23.28	Monoterpenic alcohol
Hotrienol	0.02	Monoterpenic alcohol
Dehydrosabinaketone	0.01	Normonoterpenic ketone
allo-Ocimene	0.01	Monoterpene
<i>trans</i> -Sabinol	0.06	Monoterpenic alcohol
Camphor	0.01	Monoterpenic ketone
Nerol oxide	0.01	Aliphatic ether
Borneol	0.04	Monoterpenic alcohol
Terpinen-4-ol	0.02	Monoterpenic alcohol
$\alpha$ -Terpineol	3.52	Monoterpenic alcohol
Hodiendiol	0.03	Monoterpenic alcohol
Linalyl formate	0.04	Monoterpenic ester
Nerol	0.55	Monoterpenic alcohol
Unknown	0.02	Unknown
Neral	0.12	Monoterpenic aldehyde
Unknown	0.08	Unknown
Geraniol	1.20	Monoterpenic alcohol

Linalyl acetate	57.27	Monoterpenic ester
( <i>trans</i> ?)-Linalool oxide acetate (fur.)?	0.16	Monoterpenic ester
Geranial	0.11	Monoterpenic aldehyde
Unknown	0.03	Unknown
Bornyl acetate	0.25	Monoterpenic ester
Neryl formate	0.02	Monoterpenic ester
Geranyl formate	0.02	Monoterpenic ester
$\delta$ -Elemene	0.04	Sesquiterpene
Hodiendiol derivative	0.06	Oxygenated monoterpene
$\alpha$ -Cubebene	0.03	Sesquiterpene
$\alpha$ -Terpinyl acetate	0.07	Monoterpenic ester
Unknown	0.04	Monoterpenic ester
Unknown	0.03	Oxygenated monoterpene
Neryl acetate	0.80	Monoterpenic ester
$\alpha$ -Copaene	0.07	Sesquiterpene
$\beta$ -Bourbonene	0.05	Sesquiterpene
Geranyl acetate	1.93	Monoterpenic ester
$\beta$ -Elemene	0.06	Sesquiterpene
$\beta$ -Cubebene	0.05	Sesquiterpene
$\gamma$ -4-Dimethylbenzenebutyral	0.01	Simple phenolic
Isocaryophyllene	0.03	Sesquiterpene
$\beta$ -Caryophyllene	2.36	Sesquiterpene
$\beta$ -Copaene	0.07	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	0.01	Sesquiterpene
$\alpha$ -Humulene	0.06	Sesquiterpene
$\alpha$ -Amorphene	0.02	Sesquiterpene
Germacrene D	1.86	Sesquiterpene
$\beta$ -Selinene	0.04	Sesquiterpene
Hodiendiol derivative IV	0.02	Oxygenated monoterpene
Bicyclogermacrene	0.07	Sesquiterpene
$\alpha$ -Selinene	0.02	Sesquiterpene
$\alpha$ -Muurolene	0.02	Sesquiterpene
( <i>Z</i> )- $\alpha$ -Bisabolene	0.01	Sesquiterpene
$\gamma$ -Cadinene	0.04	Sesquiterpene
( <i>Z</i> )- $\gamma$ -Bisabolene	0.02	Sesquiterpene
$\delta$ -Cadinene	0.05	Sesquiterpene
$\beta$ -Sesquiphellandrene	0.04	Sesquiterpene
1,5-Epoxyvalial-4(14)-ene	0.01	Sesquiterpenic ether
Spathulenol	0.03	Sesquiterpenic alcohol
Caryophyllene oxide	0.05	Sesquiterpenic ether
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Guaiol	0.03	Sesquiterpenic alcohol
Torilenol	0.01	Oxygenated sesquiterpene
Unknown	0.04	Unknown
$\tau$ -Cadinol	0.02	Sesquiterpenic alcohol
$\beta$ -Eudesmol	0.02	Sesquiterpenic alcohol
$\alpha$ -Eudesmol	0.02	Sesquiterpenic alcohol
$\alpha$ -Cadinol	0.02	Sesquiterpenic alcohol
Bulnesol	0.04	Sesquiterpenic alcohol
Sclareol	0.52	Diterpenic alcohol
<b>Consolidated total</b>	<b>99.08%</b>	

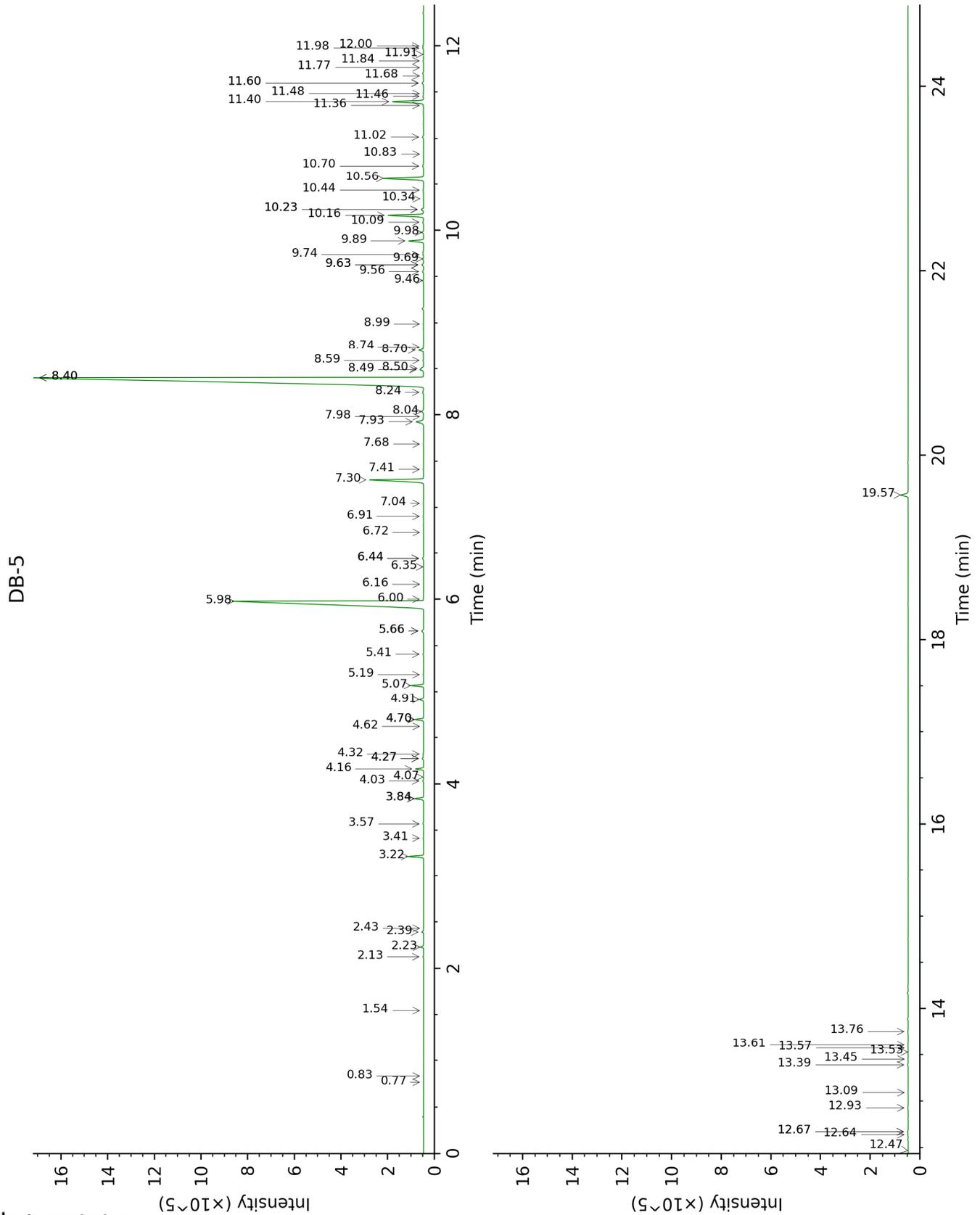
tr: The compound has been detected below 0.005% of total signal.

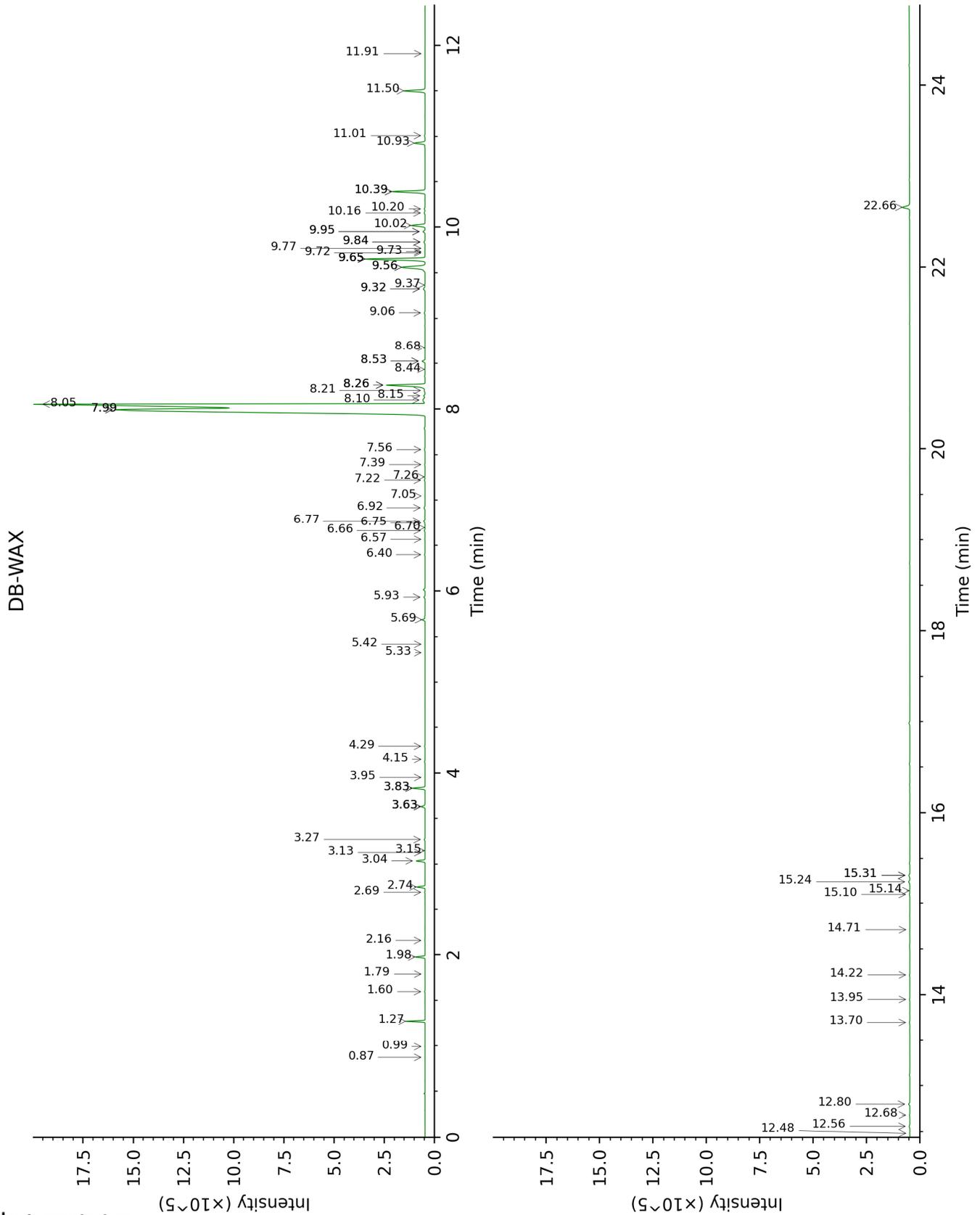
Note: no correction factor was applied

**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	%
2-Pentanone	0.77	680	tr	0.99	939	tr
2-Ethylfuran	0.83	701	tr	0.87	918	tr
Hexanal	1.54	799	0.01	1.79	1044	0.01
(2E)-Hexenal	2.13	848	0.03	3.27	1175	0.04
(3Z)-Hexenol	2.23	857	0.13	5.69	1353	0.15
(2E)-Hexenol	2.39	870	0.08	5.93	1370	0.06
Hexanol	2.43	873	0.01	5.33	1327	0.01
α-Pinene	3.22	931	0.71	1.27	989	0.70
Camphene	3.41	944	0.03	1.60	1024	0.02
Benzaldehyde	3.57	954	0.04	7.22	1466	0.04
β-Pinene	3.84*	972	0.45	1.98	1064	0.43
Sabinene	3.84*	972	[0.45]	2.16	1083	0.01
Octen-3-ol	4.03	984	0.04	6.66	1424	0.05
Octan-3-one	4.07	987	0.01	3.83*	1219	0.61
Myrcene	4.16	992	0.37	2.74	1132	0.38
Octanal	4.27*	1000	0.08	4.29	1254	0.03
α-Phellandrene	4.27*	1000	[0.08]	2.69	1128	0.02
cis-Dehydroxylinalool oxide	4.32	1003	0.03	3.63*	1204	0.21
para-Cymene	4.62	1022	0.01	3.95	1228	0.02
Limonene	4.70*	1026	0.42	3.04	1156	0.42
β-Phellandrene	4.70*	1026	[0.42]	3.13	1164	0.01
1,8-Cineole	4.70*	1026	[0.42]	3.15	1166	0.01
(Z)-β-Ocimene	4.91	1040	0.19	3.63*	1204	[0.21]
(E)-β-Ocimene	5.07	1050	0.60	3.83*	1219	[0.61]
γ-Terpinene	5.19	1057	0.02	3.63*	1204	[0.21]
cis-Linalool oxide (fur.)	5.41	1071	0.03	6.40	1404	0.03
Terpinolene	5.66*	1086	0.11	4.15	1243	0.01
trans-Linalool oxide (fur.)	5.66*	1086	[0.11]	6.77	1432	0.09
Linalool	5.98	1106	23.28	7.99*†	1524	80.59
Hotrienol	6.00	1108	0.02	8.68	1578	0.01
Dehydrosabinaketone	6.16	1118	0.01	8.53*	1566	0.17
allo-Ocimene	6.35	1130	0.01	5.42	1333	0.01
trans-Sabinol	6.44*	1136	0.08	9.65*	1656	3.56
Camphor	6.44*	1136	[0.08]	7.05	1453	0.01
Nerol oxide	6.72	1154	0.01	6.70	1427	0.01
Borneol	6.90	1165	0.04	9.65*	1656	[3.56]
Terpinen-4-ol	7.04	1174	0.02	8.44	1559	0.02
α-Terpineol	7.30	1190	3.52	9.65*	1656	[3.56]
Hodiendiol	7.41	1197	0.03	12.68	1916	0.04
Linalyl formate	7.68	1215	0.04	8.26*	1545	2.43
Nerol	7.93	1231	0.55	10.93	1762	0.60
Unknown [m/z 43, 93 (49), 41 (22), 80 (22), 69 (17), 121 (14)...]	7.98	1235	0.02	7.39	1478	0.03
Neral	8.04	1238	0.12	9.32*	1629	0.13

Unknown [m/z 69, 41 (75), 109 (35), 95 (34), 55 (28), 43 (27), 110 (26)...]	8.24	1252	0.08			
Geraniol	8.40*	1263	58.53	11.50	1811	1.20
Linalyl acetate	8.40*	1263	[58.53]	8.06†	1529	[80.59]
( <i>trans</i> ?) - Linalool oxide acetate (fur.)?	8.49†	1269	0.31	8.53*	1566	[0.17]
Geranial	8.50†	1270	[0.31]	9.95*	1680	0.12
Unknown [m/z 121, 43 (75), 95 (57), 41 (34), 93 (33), 69 (28)...]	8.59	1275	0.03			
Bornyl acetate	8.70	1283	0.25	8.10	1532	0.26
Neryl formate	8.74	1285	0.02	9.32*	1629	[0.13]
Geranyl formate	8.99	1302	0.02	9.77	1665	0.01
δ-Elementene	9.46	1335	0.04	6.75	1430	0.02
Hodiendiol derivative	9.56	1342	0.06	12.80	1927	0.08
α-Cubebene	9.63*	1347	0.10	6.57	1417	0.03
α-Terpinyl acetate	9.63*	1347	[0.10]	9.56*	1648	1.94
Unknown [m/z 43, 121 (52), 93 (48), 79 (33), 41 (30), 136 (26), 81 (25)...]	9.69	1351	0.04			
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.74	1355	0.03	11.01	1769	0.04
Neryl acetate	9.89	1365	0.80	10.02	1685	0.81
α-Copaene	9.98	1371	0.07	6.92	1443	0.08
β-Bourbonene	10.09	1379	0.05	7.26	1468	0.03
Geranyl acetate	10.16	1384	1.93	10.39*	1716	1.94
β-Elementene	10.23*	1389	0.14	8.20	1541	0.06
β-Cubebene	10.23*	1389	[0.14]	7.56	1491	0.05
γ-4-Dimethylbenzenebutyral	10.34	1397	0.01			
Isocaryophyllene	10.44	1404	0.03	7.99*†	1524	[80.59]
β-Caryophyllene	10.56	1413	2.36	8.26*	1545	[2.43]
β-Copaene	10.70	1423	0.07	8.15	1536	0.08
<i>trans</i> -α-Bergamotene	10.83	1433	0.01	8.26*	1545	[2.43]
α-Humulene	11.02	1447	0.06	9.06	1608	0.05
α-Amorphene	11.36	1472	0.02	9.37	1632	0.02
Germacrene D	11.40	1475	1.86	9.56*	1648	[1.94]
β-Selinene	11.46	1479	0.04	9.65*	1656	[3.56]
Hodiendiol derivative IV	11.48	1481	0.02			
Bicyclgermacrene	11.60*	1490	0.10	9.84*	1671	0.08
α-Selinene	11.60*	1490	[0.10]	9.73	1662	0.02
α-Murolene	11.68	1496	0.02	9.84*	1671	[0.08]
( <i>Z</i> )-α-Bisabolene	11.76	1502	0.01	9.95*	1680	[0.12]
γ-Cadinene	11.84	1508	0.04	10.16	1697	0.06
( <i>Z</i> )-γ-Bisabolene	11.91	1513	0.02	9.72	1661	0.01
δ-Cadinene	11.98	1519	0.05	10.20	1700	0.05
β-Sesquiphellandrene	12.00	1520	0.04	10.39*	1716	[1.94]
1,5-Epoxysalvial-4(14)-ene	12.47	1557	0.01	11.91	1847	0.01
Spathulenol	12.64	1571	0.03	14.22	2060	0.03

Caryophyllene oxide	12.67*	1573	0.06	12.56	1905	0.05
Caryophyllene oxide isomer	12.67*	1573	[0.06]	12.48	1898	0.01
Guaiol	12.93	1593	0.03	13.95	2034	0.03
Torilenol	13.09	1606	0.01	15.31*	2167	0.08
Unknown [m/z 43, 93 (89), 91 (88), 79 (87), 123 (76), 81 (75)...]	13.39	1631	0.04	13.70	2010	0.04
τ-Cadinol	13.45	1636	0.02	14.71	2108	0.01
β-Eudesmol	13.53	1642	0.02	15.24	2160	0.09
α-Eudesmol	13.57	1646	0.02	15.14	2150	0.02
α-Cadinol	13.60	1648	0.02	15.31*	2167	[0.08]
Bulnesol	13.76	1661	0.04	15.10	2146	0.03
Sclareol	19.57	2204	0.52	22.66	3020	0.51
<b>Total identified</b>		<b>99.01%</b>			<b>98.80%</b>	
<b>Total reported</b>		<b>99.26%</b>			<b>98.91%</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