

Date : May 04, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21D20-ORA10


Customer identification : Citronella - China - 3 years - 048762A

Type : Essential oil

Source : *Cymbopogon winterianus*

Customer : Organic Aromas Inc.

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 : Benoit Roger, Ph. D.

Analysis date : May 03, 2021

Checked and approved by :

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

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia. This report is digitally signed, it is only considered valid if the digital signature is intact. The results only describe the samples that were submitted to the assays.

PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4705 ± 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
3-Methylcyclopentene	0.02	Alkene
3-Methylcyclopentane	0.01	Alkane
Isovaleral	tr	Aliphatic aldehyde
Unknown	0.02	Unknown
Unknown	0.02	Unknown
Tricyclene	0.02	Monoterpene
α -Thujene	tr	Monoterpene
α -Pinene	0.07	Monoterpene
Camphene	0.06	Monoterpene
Sabinene	0.02	Monoterpene
6-Methyl-5-hepten-2-one	0.08	Aliphatic ketone
Myrcene	0.03	Monoterpene
α -Phellandrene	0.01	Monoterpene
Octanal	0.01	Aliphatic aldehyde
α -Terpinene	0.01	Monoterpene
para-Cymene	0.02	Monoterpene
Limonene	2.90	Monoterpene
β -Phellandrene	0.01	Monoterpene
Unknown	0.04	Unknown
(Z)- β -Ocimene	0.23	Monoterpene
(E)- β -Ocimene	0.16	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.11	Aliphatic aldehyde
γ -Terpinene	0.01	Monoterpene
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.06	Monoterpene
Linalool	0.76	Monoterpenic alcohol
Nonanal	0.01	Aliphatic aldehyde
Unknown	0.04	Oxygenated monoterpene
<i>trans</i> -Rose oxide	0.01	Monoterpenic ether
Melonol ?	0.08	Normonoterpene
Unknown	0.02	Unknown
Isopulegol	1.19	Monoterpenic alcohol
Menthone	0.05	Monoterpenic ketone
Citronellal	33.53	Monoterpenic aldehyde
iso-Isopulegol	0.39	Monoterpenic alcohol
Isomenthone	0.04	Monoterpenic ketone
Borneol	0.03	Monoterpenic alcohol
neoiso-Isopulegol	0.10	Monoterpenic alcohol
Isopulegol isomer	0.04	Monoterpenic alcohol
Terpinen-4-ol	0.03	Monoterpenic alcohol
α -Terpineol	0.07	Monoterpenic alcohol
(4Z)-Decenal	0.03	Aliphatic aldehyde
Decanal	0.11	Aliphatic aldehyde
Nerol	0.20	Monoterpenic alcohol
Citronellol	9.38	Monoterpenic alcohol

Neral	0.43	Monoterpenic aldehyde
Geraniol	23.19	Monoterpenic alcohol
Geranial	0.78	Monoterpenic aldehyde
Citronellyl formate	0.09	Monoterpenic ester
Geranyl formate	0.09	Monoterpenic ester
Unknown	0.05	Norsesquiterpene
Citronellic acid	0.39	Monoterpenic acid
8-Hydroxy-neo-menthol	0.13	Monoterpenic alcohol
Eugenol	0.54	Phenylpropanoid
Citronellyl acetate	2.66	Monoterpenic ester
Neryl acetate	0.05	Monoterpenic ester
α -Copaene	0.04	Sesquiterpene
<i>cis</i> - β -Elemene	0.09	Sesquiterpene
Geranyl acetate	4.60	Monoterpenic ester
β -Elemene	1.35	Sesquiterpene
Methyleugenol	0.06	Phenylpropanoid
Dodecanal	0.01	Aliphatic aldehyde
β -Caryophyllene	0.68	Sesquiterpene
β -Copaene	0.04	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.15	Sesquiterpene
α -Humulene	0.17	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.05	Sesquiterpene
γ -Murolene	0.13	Sesquiterpene
Germacrene D	1.06	Sesquiterpene
β -Selinene	0.02	Sesquiterpene
epi-Cubebol	0.15	Sesquiterpenic alcohol
α -Selinene	0.03	Sesquiterpene
α -Murolene	0.44	Sesquiterpene
Germacrene A	0.45	Sesquiterpene
Methyl (<i>E</i>)-isoeugenol	0.43	Phenylpropanoid
γ -Cadinene	0.44	Sesquiterpene
Cubebol	0.24	Sesquiterpenic alcohol
<i>trans</i> -Calamenene	0.03	Sesquiterpene
δ -Cadinene	1.34	Sesquiterpene
Unknown	0.04	Sesquiterpene
α -Cadinene	0.09	Sesquiterpene
α -Elemol	2.23	Sesquiterpenic alcohol
Geranyl butyrate	0.26	Monoterpenic ester
Germacrene D-4-ol	0.92	Sesquiterpenic alcohol
Caryophyllene oxide	0.04	Sesquiterpenic ether
10-epi-Cubebol	0.07	Sesquiterpenic alcohol
Unknown	0.08	Unknown
γ -Eudesmol	0.18	Sesquiterpenic alcohol
τ -Cadinol	0.25	Sesquiterpenic alcohol
τ -Muurolol	0.30	Sesquiterpenic alcohol
β -Eudesmol	0.25	Sesquiterpenic alcohol
α -Eudesmol	0.18	Sesquiterpenic alcohol
α -Cadinol	0.51	Sesquiterpenic alcohol
Unknown	0.66	Oxygenated sesquiterpene
(2 <i>E</i> ,6 <i>Z</i>)-Farnesal	0.02	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>E</i>)-Farnesol	0.09	Sesquiterpenic alcohol
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	0.03	Sesquiterpenic aldehyde

Cryptomeridiol	0.02	Sesquiterpenic alcohol
Unknown	0.01	Oxygenated diterpene
Unknown	0.08	Oxygenated diterpene
Citronellyl citronellate	0.01	Monoterpenic ester
Unknown	0.13	Unknown
Unknown	0.30	Unknown
Unknown	0.29	Unknown
Consolidated total	97.44%	

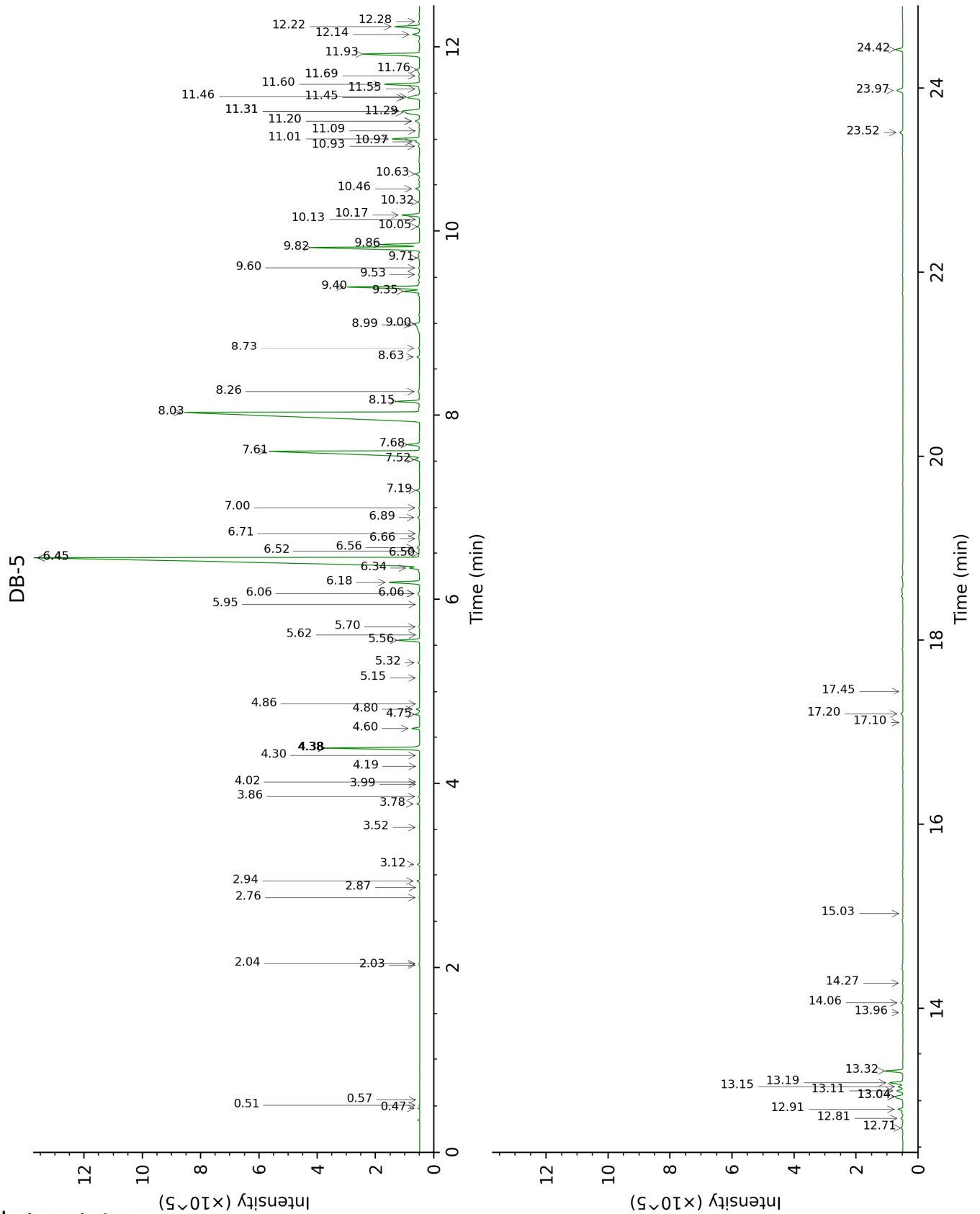
tr: The compound has been detected below 0.005% of total signal.

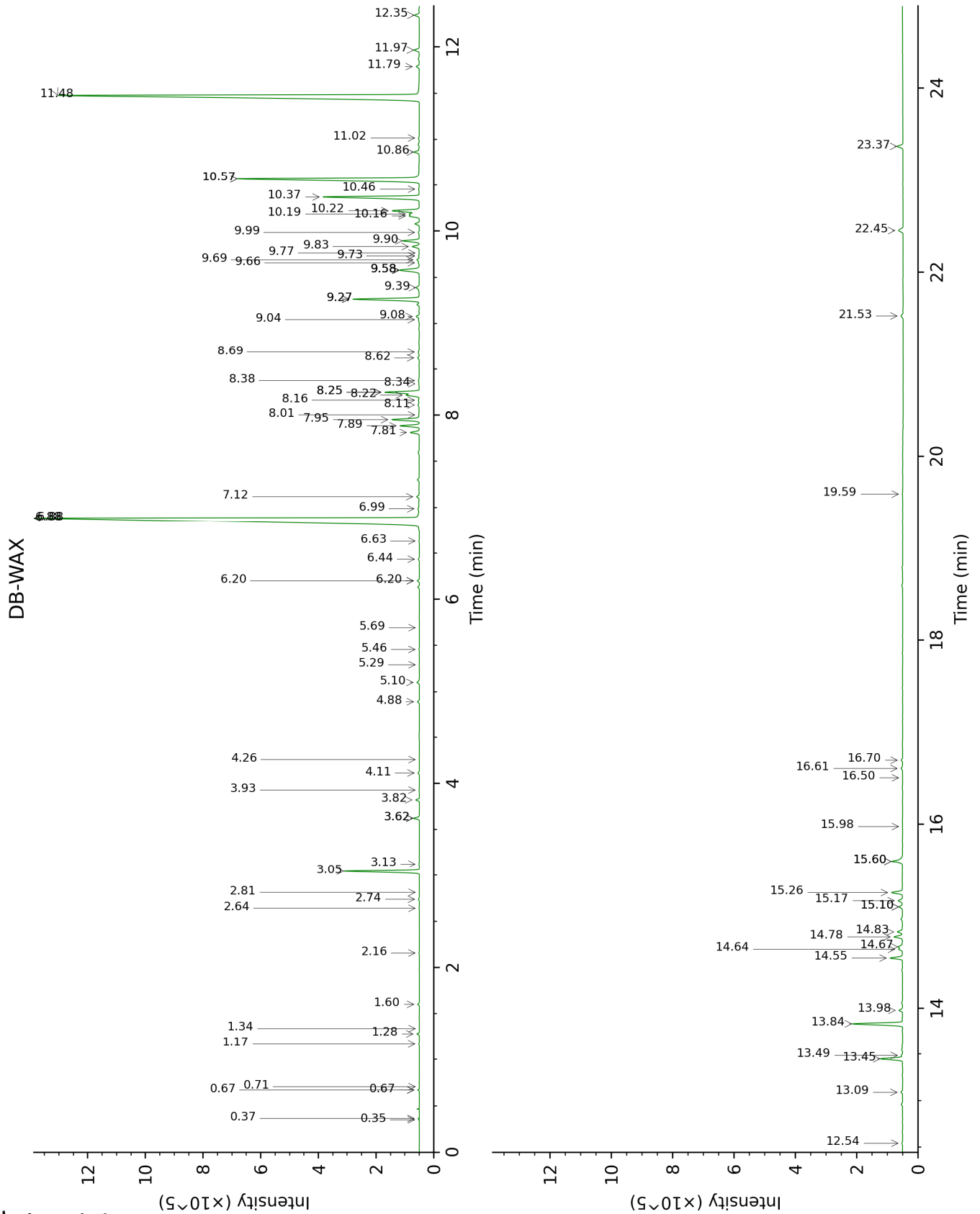
Note: no correction factor was applied

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	%
3-Methylcyclopentene	0.48	602	0.02	0.37	672	0.01
3-Methylcyclopentane	0.51	616	0.01	0.35	642	0.01
Isovaleral	0.57	640	tr	0.71	887	tr
Unknown [m/z 55, 83 (89), 82 (70), 67 (66), 41 (55), 69 (46), 111 (37)... 126 (2)]	2.03	860	0.02	0.67*	873	0.04
Unknown [m/z 55, 83 (79), 67 (65), 41 (63), 82 (60), 69 (58)... 111 (27), 126 (9)]	2.04	862	0.02	0.67*	873	[0.04]
Tricyclene	2.76	920	0.02	1.17	972	0.02
α -Thujene	2.87	927	tr	1.34	1001	tr
α -Pinene	2.94	932	0.07	1.28	992	0.07
Camphene	3.12	944	0.06	1.60	1027	0.06
Sabinene	3.52	971	0.02	2.16	1084	0.01
6-Methyl-5-hepten-2-one	3.78	988	0.08	4.88	1298	0.08
Myrcene	3.86	994	0.03	2.74	1133	0.03
α -Phellandrene	3.99	1003	0.01	2.64	1126	0.01
Octanal	4.02	1005	0.01	4.26	1251	0.01
α -Terpinene	4.19	1015	0.01	2.82	1139	0.01
para-Cymene	4.30	1023	0.02	3.93	1227	0.02
Limonene	4.38*	1028	3.05	3.05	1158	2.90
β -Phellandrene	4.38*	1028	[3.05]	3.13	1164	0.01
Unknown [m/z 59, 43 (12), 109 (11), 41 (10), 127 (8)...]	4.38*	1028	[3.05]	6.20*	1390	0.09
(Z)- β -Ocimene	4.60	1041	0.23	3.62*	1204	0.23
(E)- β -Ocimene	4.75	1051	0.16	3.82	1219	0.13
2,6-Dimethyl-5-heptenal (melonal)	4.80	1054	0.11	5.10	1311	0.12
γ -Terpinene	4.86	1058	0.01	3.62*	1204	[0.23]
Octanol	5.15	1076	0.02	8.00	1526	0.03
Terpinolene	5.32	1087	0.06	4.11	1240	0.05
Linalool	5.56	1102	0.76	7.89	1517	0.78
Nonanal	5.62	1106	0.01	5.69	1354	0.01
Unknown [m/z 111, 69 (70), 41 (68), 55 (53), 43 (51)... 154 (7)]	5.70	1112	0.04	5.46	1336	0.02
trans-Rose oxide	5.94	1127	0.01	5.29	1325	0.01
Melonol ?	6.06*	1135	0.11			
Unknown [m/z 81, 70 (98), 67 (63), 82	6.06*	1135	[0.11]	6.63	1422	0.02

(53), 41 (46), 69 (46), 109 (43)...						
Isopulegol	6.18	1142	1.19	7.95	1522	1.24
Menthone	6.34†	1152	34.27	6.44	1408	0.05
Citronellal	6.45*†	1160	[34.27]	6.88*	1441	33.57
iso-Isopulegol	6.45*†	1160	[34.27]	7.81	1511	0.39
Isomenthone	6.50	1162	0.04	6.88*	1441	[33.57]
Borneol	6.52	1164	0.03	9.58*	1651	1.14
neoiso-Isopulegol	6.56	1167	0.10	8.62	1574	0.07
Isopulegol isomer	6.66	1173	0.04	8.38	1555	0.04
Terpinen-4-ol	6.71	1176	0.03	8.34	1552	0.03
α-Terpineol	6.89	1188	0.07	9.58*	1651	[1.14]
(4Z)-Decenal	7.00	1195	0.03			
Decanal	7.19	1207	0.11	7.12	1459	0.10
Nerol	7.52	1230	0.20	10.86	1759	0.26
Citronellol	7.61	1236	9.38	10.57*	1734	9.52
Neral	7.68	1240	0.43	9.26*	1626	3.00
Geraniol	8.03	1264	23.19	11.48	1812	23.65
Geranial	8.15	1272	0.78	9.90	1677	0.73
Citronellyl formate	8.26	1279	0.09	8.69	1579	0.07
Geranyl formate	8.63	1304	0.09	9.69	1660	0.12
Unknown [m/z 135, 121 (81), 177 (78), 107 (60), 192 (42), 149 (35)]	8.73	1311	0.05	6.20*	1390	[0.09]
Citronellic acid	8.99	1329	0.39	15.60*	2203	0.64
8-Hydroxy-neo- menthol	9.00	1330	0.13	13.98	2042	0.18
Eugenol	9.35	1355	0.54	14.55	2097	0.57
Citronellyl acetate	9.40	1358	2.66	9.26*	1626	[3.00]
Neryl acetate	9.53	1368	0.05	9.99	1685	0.04
α-Copaene	9.60	1373	0.04	6.99	1449	0.05
cis-β-Elemene	9.71	1380	0.09	8.11	1534	0.07
Geranyl acetate	9.82	1388	4.60	10.37	1717	4.58
β-Elemene	9.86	1391	1.35	8.25*†	1545	[2.11]
Methyleugenol	10.05	1404	0.06	13.09	1958	0.07
Dodecanal	10.13	1410	0.01	9.76	1667	0.01
β-Caryophyllene	10.17	1414	0.68	8.22†	1543	2.11
β-Copaene	10.32	1424	0.04	8.16	1539	0.04
trans-α- Bergamotene	10.46	1435	0.15	8.25*†	1545	[2.11]
α-Humulene	10.63	1448	0.17	9.08	1610	0.14
trans-Cadina-1(6),4- diene	10.93	1470	0.05	9.04	1608	0.05
γ-Murolene	10.98	1474	0.13	9.39	1636	0.20
Germacrene D	11.01	1476	1.06	9.58*	1651	[1.14]
β-Selinene	11.09	1482	0.02	9.66	1658	0.04
epi-Cubebol	11.20*	1490	0.22	11.79	1840	0.15
α-Selinene	11.20*	1490	[0.22]	9.73	1664	0.03
α-Murolene	11.29	1497	0.44	9.83	1672	0.33
Germacrene A	11.31*	1498	0.85	10.16	1699	0.45

Methyl (E)-isoeugenol	11.31*	1498	[0.85]	14.78	2120	0.43
γ-Cadinene	11.45	1509	0.44	10.19	1701	0.41
Cubebol	11.46	1510	0.24	12.34	1889	0.23
trans-Calamenene	11.55	1517	0.03	11.02	1772	0.04
δ-Cadinene	11.60	1521	1.34	10.22	1704	1.35
Unknown [m/z 119, 105 (53), 161 (33), 93 (28), 91 (25), 40 (20)...204]	11.69	1528	0.04	10.46	1724	0.04
α-Cadinene	11.76	1533	0.09	10.57*	1734	[9.52]
α-Elemol	11.92	1547	2.23	13.84	2028	2.26
Geranyl butyrate	12.14	1563	0.26	11.97	1856	0.26
Germacrene D-4-ol	12.22	1570	0.92	13.45	1992	0.98
Caryophyllene oxide	12.28	1574	0.04	12.54	1907	0.04
10-epi-Cubebol	12.71	1608	0.07	13.49	1995	0.06
Unknown [m/z 69, 41 (42), 109 (25), 123 (22), 64 (22), 179 (18)...]	12.81	1617	0.08			
γ-Eudesmol	12.91	1625	0.18	14.64	2107	0.19
τ-Cadinol	13.04*	1636	0.45	14.67	2109	0.25
τ-Muurolol	13.04*	1636	[0.45]	14.83	2126	0.30
β-Eudesmol	13.11	1641	0.25	15.17	2160	0.25
α-Eudesmol	13.15	1645	0.18	15.10*	2153	0.22
α-Cadinol	13.19	1648	0.51	15.26	2169	0.59
Unknown [suspected m/z 59, 93 (79), 161 (61), 107 (47), 81 (44), 121 (37)...]	13.32	1659	0.66			
(2E,6Z)-Farnesal	13.96	1712	0.02	15.10*	2153	[0.22]
(2E,6E)-Farnesol	14.06	1721	0.09	16.61	2309	0.09
(2E,6E)-Farnesal	14.27	1740	0.03	15.60*	2203	[0.64]
Cryptomeridiol	15.03	1805	0.02	19.59	2648	0.02
Unknown [m/z 81, 137 (70), 95 (46), 69 (45), 41 (39), 55 (29)...]	17.10	1998	0.01	15.98	2243	0.01
Unknown [m/z 41, 69 (98), 55 (55), 81 (46), 109 (46)... 290 (8)]	17.20	2008	0.08	16.70	2319	0.08
Citronellyl citronellate	17.45	2032	0.01	16.50	2298	0.01
Unknown [m/z 69, 81 (79), 81 (70), 137 (53), 139 (35), 95 (30)...]	23.52	2716	0.13	21.53	2889	0.12
Unknown [m/z 69, 81 (84), 137 (53), 83	23.97	2774	0.30	22.45	3011	0.29

(30), 95 (27), 41 (19)...						
Unknown [m/z 69, 81 (64), 95 (29), 137 (19), 41 (19)...	24.42	2833	0.29	23.37	3137	0.28
Total identified	96.04%			96.44%		
Total reported	97.74%			97.30%		

*: 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