

Date : 2023-09-01

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23H28-PTH01

Customer Identification : Lemon Petitgrain - Spain - LY1100R

Type : Essential Oil

Source : *Citrus x limon*

Customer : Plant Therapy

Checked and approved by:

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

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GAS CHROMATOGRAPHIC ANALYSIS

Method : PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID

***ISO**

Results : See analysis summary (next page)

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

Date : 2023-08-30

PHYSICOCHEMICAL DATA

Refractive index : 1.4757 ± 0.0003 (20 °C)

Method : PC-MAT-016 - Measure of the refractive index of a liquid.

Analyst : Cindy Caron B. Sc.

Date : 2023-08-28

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	0.03	Aliphatic alcohol
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Hexanal	0.01	Aliphatic aldehyde
Octane	tr	Alkane
(3Z)-Hexenol	0.01	Aliphatic alcohol
Unknown	0.01	Unknown
Hexanol	0.02	Aliphatic alcohol
Unknown	0.01	Unknown
Tricyclene	0.02	Monoterpene
α -Thujene	0.12	Monoterpene
α -Pinene	1.56	Monoterpene
Camphene	0.11	Monoterpene
α -Fenchene	0.01	Monoterpene
β -Pinene	15.31	Monoterpene
Sabinene	2.81	Monoterpene
6-Methyl-5-hepten-2-one	2.59	Aliphatic ketone
Myrcene	1.05	Monoterpene
Pseudolimonene	0.02	Monoterpene
α -Phellandrene	0.11	Monoterpene
Octanal	0.02	Aliphatic aldehyde
Δ^3 -Carene	1.56	Monoterpene
α -Terpinene	0.18	Monoterpene
<i>para</i> -Cymene	0.25	Monoterpene
Limonene	42.84	Monoterpene
β -Phellandrene	0.15	Monoterpene
1,8-Cineole	2.37	Monoterpenic ether
(Z)- β -Ocimene	0.45	Monoterpene
(E)- β -Ocimene	2.02	Monoterpene
Unknown	0.02	Monoterpene
γ -Terpinene	0.51	Monoterpene
<i>cis</i> -Sabinene hydrate	0.04	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
α -Pinene oxide analog	0.01	Monoterpenic ether
Terpinolene isomer	0.01	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.04	Monoterpenic alcohol
Terpinolene	0.38	Monoterpene
<i>trans</i> -Sabinene hydrate	0.02	Monoterpenic alcohol
Rosefuran	0.03	Monoterpenic ether

Linalool	1.16	Monoterpenic alcohol
Nonanal	0.10	Aliphatic aldehyde
<i>cis</i> -Rose oxide	0.01	Monoterpenic ether
endo-Fenchol	0.02	Monoterpenic alcohol
<i>trans-para</i> -Mentha-2,8-dien-1-ol	0.06	Monoterpenic alcohol
<i>cis</i> -Limonene oxide	0.02	Monoterpenic ether
allo-Ocimene	0.02	Monoterpene
<i>trans</i> -Limonene oxide	0.02	Monoterpenic ether
<i>cis-para</i> -Mentha-2,8-dien-1-ol	0.07	Monoterpenic alcohol
Camphor	0.67	Monoterpenic ketone
(<i>E</i>)-Myroxide	0.01	Monoterpenic ether
Isopulegol	0.05	Monoterpenic alcohol
Citronellal	0.57	Monoterpenic aldehyde
iso-Isopulegol	0.03	Monoterpenic alcohol
Isoneral	0.01	Monoterpenic aldehyde
δ -Terpineol	0.17	Monoterpenic alcohol
Terpinen-4-ol	0.59	Monoterpenic alcohol
Unknown	0.05	Oxygenated monoterpene
Isogeranial	0.04	Monoterpenic aldehyde
<i>para</i> -Cymen-8-ol	0.02	Monoterpenic alcohol
α -Terpineol	0.77	Monoterpenic alcohol
Unknown	0.05	Unknown
Unknown	0.03	Unknown
Unknown	0.27	Oxygenated monoterpene
Decanal	0.04	Aliphatic aldehyde
<i>trans</i> -Carveol	0.03	Monoterpenic alcohol
Nerol	1.05	Monoterpenic alcohol
Citronellol	0.43	Monoterpenic alcohol
Neral	3.64	Monoterpenic aldehyde
(<i>Z</i>)-Isogeraniol	0.03	Monoterpenic alcohol
Geraniol	0.82	Monoterpenic alcohol
Geranial	5.46	Monoterpenic aldehyde
Neryl formate	tr	Monoterpenic ester
Unknown	0.03	Oxygenated monoterpene
Citronellyl formate	0.04	Monoterpenic ester
(<i>E</i>)-Anethole	0.05	Phenylpropanoid
Geranyl formate	0.07	Monoterpenic ester
Undecanal	0.03	Aliphatic aldehyde
4-Vinylguaiacol	0.04	Simple phenolic
δ -Elemene	0.06	Sesquiterpene
Limonene <i>trans</i> -glycol	0.03	Monoterpenic alcohol
Citronellyl acetate	0.15	Monoterpenic ester
Neryl acetate	1.66	Monoterpenic ester
Geranyl acetate	1.65	Monoterpenic ester
β -Elemene	0.02	Sesquiterpene

β -Caryophyllene	1.84	Sesquiterpene
<i>cis</i> - α -Bergamotene	0.02	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.19	Sesquiterpene
α -Humulene	0.17	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.03	Sesquiterpene
Geranyl propionate	0.05	Monoterpenic ester
<i>trans</i> - β -Bergamotene	0.02	Sesquiterpene
Bicyclogermacrene	0.19	Sesquiterpene
(<i>Z</i>)- α -Bisabolene	0.03	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	0.05	Sesquiterpene
β -Bisabolene	0.28	Sesquiterpene
δ -Cadinene	0.05	Sesquiterpene
(<i>E</i>)-Nerolidol	0.01	Sesquiterpenic alcohol
Spathulenol	0.05	Sesquiterpenic alcohol
Caryophyllene oxide	0.08	Sesquiterpenic ether
Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
<i>trans</i> -Sesquisabinene hydrate	0.01	Sesquiterpenic alcohol
Humulene epoxide II	0.01	Sesquiterpenic ether
Isospathulenol	0.01	Sesquiterpenic alcohol
τ -Cadinol	0.02	Sesquiterpenic alcohol
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
α -Bisabolol	0.03	Sesquiterpenic alcohol
Phytone	0.01	Terpenic ketone
Unknown	0.01	Unknown
<i>meta</i> -Camphorene	0.02	Diterpene
<i>para</i> -Camphorene	0.03	Diterpene
Unknown	0.03	Unknown
Unknown	0.01	Unknown
Unknown	0.02	Unknown
6-Methyl-4,6-bis(4-methylpent-3-en-1-yl)cyclohexa-1,3-dienecarbaldehyde?	0.06	Diterpenic aldehyde
Phytol	0.10	Diterpenic alcohol
(<i>E</i>)-Phytyl acetate	0.02	Diterpenic ester
Consolidated total	98.36	

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

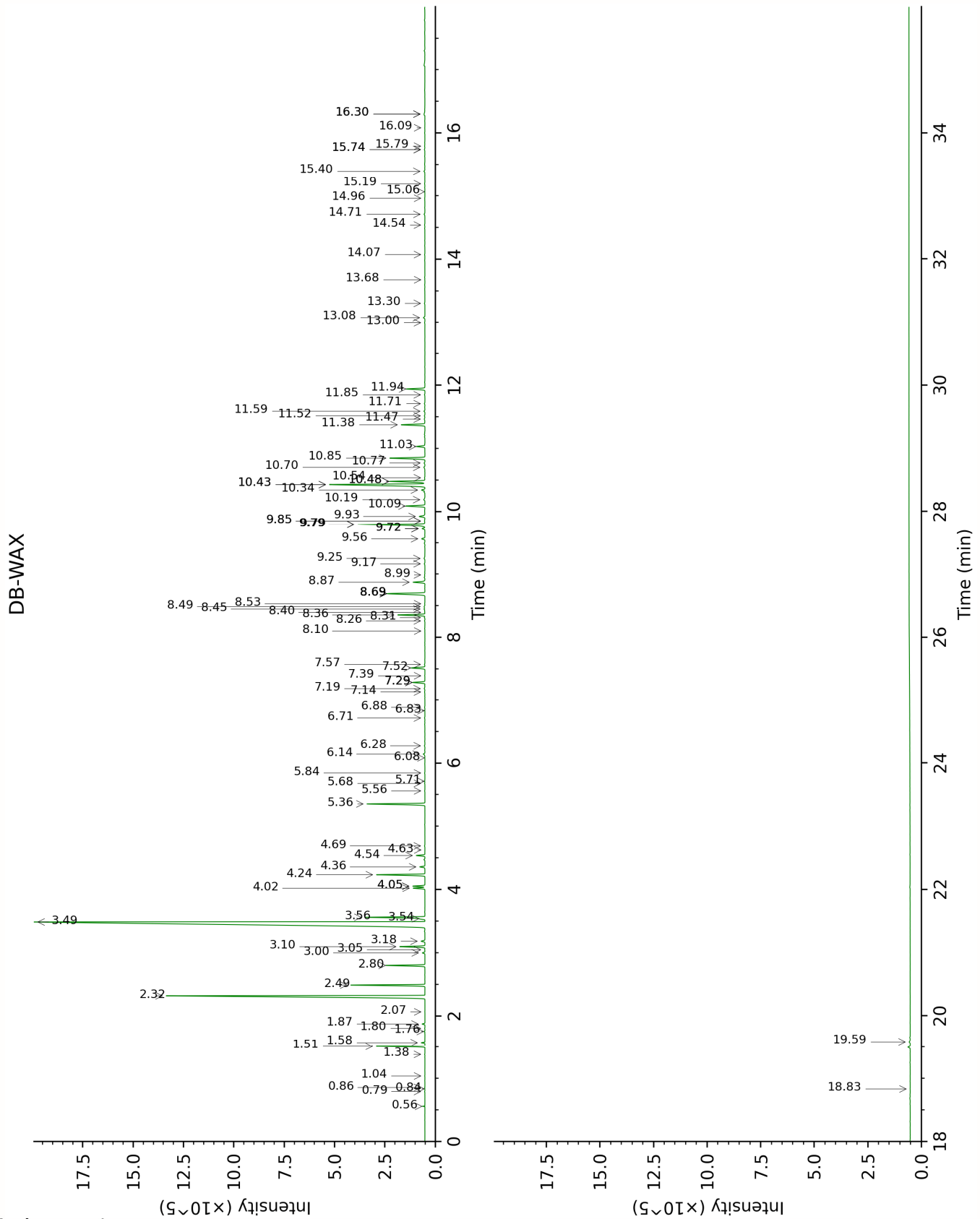
Note: no correction factor was applied

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.

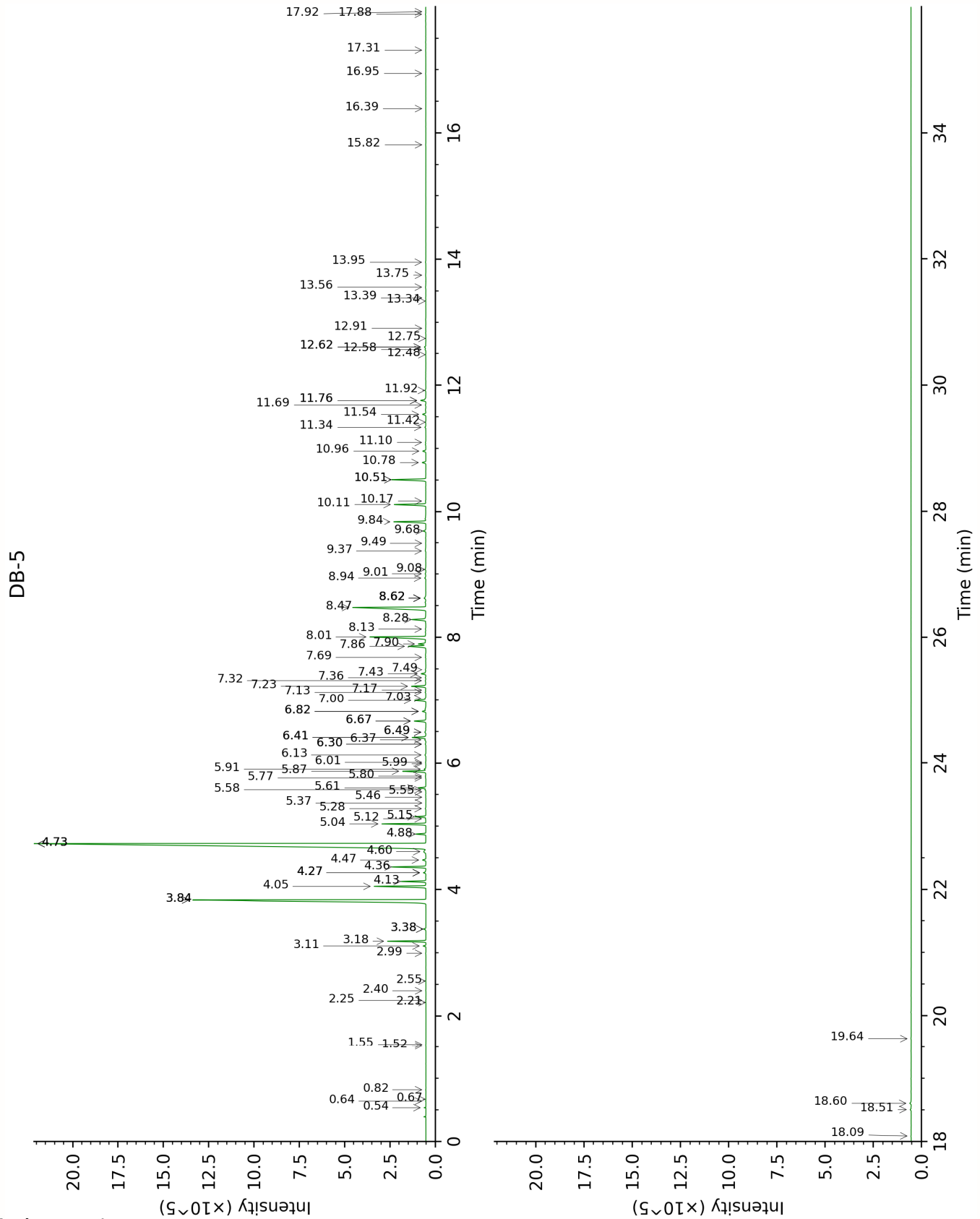
Unknowns: Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

Bracketed value (xx): A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

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



Lemon Petitgrain - Spain - LY1100R



FULL ANALYSIS DATA

2-Methyl-3-buten-2-ol	Column DB-WAX			Column DB-5		
	1.76	1015.2	0.03	0.54	607.2	0.03
Isovaleral	0.86	890.3	0.01	0.64	642.0	tr
2-Methylbutyral	0.84	883.3	tr	0.67	652.1	tr
2-Ethylfuran	1.04	920.9	tr	0.82	702.3	tr
Hexanal	2.07	1044.5	0.01	1.52	800.5	0.01
Octane	0.56	785.2	0.04	1.55	803.9	tr
(3Z)-Hexenol	6.08	1350.1	0.01	2.22	859.0	0.01
Unknown COCI I [m/z 55, 83 (89), 82 (70), 67 (66), 41 (55), 69 (46), 111 (37)... 126 (2)]	0.79	869.4	0.01	2.25	861.7	0.01
Hexanol	5.68	1321.3	0.02	2.40	874.2	0.02
Unknown CULE I [m/z 69, 41 (57), 81 (57), 80 (18), 79 (18), 67 (17)...]				2.55	886.7	0.01
Tricyclene	1.38	971.9	0.01	2.99	919.2	0.02
α -Thujene	1.58	998.5	0.11	3.11	926.8	0.12
α -Pinene	1.51	991.4	1.55	3.18	931.7	1.56
Camphene	1.87	1026.4	0.11	3.38*	944.3	[0.12]
α -Fenchene	1.80	1019.8	0.01	3.38*	944.3	[0.12]
β -Pinene	2.32	1068.5	15.31	3.84*	974.5	[18.22]
Sabinene	2.49	1084.7	2.81	3.84*	974.5	[18.22]
6-Methyl-5-hepten-2-one	5.36	1298.1	2.58	4.05	988.7	2.59
Myrcene	3.10	1133.0	1.03	4.13	993.7	1.05
Pseudolimonene	3.05	1129.2	0.02	4.27*	1002.8	[0.15]
α -Phellandrene	3.00	1125.4	0.11	4.27*	1002.8	[0.15]
Octanal	4.69	1252.5	0.02	4.27*	1002.8	[0.15]
Δ 3-Carene	2.80	1110.3	1.54	4.36	1008.6	1.56
α -Terpinene	3.18	1139.6	0.18	4.47	1015.4	0.18
<i>para</i> -Cymene	4.36	1228.3	0.23	4.60	1023.7	0.25
Limonene	3.49	1163.0	42.84	4.73*	1031.5	[45.62]
β -Phellandrene	3.54	1167.1	0.15	4.73*	1031.5	[45.62]
1,8-Cineole	3.56	1168.7	2.37	4.73*	1031.5	[45.62]
(Z)- β -Ocimene	4.02	1203.8	0.47	4.88	1041.0	0.45
(E)- β -Ocimene	4.24	1219.2	2.02	5.04	1051.0	2.02
Unknown CUSE I [m/z 93, 91 (54), 92 (31), 77 (29), 79 (17), 43 (13), 41 (10), 136 (9)]	4.06*	1206.1	[0.51]	5.12	1056.1	0.02

γ-Terpinene	4.06*	1206.1	[0.51]	5.15	1058.0	0.51
cis-Sabinene hydrate	7.14	1426.3	0.03	5.28	1066.1	0.04
cis-Linalool oxide (fur.)	6.83	1403.7	0.01	5.37	1071.6	0.01
α-Pinene oxide analog	5.71	1323.7	0.01	5.46	1077.3	0.01
Terpinolene isomer	4.63	1247.8	0.01	5.55	1082.6	0.01
trans-Linalool oxide (fur.)	7.19	1430.3	0.05	5.58	1084.7	0.04
Terpinolene	4.54	1241.4	0.37	5.61	1086.5	0.38
trans-Sabinene hydrate	8.26	1510.0	0.02	5.77	1096.4	0.02
Rosefuran	6.28	1363.8	0.03	5.80	1098.2	0.03
Linalool	8.36	1517.2	1.16	5.87	1103.0	1.16
Nonanal	6.14	1354.4	0.09	5.90	1104.9	0.10
cis-Rose oxide	5.56	1312.8	0.02	5.99	1110.5	0.01
endo-Fenchol	8.69*	1543.1	[2.05]	6.01	1111.9	0.02
trans-para-Mentha-2,8-dien-1-ol	9.25	1585.9	0.06	6.13	1119.3	0.06
cis-Limonene oxide	6.72	1395.1	0.02	6.30*	1130.1	[0.04]
allo-Ocimene	5.84	1333.0	0.02	6.30*	1130.1	[0.04]
trans-Limonene oxide	6.88	1407.6	0.02	6.37*†	1134.6	[0.07]
cis-para-Mentha-2,8-dien-1-ol	9.79*	1629.3	[3.71]	6.41*†	1136.9	[0.70]
Camphor	7.52	1454.4	0.67	6.41*†	1136.9	[0.70]
(E)-Myroxide	7.39	1445.3	0.01	6.49*	1142.2	[0.08]
Isopulegol	8.45	1524.4	0.05	6.49*	1142.2	[0.08]
Citronellal	7.29*	1437.4	[0.56]	6.67*	1153.4	[0.60]
iso-Isopulegol	8.32	1514.0	0.03	6.67*	1153.4	[0.60]
Isoneral	8.10	1497.6	0.01	6.82*	1163.2	[0.18]
δ-Terpineol	9.72*	1623.6	[0.13]	6.82*	1163.2	[0.18]
Terpinen-4-ol	8.87	1557.0	0.58	7.00	1174.3	0.59
Unknown CYFL V [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	9.93	1639.9	0.32	7.03	1176.6	0.05
Isogeranial	8.49	1527.3	0.06	7.13	1183.0	0.04
para-Cymen-8-ol	11.85	1799.5	0.03	7.17	1185.2	0.02
α-Terpineol	10.09	1653.1	0.90	7.23	1189.1	0.77
Unknown ABCO I [m/z 79, 107 (72), 41 (58), 55 (47), 77 (41), 67 (41)...]				7.32	1194.8	0.05

Unknown MISC XXXII [m/z 121, 79 (61), 93 (55), 94 (40), 91 (39), 84 (37)...]	8.40	1520.2	0.01	7.36	1197.8	0.03
Unknown CYFL VI [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]	10.48*	1684.4	[1.73]	7.43	1201.7	0.27
Decanal	7.57	1458.5	0.03	7.49	1205.9	0.04
<i>trans</i> -Carveol	11.71	1787.3	0.03	7.69	1218.9	0.03
Nerol	11.38	1759.3	1.13	7.86	1230.6	1.05
Citronellol	11.03	1730.5	0.40	7.90	1233.0	0.43
Neral	9.79*	1629.3	[3.71]	8.01	1240.5	3.64
(<i>Z</i>)-Isogeraniol	11.52	1771.2	0.03	8.13	1248.7	0.03
Geraniol	11.94	1807.6	0.87	8.28	1258.8	0.82
Geranial	10.43*	1680.4	[5.71]	8.48	1271.5	5.46
Neryl formate	9.79*	1629.3	[3.71]	8.62*	1281.3	[0.12]
Unknown CYFL VII [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	13.30	1928.5	0.03	8.62*	1281.3	[0.12]
Citronellyl formate	9.17	1579.4	0.04	8.62*	1281.3	[0.12]
(<i>E</i>)-Anethole	11.47	1766.9	0.05	8.62*	1281.3	[0.12]
Geranyl formate	10.19	1661.2	0.08	8.94	1302.5	0.07
Undecanal	8.99	1565.9	0.02	9.01	1307.3	0.03
4-Vinylguaiacol	15.40	2126.3	0.05	9.08	1312.0	0.04
δ -Elemene	7.29*	1437.4	[0.56]	9.37	1332.6	0.06
Limonene <i>trans</i> - glycol	16.30*	2216.9	[0.09]	9.49	1341.2	0.03
Citronellyl acetate	9.72*	1623.6	[0.13]	9.68	1354.8	0.15
Neryl acetate	10.48*	1684.4	[1.73]	9.84	1365.9	1.66
Geranyl acetate	10.85	1715.1	1.66	10.11	1385.1	1.65
β -Elemene	8.69*	1543.1	[2.05]	10.17	1388.9	0.02
β -Caryophyllene	8.69*	1543.1	[2.05]	10.51*	1413.3	[1.86]
<i>cis</i> - α -Bergamotene	8.53	1530.8	0.02	10.51*	1413.3	[1.86]
<i>trans</i> - α - Bergamotene	8.69*	1543.1	[2.05]	10.78	1433.4	0.19
α -Humulene	9.56	1610.7	0.17	10.96	1446.8	0.17
(<i>E</i>)- β -Farnesene	9.85*	1634.0	[0.04]	11.10	1457.0	0.03
Geranyl propionate	11.59	1777.3	0.05	11.34	1474.8	0.05
<i>trans</i> - β - Bergamotene	9.85*	1634.0	[0.04]	11.42	1480.8	0.02
Bicyclogermacrene	10.34	1673.5	0.18	11.54	1490.0	0.19

(Z)- α -Bisabolene	10.54	1689.1	0.03	11.69	1501.0	0.03
(3E,6E)- α -Farnesene	10.77	1708.6	0.05	11.76*	1506.4	[0.32]
β -Bisabolene	10.43*	1680.4	[5.71]	11.76*	1506.4	[0.32]
δ -Cadinene	10.70	1702.9	0.08	11.92	1518.9	0.05
(E)-Nerolidol	14.07	1999.2	0.02	12.48	1563.2	0.01
Spathulenol	14.71	2059.3	0.05	12.58	1570.5	0.05
Caryophyllene oxide	13.08	1907.9	0.08	12.62*	1573.5	[0.09]
Caryophyllene oxide isomer	13.00	1900.7	0.02	12.62*	1573.5	[0.09]
<i>trans</i> - Sesquisabinene hydrate	14.54	2043.3	0.03	12.75	1584.1	0.01
Humulene epoxide II	13.68	1962.4	0.01	12.91	1596.6	0.01
Isospathulenol	15.79	2165.6	0.02	13.34	1631.6	0.01
τ -Cadinol	15.19	2105.9	0.02	13.39	1635.8	0.02
Unknown SCCH IV [m/z 94, 122 (67), 95 (46), 69 (30), 109 (25), 121 (25), 93 (22)... 204 (11), 222 (1)]				13.56	1649.7	0.04
Unknown CILI II [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	16.30*	2216.9	[0.09]	13.75	1665.2	0.01
α -Bisabolol	15.74*	2160.2	[0.03]	13.95	1682.0	0.03
Phytone	15.06	2093.3	0.01	15.82	1844.3	0.01
Unknown COGU XXIII [m/z 93, 69 (93), 109 (84), 135 (82), 203 (74), 41 (49)...]	14.96	2083.3	0.01	16.39	1896.3	0.01
<i>meta</i> -Camphorene	15.74*	2160.2	[0.03]	16.95	1949.0	0.02
<i>para</i> -Camphorene	16.09	2194.7	0.01	17.31	1983.9	0.03
Unknown LICU VII [m/z 69, 41 (94), 81 (42), 109 (39), 107 (33), 43 (31)...]				17.88	2039.3	0.03
Unknown LICU III [m/z 69, 41 (78), 95 (56), 109 (46), 55 (41), 81 (36), 219 (32)...]				17.92	2043.6	0.01

Unknown DRMO VII [m/z 69, 41 (49), 81 (47), 93 (21), 95 (30), 43 (26)...]				18.08	2059.6	0.02
6-Methyl-4,6-bis(4- methylpent-3-en-1- yl)cyclohexa-1,3- dienecarbaldehyde?				18.51	2101.2	0.06
Phytol	19.59	2573.1	0.06	18.60	2111.4	0.10
(E)-Phytol acetate	18.83	2487.3	0.01	19.64	2219.2	0.02
Total reported		98.10%			98.73%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is 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