

Date : March 02, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23B27-PTH01


Customer identification : Citronella ORGANIC - China - CD0107R

Type : Essential oil

Source : *Cymbopogon winterianus*

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 : February 28, 2023

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4703 ± 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-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
3-Methylcyclopentane	tr	Alkane
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	tr	Aliphatic alcohol
Hexanal	tr	Aliphatic aldehyde
Unknown	0.01	Unknown
Unknown	0.01	Unknown
α -Thujene	0.01	Monoterpene
α -Pinene	0.05	Monoterpene
Camphene	0.01	Monoterpene
Sabinene	0.02	Monoterpene
β -Pinene	0.04	Monoterpene
6-Methyl-5-hepten-2-one	0.09	Aliphatic ketone
Myrcene	0.10	Monoterpene
Octanal	0.01	Aliphatic aldehyde
α -Phellandrene	0.03	Monoterpene
Δ^3 -Carene	0.03	Monoterpene
α -Terpinene	0.02	Monoterpene
para-Cymene	0.04	Monoterpene
β -Phellandrene	0.06	Monoterpene
Limonene	3.69	Monoterpene
1,8-Cineole	0.05	Monoterpenic ether
(Z)- β -Ocimene	0.03	Monoterpene
(E)- β -Ocimene	0.04	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.07	Aliphatic aldehyde
γ -Terpinene	0.04	Monoterpene
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.09	Monoterpene
<i>trans</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
Linalool	0.92	Monoterpenic alcohol
Nonanal	0.01	Aliphatic aldehyde
Unknown	0.03	Oxygenated monoterpene
<i>cis</i> -Rose oxide	0.01	Monoterpenic ether
<i>trans</i> -para-Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol
<i>trans</i> -Rose oxide	0.02	Monoterpenic ether
Unknown	0.01	Unknown
Melonol ?	0.08	Normonoterpene
Isopulegol	2.07	Monoterpenic alcohol
Menthone	0.07	Monoterpenic ketone
iso-Isopulegol	0.89	Monoterpenic alcohol
Citronellal	32.99	Monoterpenic aldehyde
Borneol	0.05	Monoterpenic alcohol
neoiso-Isopulegol	0.17	Monoterpenic alcohol

Isopulegol isomer	0.06	Monoterpenic alcohol
Terpinen-4-ol	0.06	Monoterpenic alcohol
α -Terpineol	0.08	Monoterpenic alcohol
(4Z)-Decenal	0.03	Aliphatic aldehyde
Decanal	0.12	Aliphatic aldehyde
2,3-Epoxyneral?	0.03	Monoterpenic aldehyde
Nerol	0.18	Monoterpenic alcohol
Citronellol	12.63	Monoterpenic alcohol
Neral	0.37	Monoterpenic aldehyde
Piperitone	0.04	Monoterpenic ketone
Geraniol	20.27	Monoterpenic alcohol
Geranial	0.47	Monoterpenic aldehyde
Citronellyl formate	0.06	Monoterpenic ester
Geranyl formate	0.04	Monoterpenic ester
Unknown	0.06	Norsesquiterpene
8-Hydroxy-neo-menthol	0.22	Monoterpenic alcohol
Citronellic acid	0.02	Monoterpenic acid
Citronellyl acetate	1.99	Monoterpenic ester
Eugenol	1.06	Phenylpropanoid
Neryl acetate	0.03	Monoterpenic ester
α -Copaene	0.05	Sesquiterpene
β -Bourbonene	0.14	Sesquiterpene
<i>cis</i> - β -Elemene	0.08	Sesquiterpene
Geranyl acetate	2.00	Monoterpenic ester
β -Elemene	1.83	Sesquiterpene
β -Cubebene	0.03	Sesquiterpene
Dodecanal	0.01	Aliphatic aldehyde
β -Caryophyllene	0.18	Sesquiterpene
β -Copaene	0.05	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.01	Sesquiterpene
Isogermacrene D	0.02	Sesquiterpene
α -Humulene	0.13	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.08	Sesquiterpene
γ -Muurolene	0.27	Sesquiterpene
Germacrene D	2.38	Sesquiterpene
β -Selinene	0.07	Sesquiterpene
epi-Cubebol	0.08	Sesquiterpenic alcohol
α -Selinene	0.05	Sesquiterpene
α -Muurolene	0.58	Sesquiterpene
Germacrene A	0.51	Sesquiterpene
Methyl (<i>E</i>)-isoeugenol	0.08	Phenylpropanoid
γ -Cadinene	0.62	Sesquiterpene
Cubebol	0.06	Sesquiterpenic alcohol
δ -Cadinene	2.12	Sesquiterpene
<i>trans</i> -Calamenene	0.03	Sesquiterpene
Unknown	0.06	Sesquiterpene
α -Cadinene	0.15	Sesquiterpene
α -Elemol	2.48	Sesquiterpenic alcohol
Geranyl butyrate	0.01	Monoterpenic ester
Germacrene D-4-ol	0.49	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
10-epi-Cubebol	0.05	Sesquiterpenic alcohol

Unknown	0.10	Unknown
γ-Eudesmol	0.30	Sesquiterpenic alcohol
τ-Cadinol	0.60	Sesquiterpenic alcohol
β-Eudesmol	0.34	Sesquiterpenic alcohol
α-Muurolol	0.13	Sesquiterpenic alcohol
α-Eudesmol	0.28	Sesquiterpenic alcohol
α-Cadinol	0.60	Sesquiterpenic alcohol
Unknown	0.43	Oxygenated sesquiterpene
(2E,6Z)-Farnesal	0.01	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	0.07	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
Cryptomeridiol	0.03	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated diterpene
Unknown	0.14	Oxygenated diterpene
Unknown	0.01	Unknown
Consolidated total	97.54%	

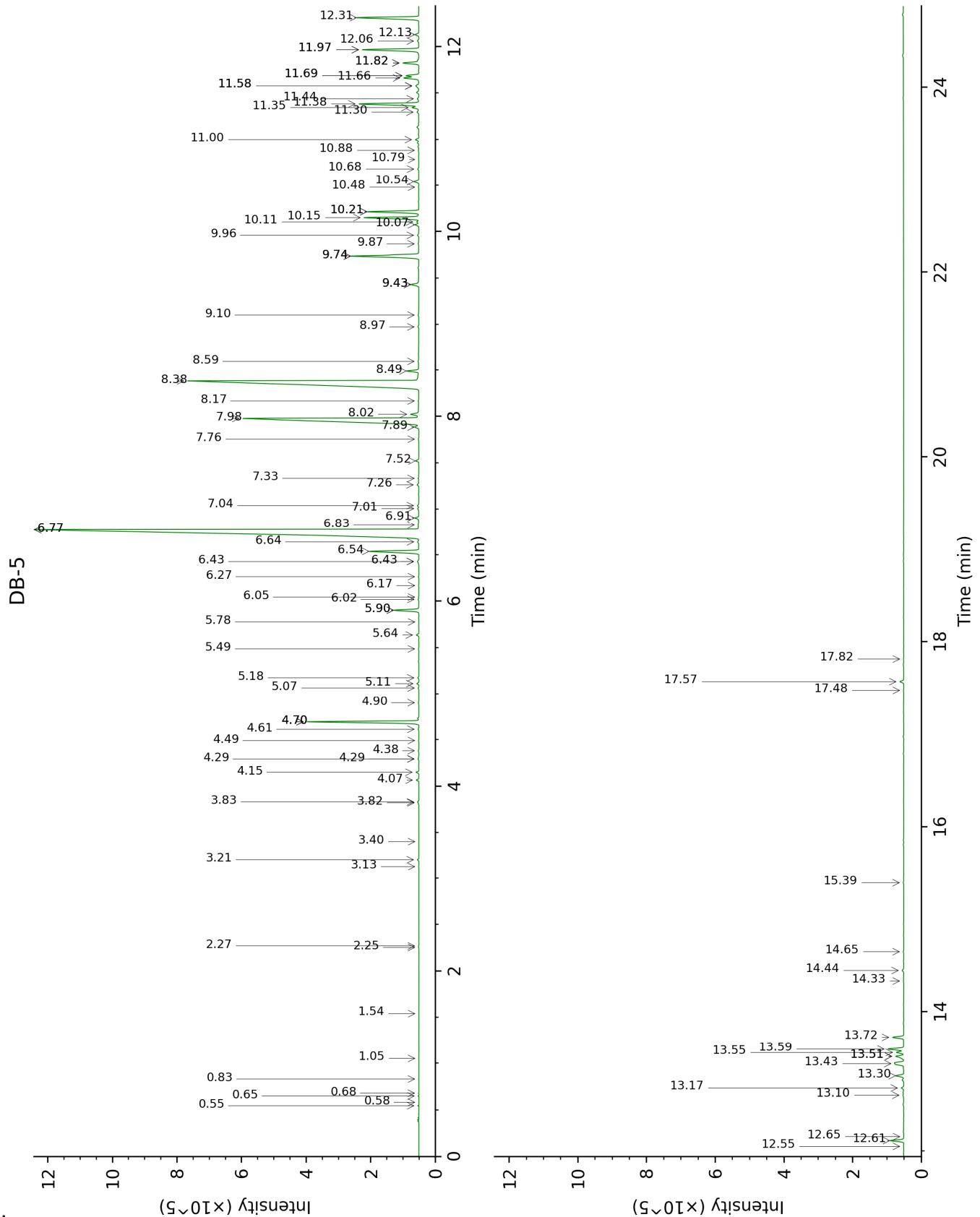
tr: The compound has been detected below 0.005% of total signal.

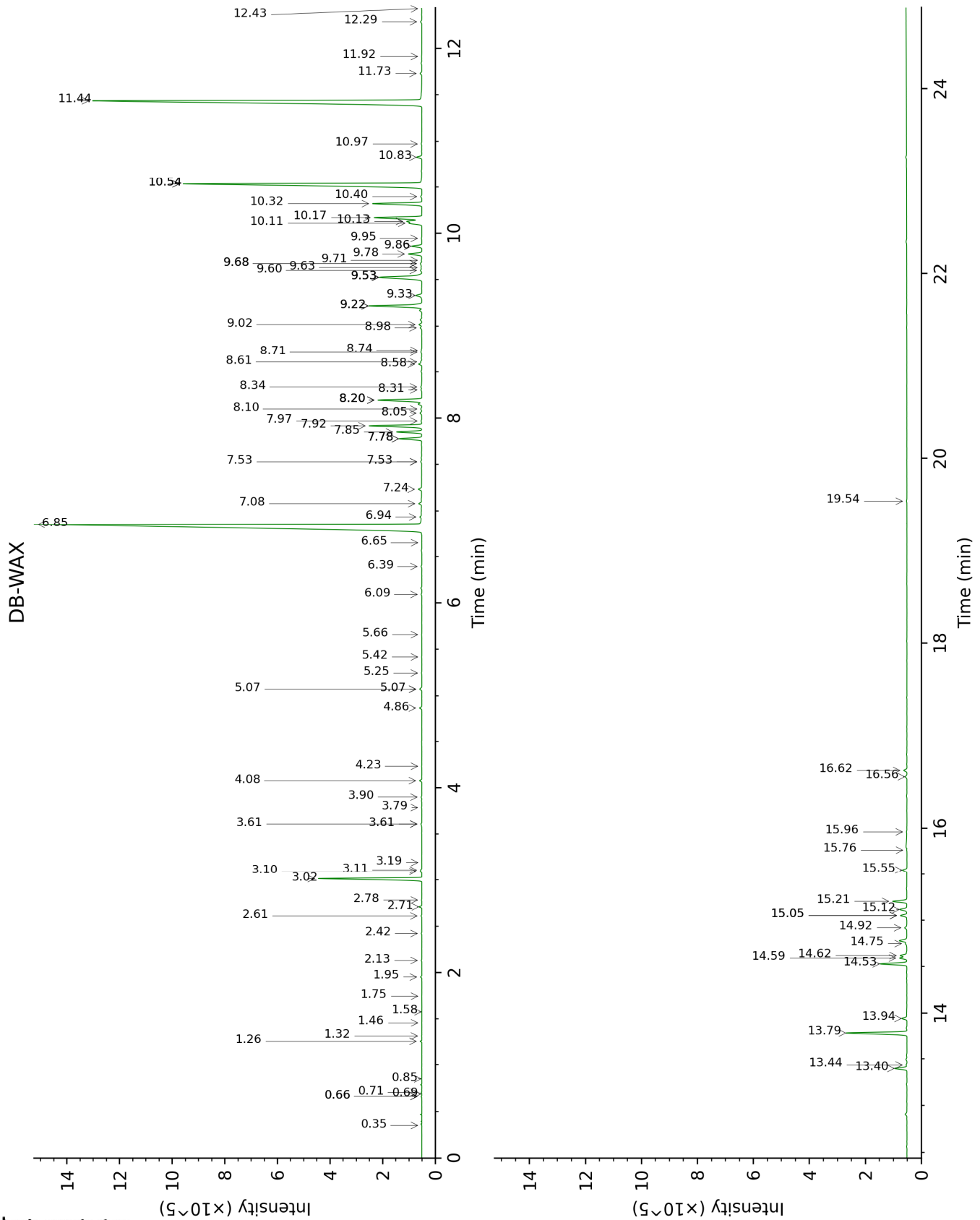
Note: no correction factor was applied

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-Methyl-3-buten-2-ol	0.55	606	0.01	1.46	1012	tr
3-Methylcyclopentane	0.58	618	tr	0.35	640	tr
Isovaleral	0.65	640	0.01	0.71	886	0.01
2-Methylbutyral	0.68	651	0.01	0.69	880	tr
2-Ethylfuran	0.83	701	tr	0.85	917	tr
Isoamyl alcohol	1.05	733	tr	3.19	1172	0.01
Hexanal	1.54	799	tr	1.75	1042	tr
Unknown [m/z 55, 83 (89), 82 (70), 67 (66), 41 (55), 69 (46), 111 (37)... 126 (2)]	2.26	859	0.01	0.66*	869	0.01
Unknown [m/z 55, 83 (79), 67 (65), 41 (63), 82 (60), 69 (58)... 111 (27), 126 (9)]	2.27	861	0.01	0.66*	869	[0.01]
α-Thujene	3.13	926	0.01	1.32	998	0.01
α-Pinene	3.21	930	0.05	1.26	990	0.04
Camphene	3.40	943	0.01	1.58	1025	tr
Sabinene	3.82†	971	0.07	2.13	1082	0.02
β-Pinene	3.83†	971	[0.07]	1.95	1064	0.04
6-Methyl-5-hepten-2-one	4.07	987	0.09	4.86	1302	0.09
Myrcene	4.15	992	0.10	2.71	1133	0.09
Octanal	4.29*	1002	0.05	4.23	1254	0.01
α-Phellandrene	4.29*	1002	[0.05]	2.61	1124	0.03
Δ ³ -Carene	4.38	1007	0.03	2.42	1109	0.02
α-Terpinene	4.49	1014	0.02	2.78	1139	0.01
para-Cymene	4.61	1022	0.04	3.90	1228	0.03
β-Phellandrene	4.70*	1027	3.78	3.10	1164	0.06
Limonene	4.70*	1027	[3.78]	3.02	1158	3.69
1,8-Cineole	4.70*	1027	[3.78]	3.11	1166	0.05
(Z)-β-Ocimene	4.90	1040	0.03	3.61*	1206	0.05
(E)-β-Ocimene	5.07	1050	0.04	3.79	1220	0.02
2,6-Dimethyl-5-heptenal (melonal)	5.11	1053	0.07	5.07*	1312	0.10
γ-Terpinene	5.18	1057	0.04	3.61*	1206	[0.05]
Octanol	5.49	1076	0.02	7.97	1526	0.05
Terpinolene	5.64	1086	0.09	4.08	1242	0.08
trans-Sabinene hydrate	5.78	1094	0.01	7.78*	1512	0.90
Linalool	5.90*	1102	0.93	7.85	1517	0.92
Nonanal	5.90*	1102	[0.93]	5.66	1355	0.01
Unknown [m/z 111, 69 (70), 41 (68), 55	6.02	1110	0.03	5.42	1337	0.01

(53), 43 (51)... 154 (7)]						
<i>cis</i> -Rose oxide	6.05	1111	0.01	5.07*	1312	[0.10]
<i>trans</i> -para-Mentha-2,8-dien-1-ol	6.17	1119	0.02	8.74	1586	0.03
<i>trans</i> -Rose oxide	6.27	1125	0.02	5.25	1325	0.02
Unknown [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	6.43*	1136	0.09	6.65	1427	0.01
Melonol ?	6.43*	1136	[0.09]			
Isopulegol	6.54	1143	2.07	7.92	1522	2.13
Menthone	6.64	1149	0.07	6.39	1408	0.04
iso-Isopulegol	6.77*	1158	34.36	7.78*	1512	[0.90]
Citronellal	6.77*	1158	[34.36]	6.85	1442	32.99
Borneol	6.82	1161	0.05	9.53*	1649	2.50
neoiso-Isopulegol	6.91	1166	0.17	8.58	1574	0.13
Isopulegol isomer	7.01	1172	0.06	8.31	1552	0.04
Terpinen-4-ol	7.04	1175	0.06	8.34	1555	0.08
α -Terpineol	7.26	1189	0.08	9.53*	1649	[2.50]
(4Z)-Decenal	7.33	1193	0.03	7.53*	1492	0.06
Decanal	7.52	1205	0.12	7.08	1459	0.15
2,3-Epoxyneral?	7.76	1221	0.03			
Nerol	7.89	1230	0.18	10.83	1758	0.22
Citronellol	7.98	1236	12.63	10.54*	1733	13.04
Neral	8.02	1239	0.37	9.22*	1624	2.35
Piperitone	8.17	1248	0.04	9.63	1658	0.04
Geraniol	8.38	1263	20.27	11.44	1810	20.52
Geranial	8.49	1270	0.47	9.86	1677	0.40
Citronellyl formate	8.59	1277	0.06	8.61	1576	0.05
Geranyl formate	8.97	1302	0.04	9.68*	1661	0.09
Unknown [m/z 135, 121 (81), 177 (78), 107 (60), 192 (42), 149 (35)]	9.10	1311	0.06	6.09	1386	0.03
8-Hydroxy-neomenthol	9.43*	1334	0.34	13.94	2040	0.22
Citronellic acid	9.43*	1334	[0.34]	15.76	2222	0.02
Citronellyl acetate	9.74*	1356	3.18	9.22*	1624	[2.35]
Eugenol	9.74*	1356	[3.18]	14.53	2097	1.06
Neryl acetate	9.87	1365	0.03	9.95	1684	0.02
α -Copaene	9.96	1372	0.05	6.94	1448	0.10
β -Bourbonene	10.07	1380	0.14	7.24	1470	0.18
<i>cis</i> - β -Elemene	10.10	1382	0.08	8.06	1533	0.09
Geranyl acetate	10.15	1385	2.00	10.32	1715	1.98
β -Elemene	10.22*	1389	1.86	8.20*†	1544	2.03
β -Cubebene	10.22*	1389	[1.86]	7.53*	1492	[0.06]
Dodecanal	10.48	1408	0.01	9.71	1664	0.02
β -Caryophyllene	10.54	1413	0.18	8.20*†	1544	[2.03]
β -Copaene	10.68	1423	0.05	8.10	1536	0.05
<i>trans</i> - α -Bergamotene	10.78	1431	0.01	8.20*†	1544	[2.03]

Isogermacrene D	10.88	1438	0.02	8.71	1584	0.04
α-Humulene	11.00	1447	0.13	9.02	1608	0.12
<i>trans</i> -Cadina-1(6),4-diene	11.30	1469	0.08	8.98	1605	0.08
γ-Muurolene	11.34	1473	0.27	9.33	1634	0.29
Germacrene D	11.38	1476	2.38	9.53*	1649	[2.50]
β-Selinene	11.44	1480	0.07	9.60	1655	0.07
epi-Cubebol	11.58*	1490	0.18	11.73	1836	0.08
α-Selinene	11.58*	1490	[0.18]	9.68*	1661	[0.09]
α-Muurolene	11.66†	1496	1.06	9.78	1670	0.58
Germacrene A	11.69*†	1498	[1.06]	10.11	1697	0.51
Methyl (E)-isoeugenol	11.69*†	1498	[1.06]	14.75	2119	0.08
γ-Cadinene	11.82*	1508	0.60	10.13	1698	0.62
Cubebol	11.82*	1508	[0.60]	12.29	1885	0.06
δ-Cadinene	11.97*	1520	2.19	10.17	1702	2.12
<i>trans</i> -Calamenene	11.97*	1520	[2.19]	10.97	1770	0.03
Unknown [m/z 119, 105 (53), 161 (33), 93 (28), 91 (25), 40 (20)...204]	12.06	1527	0.06	10.40	1721	0.05
α-Cadinene	12.13	1532	0.15	10.54*	1733	[13.04]
α-Elemol	12.31	1547	2.48	13.79	2025	2.48
Geranyl butyrate	12.55	1565	0.01	11.92	1852	0.02
Germacrene D-4-ol	12.61	1570	0.49	13.40	1988	0.51
Caryophyllene oxide isomer	12.65	1573	0.01	12.43	1898	0.01
10-epi-Cubebol	13.10	1608	0.05	13.44	1991	0.04
Unknown [m/z 69, 41 (42), 109 (25), 123 (22), 64 (22), 179 (18)...]	13.17	1615	0.10			
γ-Eudesmol	13.30	1626	0.30	14.62	2106	0.28
τ-Cadinol	13.43	1636	0.60	14.59	2103	0.29
β-Eudesmol	13.51*	1643	0.39	15.12	2156	0.34
α-Muurolol	13.51*	1643	[0.39]	14.92	2136	0.13
α-Eudesmol	13.55	1646	0.28	15.05*	2149	0.28
α-Cadinol	13.59	1649	0.60	15.21	2164	0.60
Unknown [suspected m/z 59, 93 (79), 161 (61), 107 (47), 81 (44), 121 (37)...]	13.72	1660	0.43			
(2E,6Z)-Farnesal	14.33	1710	0.01	15.05*	2149	[0.28]
(2E,6E)-Farnesol	14.44	1720	0.07	16.56	2305	0.08
(2E,6E)-Farnesal	14.65	1738	0.02	15.55	2199	0.19
Cryptomeridiol	15.39	1802	0.03	19.54	2644	0.02
Unknown [m/z 81, 137 (70), 95 (46), 69 (45), 41 (39), 55 (29)...]	17.48	1996	0.02	15.96	2242	0.03

Unknown [m/z 41, 69 (98), 55 (55), 81 (46), 109 (46)... 290 (8)]	17.57	2005	0.14	16.62	2312	0.14
Unknown [m/z 69, 41 (96), 55 (53), 109 (48), 95 (43), 67 (35)...]	17.82	2029	0.01			
Total identified		97.20%			96.99%	
Total reported		98.07%			97.26%	

*: 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