

Date : February 20, 2020

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20B06-PSC01

Customer identification : Clary Sage - Bulgaria - CS2019

Type : Essential oil

Source : *Salvia sclarea*

Customer : Pacha Soap Co.

ANALYSIS

Method: PC-MAT-007 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID (in French); identifications validated by GC-MS.

Analyst : Sylvain Mercier, M. Sc., Chimiste

Analysis date : February 11, 2020

Checked and approved by :

Alexis St-Gelais, M. Sc., chimiste 2013-174

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PHYSICOCHEMICAL DATA

Physical aspect: Light yellow liquid
Refractive index: 1.4632 ± 0.0003 (20 °C)
Optical rotation: -10.72°

NFT 75-255:1992 - CLARY SAGE OIL - FRESHLY CRUSHED

Compound	Min. %	Max. %	Observed %	Complies?
Sclareol	0.4	2.6	0.7	Yes
Germacrene D	1.2	7.5	3.0	Yes
α-Terpineol	1	5	3	Yes
Linalyl acetate	56.0	70.5	51.3	No
Linalool	13	24	20	Yes
Optical rotation	-20.0°	-10.0°	-10.7°	Yes
Refractive index	1.456	1.466	1.463	Yes

CONCLUSION

This sample features significant (>1%) amounts of matricaria esters and (E)-β-farnesene, neither of which are typical constituents of clary sage. We recommend that this observation is taken into account when evaluating this batch. The oil marginally does not comply with the AFNOR standard for freshly crushed clary sage oil.

ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

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

Identification	%	Classe
Ethanol	tr	Aliphatic alcohol
Isobutyral	tr	Aliphatic aldehyde
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
2-Methylbutanol	tr	Aliphatic alcohol
Toluene	tr	Simple phenolic
Hexanal	tr	Aliphatic aldehyde
(2E)-Hexenal	0.01	Aliphatic aldehyde
(3Z)-Hexenal	0.15	Aliphatic alcohol
(2E)-Hexenal	0.03	Aliphatic alcohol
Hexanol	0.05	Aliphatic alcohol
α -Thujene	tr	Monoterpene
α -Pinene	0.03	Monoterpene
Camphene	0.01	Monoterpene
Sabinene	0.01	Monoterpene
β -Pinene	0.04	Monoterpene
Octen-3-ol	0.04	Aliphatic alcohol
Octan-3-one	0.02	Aliphatic ketone
<i>trans</i> -Dehydroxylinalool oxide	0.05	Monoterpenic ether
Myrcene	1.21	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.06	Monoterpenic ether
α -Terpinene	0.02	Monoterpene
para-Cymene	0.03	Monoterpene
β -Phellandrene	0.02	Monoterpene
Limonene	0.41	Monoterpene
(Z)- β -Ocimene	0.48	Monoterpene
(E)- β -Ocimene	0.91	Monoterpene
γ -Terpinene	0.03	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Terpinolene	0.26	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Hotrienol	0.03	Monoterpenic alcohol
Linalool	20.11	Monoterpenic alcohol
Dehydrosabinaketone	0.01	Normoterpenic ketone
Unknown	0.01	Unknown
allo-Ocimene	0.01	Monoterpene
Nerol oxide	0.03	Aliphatic ether
Borneol	0.02	Monoterpenic alcohol
Terpinen-4-ol	0.04	Monoterpenic alcohol
α -Terpineol	3.45	Monoterpenic alcohol
Unknown	0.04	Unknown
Unknown	0.02	Unknown
Linalyl formate	0.07	Monoterpenic ester
Nerol	0.78	Monoterpenic alcohol
Linalyl acetate	51.30	Monoterpenic ester
Geraniol	2.14	Monoterpenic alcohol

Neryl formate	0.03	Monoterpenic ester
Thymol	0.03	Monoterpenic alcohol
Geranyl formate	0.04	Monoterpenic ester
δ -Elemene	0.01	Sesquiterpene
Hodiendiol derivative	0.02	Oxygenated monoterpene
α -Cubebene	0.03	Sesquiterpene
α -Terpinyl acetate	0.06	Monoterpenic ester
Unknown	0.01	Monoterpenic ester
Unknown	0.02	Oxygenated monoterpene
Neryl acetate	1.22	Monoterpenic ester
α -Copaene	0.74	Sesquiterpene
(Z)-8-Hydroxylinalool?	0.02	Monoterpenic alcohol
β -Bourbonene	0.21	Sesquiterpene
1,5-diepi- β -Bourbonene	0.02	Sesquiterpene
Geranyl acetate	2.36	Monoterpenic ester
β -Cubebene	0.16	Sesquiterpene
β -Elemene	0.08	Sesquiterpene
Isocaryophyllene	0.02	Sesquiterpene
β -Caryophyllene	1.63	Sesquiterpene
β -Copaene	0.06	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.03	Sesquiterpene
α -Humulene	0.11	Sesquiterpene
(E)- β -Farnesene	1.12	Sesquiterpene
9-epi- β -Caryophyllene	0.02	Sesquiterpene
Germacrene D	2.99	Sesquiterpene
α -Amorphene	0.02	Sesquiterpene
β -Selinene	0.03	Sesquiterpene
Hodiendiol derivative IV	0.09	Oxygenated monoterpene
Bicyclogermacrene	0.39	Sesquiterpene
(Z)- α -Bisabolene	0.08	Sesquiterpene
Hodiendiol derivative II	0.01	Oxygenated monoterpene
γ -Cadinene	0.02	Sesquiterpene
Cubebol	0.04	Sesquiterpenic alcohol
(3E,6E)- α -Farnesene	0.17	Sesquiterpene
(Z)-2-Lachnophyllum ester	0.03	Polyene ester
Matricaria ester isomer II	0.12	Polyene ester
δ -Cadinene	0.20	Sesquiterpene
<i>trans</i> -Calamenene	tr	Sesquiterpene
Matricaria ester isomer I	1.02	Polyene ester
α -Calacorene	0.05	Sesquiterpene
Isocaryophyllene epoxide B	0.01	Sesquiterpenic ether
α -Elemol	0.01	Sesquiterpenic alcohol
Salviadienol?	0.02	Sesquiterpenic alcohol
1,5-Epoxyalvial-4(14)-ene	0.06	Sesquiterpenic ether
Spathulenol	0.21	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.04	Sesquiterpenic ether
Caryophyllene oxide	0.57	Sesquiterpenic ether
Salvial-4(14)-en-1-one	0.06	Aliphatic alcohol
Unknown	0.08	Oxygenated sesquiterpene
Torilenol	0.04	Oxygenated sesquiterpene
Guaia-6,10(14)-dien-4 β -ol	0.02	Sesquiterpenic alcohol
Hinesol	0.07	Sesquiterpenic alcohol

Unknown	0.01	Unknown
Unknown	0.02	Unknown
β -Eudesmol	0.08	Sesquiterpenic alcohol
Unknown	0.02	Unknown
α -Eudesmol	0.03	Sesquiterpenic alcohol
α -Cadinol	0.02	Sesquiterpenic alcohol
Unknown	0.01	Unknown
Mustakone	0.02	Sesquiterpenic ketone
Eudesma-4(15),7-dien-1 β -ol	0.02	Sesquiterpenic alcohol
Cyclocolorenone	0.01	Sesquiterpenic ketone
Phytone	0.03	Terpenic ketone
Sclareoloxide	0.33	Terpenic ether
Geranyl- α -terpinene	0.13	Diterpene
Unknown	0.13	Unknown
Geranyl-para-cymene	0.06	Diterpene
Manoyl oxide	0.04	Diterpenic ether
13-epi-Manoyl oxide	0.02	Diterpenic ether
Manool	0.07	Diterpenic alcohol
Sclareolide?	0.01	Terpenic lactone
Sclareol	0.73	Diterpenic alcohol
Consolidated total	98.27%	

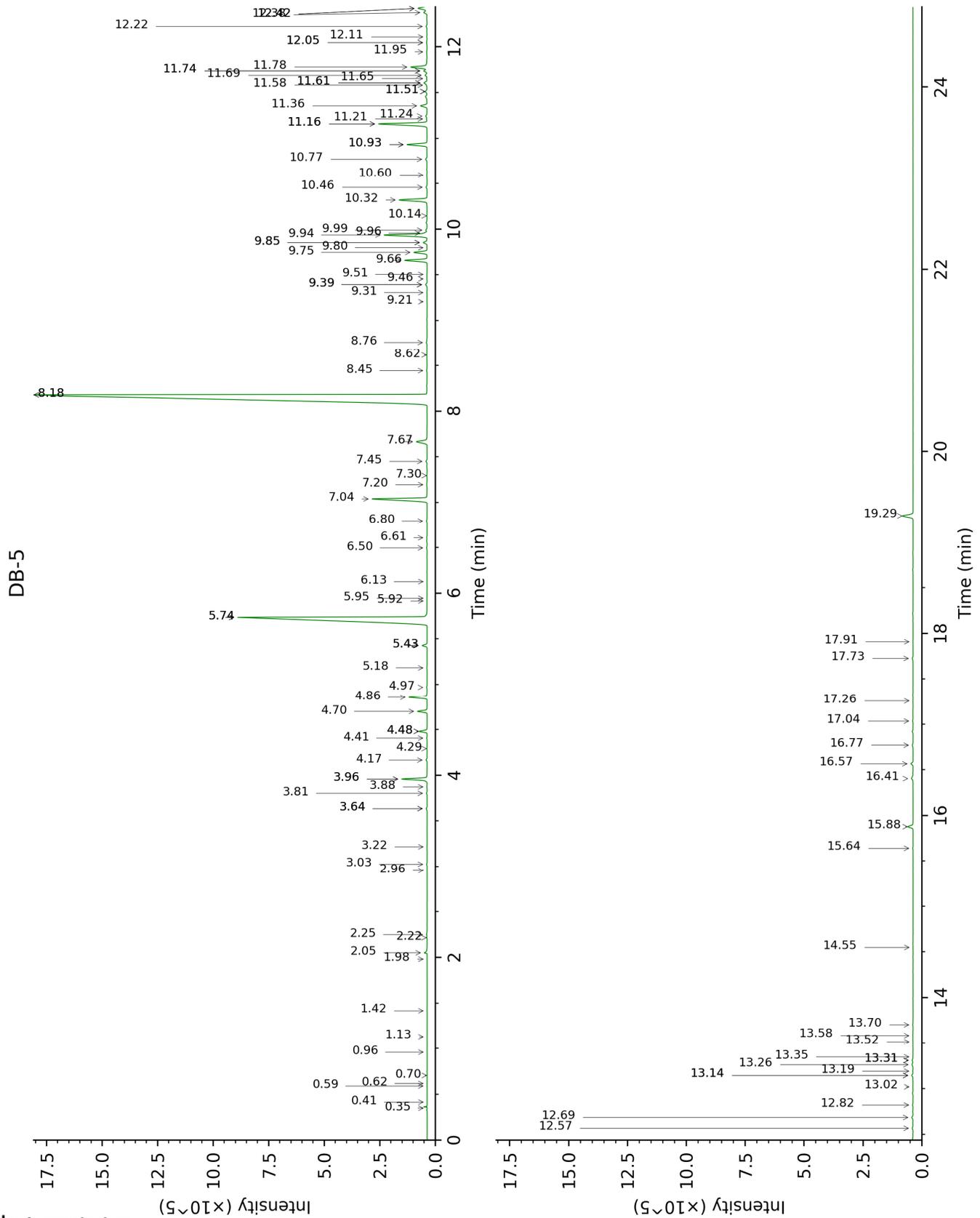
tr: The compound has been detected below 0.005% of total signal.

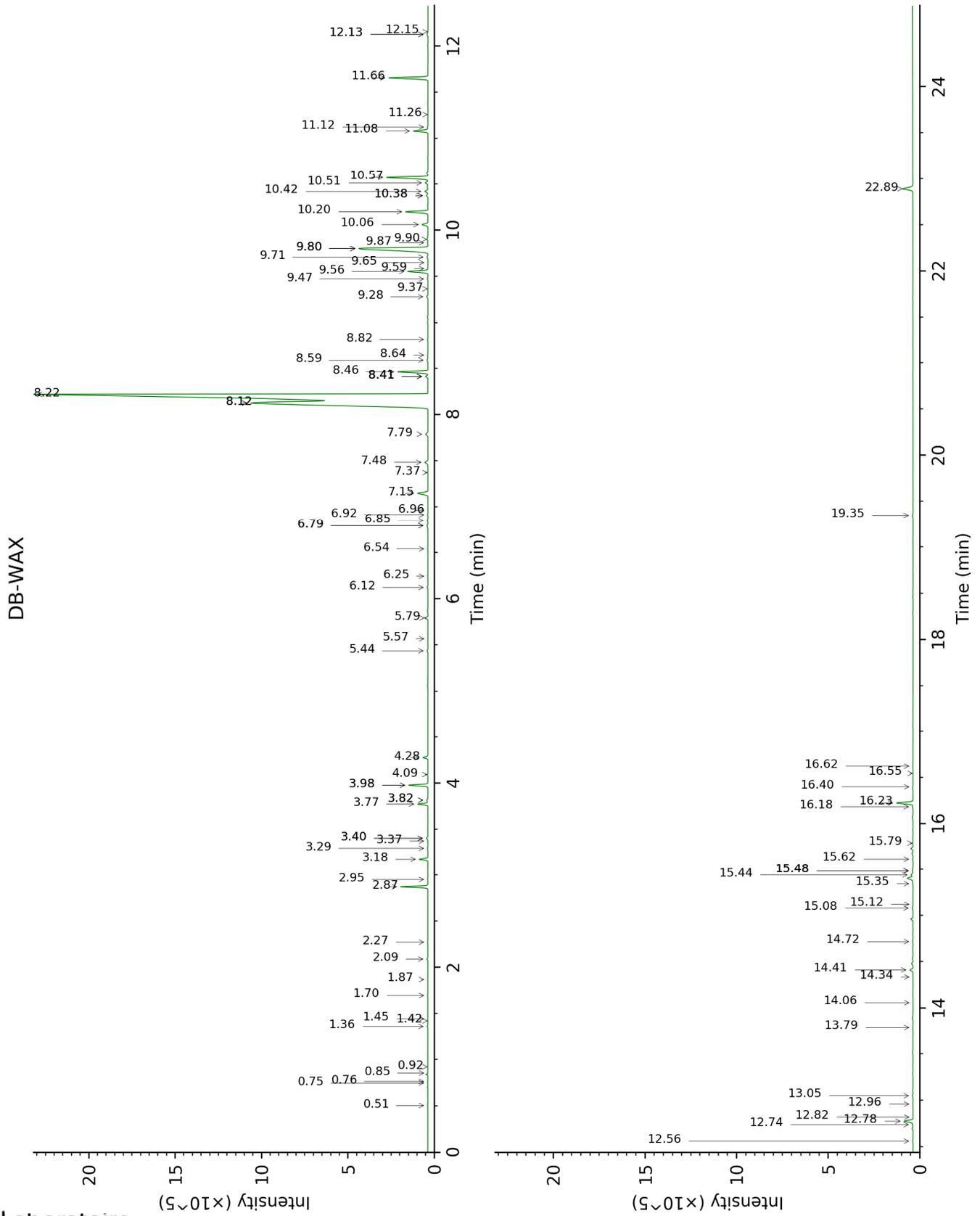
Note: no correction factor was applied

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	0.35	518	tr	0.85	906	tr
Isobutyral	0.42	528	tr	0.50	778	tr
Isovaleral	0.59	639	tr	0.76	884	tr
2-Methylbutyral	0.62	650	tr	0.75	878	tr
2-Ethylfuran	0.70	685	tr	0.92	917	tr
2-Methylbutanol	0.96	737	tr	3.40*	1174	0.07
Toluene	1.13	761	tr	1.44	1001	tr
Hexanal	1.42	801	tr	1.87	1043	tr
(2E)-Hexenal	1.98	850	0.01	3.37	1172	0.02
(3Z)-Hexenol	2.05	855	0.15	5.79	1348	0.16
(2E)-Hexenol	2.22	869	0.03	6.12	1371	0.04
Hexanol	2.25	872	0.05	5.44	1322	0.04
α-Thujene	2.96	925	tr	1.42	999	tr
α-Pinene	3.03	930	0.03	1.36	990	0.02
Camphene	3.22	942	0.01	1.70	1026	0.01
Sabinene	3.64*	970	0.06	2.27	1083	0.01
β-Pinene	3.64*	970	[0.06]	2.09	1065	0.04
Octen-3-ol	3.80	981	0.04	6.79*	1420	0.08
Octan-3-one	3.88	986	0.02	3.98*	1217	0.93
<i>trans</i> -Dehydroxylinalool oxide	3.96*	991	1.26	3.40*	1174	[0.07]
Myrcene	3.96*	991	[1.26]	2.87	1133	1.21
<i>cis</i> -Dehydroxylinalool oxide	4.17	1005	0.06	3.82*	1206	0.07
α-Terpinene	4.29	1013	0.02	2.95	1139	0.01
para-Cymene	4.41	1020	0.03	4.09	1225	0.03
β-Phellandrene	4.48*	1025	0.41	3.30	1166	0.02
Limonene	4.48*	1025	[0.41]	3.18	1156	0.41
(Z)-β-Ocimene	4.70	1039	0.48	3.77	1202	0.51
(E)-β-Ocimene	4.86	1049	0.91	3.98*	1217	[0.93]
γ-Terpinene	4.97	1056	0.03	3.82*	1206	[0.07]
<i>cis</i> -Linalool oxide (fur.)	5.18	1069	0.02	6.54	1402	0.02
Terpinolene	5.43*	1085	0.26	4.28	1238	0.26
<i>trans</i> -Linalool oxide (fur.)	5.43*	1085	[0.26]	6.92	1429	0.02
Hotrienol	5.74*	1104	20.14	8.82	1574	0.03
Linalool	5.74*	1104	[20.14]	8.12*†	1520	71.43
Dehydrosabinaketone	5.92	1116	0.01	8.64	1560	0.03
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	5.95	1118	0.01	9.65	1640	0.01
allo-Ocimene	6.13	1130	0.01	5.57	1332	0.01
Nerol oxide	6.50	1154	0.03	6.85	1425	0.05
Borneol	6.61	1161	0.02	9.80*	1652	6.47
Terpinen-4-ol	6.80	1174	0.04	8.59	1556	0.05
α-Terpineol	7.04	1190	3.45	9.80*	1652	[6.47]

Unknown [m/z 43, 71 (80), 67 (55), 59 (51), 68 (44), 41 (43)...]	7.20	1200	0.04			
Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.30	1207	0.02	6.24	1380	0.02
Linalyl formate	7.45	1217	0.07	8.41*	1542	0.12
Nerol	7.67	1232	0.78	11.08	1758	0.80
Linalyl acetate	8.18*	1268	53.81	8.22†	1527	[71.43]
Geraniol	8.18*	1268	[53.81]	11.66	1807	2.14
Neryl formate	8.44	1286	0.03	9.47	1625	0.04
Thymol	8.62	1298	0.03	15.12	2129	0.02
Geranyl formate	8.76	1308	0.04	9.90	1660	0.08
δ-Elemene	9.21	1334	0.01	6.96	1433	0.01
Hodiendiol derivative	9.31	1341	0.02	12.96	1923	0.03
α-Cubebene	9.39*	1347	0.09	6.79*	1420	[0.08]
α-Terpinyl acetate	9.39*	1347	[0.09]	9.71	1644	0.06
Unknown [m/z 43, 121 (52), 93 (48), 79 (33), 41 (30), 136 (26), 81 (25)...]	9.46	1352	0.01			
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.50	1355	0.02	11.12	1762	0.03
Neryl acetate	9.66	1366	1.22	10.20	1684	1.24
α-Copaene	9.75	1372	0.74	7.15	1447	0.73
(Z)-8-Hydroxylinalool?	9.80	1376	0.02	13.79	2000	0.03
β-Bourbonene	9.85*	1380	0.23	7.48	1471	0.21
1,5-diepi-β-Bourbonene	9.85*	1380	[0.23]	7.37	1463	0.02
Geranyl acetate	9.94†	1386	2.51	10.57	1715	2.36
β-Cubebene	9.96†	1387	[2.51]	7.79	1494	0.16
β-Elemene	9.99	1390	0.08	8.41*	1542	[0.12]
Isocaryophyllene	10.14	1401	0.02	8.12*†	1520	[71.43]
β-Caryophyllene	10.32	1413	1.63	8.46	1546	1.60
β-Copaene	10.46	1424	0.06	8.41*	1542	[0.12]
trans-α-Bergamotene	10.60	1434	0.03	8.41*	1542	[0.12]
α-Humulene	10.77	1447	0.11	9.28	1610	0.08
(E)-β-Farnesene	10.93*	1459	1.13	9.56	1632	1.12
9-epi-β-Caryophyllene	10.93*	1459	[1.13]	9.37	1617	0.02
Germacrene D	11.16*	1476	3.03	9.80*	1652	[6.47]
α-Amorphene	11.16*	1476	[3.03]	9.59	1634	0.02
β-Selinene	11.21	1480	0.03	9.87	1657	0.03
Hodiendiol derivative IV	11.24	1482	0.09			
Bicyclogermacrene	11.36	1491	0.39	10.06	1673	0.36
(Z)-α-Bisabolene	11.51*	1502	0.12	10.38*	1698	0.11
Hodiendiol derivative II	11.51*	1502	[0.12]	12.82	1910	0.01
γ-Cadinene	11.58	1508	0.02	10.38*	1698	[0.11]

Cubebol	11.61*	1510	0.20	12.56	1887	0.04
(3E,6E)- α -Farnesene	11.61*	1510	[0.20]	10.51	1710	0.17
(Z)-2-Lachnophyllum ester	11.66	1513	0.03	15.62	2178	0.03
Matricaria ester isomer II	11.69	1516	0.12			
δ -Cadinene	11.74*	1520	0.19	10.42	1702	0.20
<i>trans</i> -Calamenene	11.74*	1520	[0.19]	11.26	1773	tr
Matricaria ester isomer I	11.78	1523	1.02	16.23	2240	0.93
α -Calacorene	11.95	1536	0.05	12.13*	1848	0.08
Isocaryophyllene epoxide B	12.05*	1544	0.05	12.16	1851	0.01
α -Elemol	12.05*	1544	[0.05]	14.06	2025	0.01
Salviadienol?	12.11	1549	0.02	14.34	2052	0.01
1,5-Epoxyisoval-4(14)-ene	12.22	1558	0.06	12.13*	1848	[0.08]
Spathulenol	12.38	1570	0.21	14.41	2059	0.20
Caryophyllene oxide isomer	12.42*	1574	0.58	12.74	1903	0.04
Caryophyllene oxide	12.42*	1574	[0.58]	12.78	1906	0.57
Salvial-4(14)-en-1-one	12.57	1585	0.06	13.05	1931	0.05
Unknown [m/z 91, 119 (91), 79 (86), 93 (85), 41 (74), 107 (68), 105 (67), 134 (65)... 220 (1)]	12.69	1594	0.08			
Torilenol	12.82	1605	0.04	15.48*	2165	0.07
Guaia-6,10(14)-dien-4 β -ol	13.02	1621	0.02	15.79	2195	0.03
Hinesol	13.14*	1632	0.08	15.08	2125	0.07
Unknown [m/z 135, 93 (29), 79 (29), 41 (26), 107 (22), 67 (21), 69 (20)...]	13.14*	1632	[0.08]			
Unknown [m/z 123, 43 (86), 81 (75), 95 (73), 82 (68), 161 (64), 105 (63)... 220 (6)]	13.19	1636	0.02			
β -Eudesmol	13.26	1641	0.08	15.44	2160	0.13
Unknown [m/z 159, 91 (58), 105 (54), 93 (51), 81 (50), 177 (44)...]	13.31*	1645	0.05			
α -Eudesmol	13.31*	1645	[0.05]	15.34	2151	0.03
α -Cadinol	13.35	1648	0.02	15.48*	2165	[0.07]
Unknown [m/z 81, 41 (46), 79 (46), 93 (39), 91 (33), 107 (33)... 206 (8)]	13.52	1662	0.01			
Mustakone	13.58	1668	0.02	15.48*	2165	[0.07]
Eudesma-4(15),7-	13.70	1678	0.02			

dien-1β-ol						
Cyclocolorenone	14.55	1750	0.01	16.55	2273	0.01
Phytone	15.64	1846	0.03	14.72	2089	0.05
Sclareoloxide	15.88	1868	0.33			
Geranyl-α-terpinene	16.40	1916	0.13			
Unknown [m/z 109, 132 (88), 157 (76), 119 (66), 91 (57), 105 (55)...]	16.57	1931	0.13			
Geranyl-para-cymene	16.77	1950	0.06	16.18	2236	0.04
Manoyl oxide	17.04	1976	0.04	16.62	2282	0.02
13-epi-Manoyl oxide	17.26	1997	0.02	16.40	2258	0.01
Manool	17.73	2043	0.07	19.35	2583	0.05
Sclareolide?	17.91	2061	0.01			
Sclareol	19.29	2202	0.73	22.89	3027	0.72
Total identified		98.29%			97.05%	
Total reported		98.64%			97.11%	

*: 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