

Date : 2023-11-24

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23K17-PTH02

Customer Identification : Manuka - Australia - MF0109R

Type : Essential Oil

Source : *Leptospermum scoparium* ct. *Triketones*

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 : 2023-11-21

PHYSICOCHEMICAL DATA

Refractive index : 1.5028 ± 0.0003 (20 °C)

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

Analyst : Cindy Caron B. Sc.

Date : 2023-11-20

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-Ethylfuran	tr	Furan
2,4-Dimethyl-3-pentanone	tr	Aliphatic ketone
Octane	tr	Alkane
Ethylbenzene	0.01	Simple phenolic
(3Z)-Hexenol	0.03	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
Styrene	0.02	Simple phenolic
α -Thujene	0.01	Monoterpene
α -Pinene	0.22	Monoterpene
β -Pinene	0.07	Monoterpene
Sabinene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.09	Monoterpene
α -Phellandrene	0.01	Monoterpene
(3Z)-Hexenyl acetate	0.06	Aliphatic ester
α -Terpinene	0.01	Monoterpene
Hexyl acetate	0.01	Aliphatic ester
<i>para</i> -Cymene	0.03	Monoterpene
1,8-Cineole	0.10	Monoterpenic ether
Limonene	0.06	Monoterpene
(E)- β -Ocimene	0.01	Monoterpene
γ -Terpinene	0.03	Monoterpene
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.02	Monoterpene
Linalool	0.04	Monoterpenic alcohol
Nonanal	0.01	Aliphatic aldehyde
Isoamyl isovalerate	0.07	Aliphatic ester
Amyl isovalerate	0.03	Aliphatic ester
3-Methyl-3-butenyl isovalerate	0.05	Aliphatic ester
Prenyl isovalerate	0.01	Aliphatic ester
Dimethyloctanedione isomer	0.01	β -Diketone
2,7-Dimethyl-3,5-octanedione	0.02	β -Diketone
Terpinen-4-ol	0.03	Monoterpenic alcohol
α -Terpineol	0.05	Monoterpenic alcohol
2-Methylbutyl tiglate	0.11	Aliphatic ester
3-Methyl-3-butenyl tiglate	0.02	Aliphatic ester
Benzylacetone	0.03	Simple phenolic
Prenyl tiglate	0.02	Aliphatic ester
Geraniol	0.01	Monoterpenic alcohol
(2E)-Decenal	0.01	Aliphatic aldehyde

Geranial	0.01	Monoterpenic aldehyde
Undec-(5Z)-en-2-one	0.05	Aliphatic ketone
2-Undecanone	0.01	Aliphatic ketone
Methyl geranate	0.01	Monoterpenic ester
α -Cubebene	3.29	Sesquiterpene
α -Ylangene	0.19	Sesquiterpene
α -Copaene	4.31	Sesquiterpene
Methyl (<i>E</i>)-cinnamate	0.50	Phenylpropanoid ester
β -Bourbonene	0.08	Sesquiterpene
<i>cis</i> - β -Elemene	0.17	Sesquiterpene
Benzyl 2-methylbutyrate?	0.05	Phenolic ester
β -Cubebene	0.12	Sesquiterpene
Benzyl isovalerate	0.02	Phenolic ester
β -Elemene	3.57	Sesquiterpene
α -Gurjunene	0.52	Sesquiterpene
Unknown	0.02	Sesquiterpene
β -Ylangene	0.02	Sesquiterpene
β -Caryophyllene	1.87	Sesquiterpene
γ -Maaliene	0.03	Sesquiterpene
β -Copaene	0.12	Sesquiterpene
β -Gurjunene	0.10	Sesquiterpene
<i>cis</i> -Thujopsene	0.09	Sesquiterpene
α -Maaliene	0.05	Sesquiterpene
Aromadendrene	0.96	Sesquiterpene
<i>trans</i> - α -Bergamotene	[0.28]	Sesquiterpene
α -Guaiene	[0.28]	Sesquiterpene
Selina-5,11-diene	0.05	Sesquiterpene
6,9-Guaiadiene	0.14	Sesquiterpene
<i>trans</i> -Muuro-la-3,5-diene	2.62	Sesquiterpene
α -Humulene	0.21	Sesquiterpene
allo-Aromadendrene	0.45	Sesquiterpene
4,5-diepi-Aristolochene	0.26	Sesquiterpene
γ -Muuro-lene	0.44	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	1.33	Sesquiterpene
Selina-4,11-diene	2.29	Sesquiterpene
Germacrene D	0.18	Sesquiterpene
α -Amorphene	0.69	Sesquiterpene
allo-Aromadendr-9-ene	0.16	Sesquiterpene
β -Selinene	13.75	Sesquiterpene
<i>trans</i> -Muuro-la-4(15),5-diene	0.93	Sesquiterpene
α -Selinene	13.95	Sesquiterpene
Bicyclogermacrene	0.23	Sesquiterpene
Viridiflorene	0.40	Sesquiterpene
α -Muuro-lene	0.53	Sesquiterpene
δ -Amorphene	[1.01]	Sesquiterpene

δ-Guaiene	[1.01]	Sesquiterpene
γ-Cadinene	1.30	Sesquiterpene
Unknown	0.05	Sesquiterpene
δ-Cadinene	3.91	Sesquiterpene
<i>trans</i> -Calamenene	8.27	Sesquiterpene
<i>cis</i> -Calamenene	0.11	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	3.14	Sesquiterpene
Unknown	0.26	Sesquiterpene
α-Calacorene	0.37	Sesquiterpene
Flavesone	1.99	Norsesquiterpenic ketone
Isocaryophyllene epoxide B	0.12	Sesquiterpenic ether
Germacrene B	0.06	Sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Palustrol	0.11	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.07	Sesquiterpenic alcohol
β-Calacorene	0.02	Sesquiterpene
Spathulenol	0.27	Sesquiterpenic alcohol
Caryophyllene oxide	0.30	Sesquiterpenic ether
Globulol	0.17	Sesquiterpenic alcohol
Unknown	0.01	Terpenic ketone
Gleenol	0.15	Sesquiterpenic alcohol
Viridiflorol	0.06	Sesquiterpenic alcohol
Cubeban-11-ol	0.08	Sesquiterpenic alcohol
Ledol	0.17	Sesquiterpenic alcohol
Eudesm-5-en-11-ol	0.08	Sesquiterpenic alcohol
Unknown	0.37	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Isoleptospermone	5.90	Sesquiterpenic ketone
Leptospermone	12.49	Sesquiterpenic ketone
τ-Cadinol	[0.18]	Sesquiterpenic alcohol
Cubenol	0.43	Sesquiterpenic alcohol
τ-Muurolol	[0.18]	Sesquiterpenic alcohol
β-Eudesmol	0.10	Sesquiterpenic alcohol
α-Eudesmol	0.07	Sesquiterpenic alcohol
Selin-11-en-4α-ol	0.67	Sesquiterpenic alcohol
<i>cis</i> -Calamenen-10-ol	0.08	Sesquiterpenic alcohol
<i>trans</i> -Calamenen-10-ol	0.05	Sesquiterpenic alcohol
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5β-ol	0.09	Sesquiterpenic alcohol
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.17	Oxygenated sesquiterpene
Unknown	0.05	Unknown
<i>cis</i> -14-nor-Muurolol-5-en-4-one?	0.05	Norsesquiterpenic ketone
Unknown	0.07	Lignan
<i>trans</i> -14-nor-Cadina-5-en-4-one	0.18	Norsesquiterpenic ketone
(2 <i>E</i> ,6 <i>E</i>)-Farnesol	0.03	Sesquiterpenic alcohol

Unknown	0.03	Oxygenated sesquiterpene
14-Hydroxy- <i>trans</i> -calamenene	0.04	Sesquiterpenic alcohol
Grandiflorone	0.22	Terpenophenolic
Consolidated total	99.94	

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

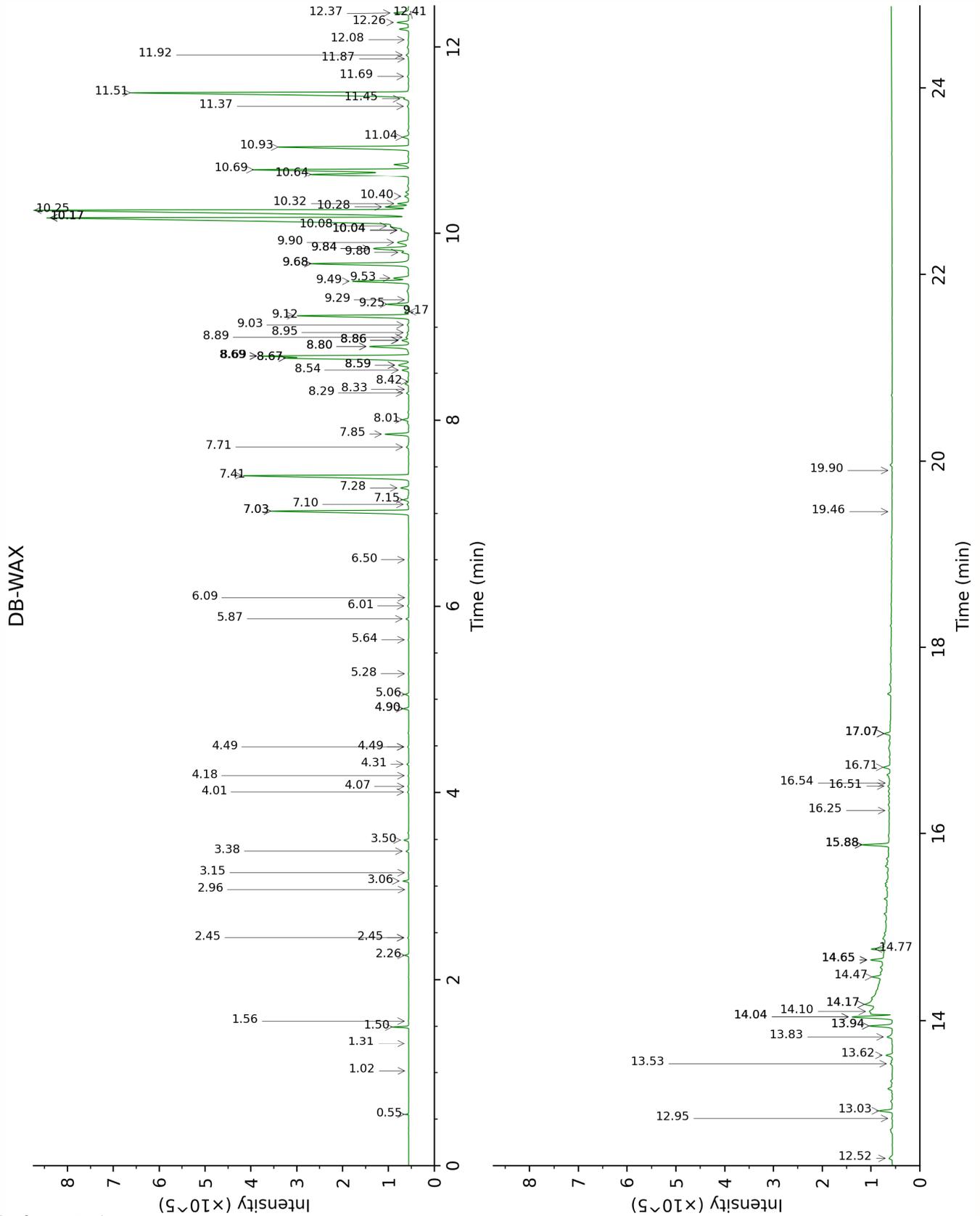
Note: no correction factor was applied

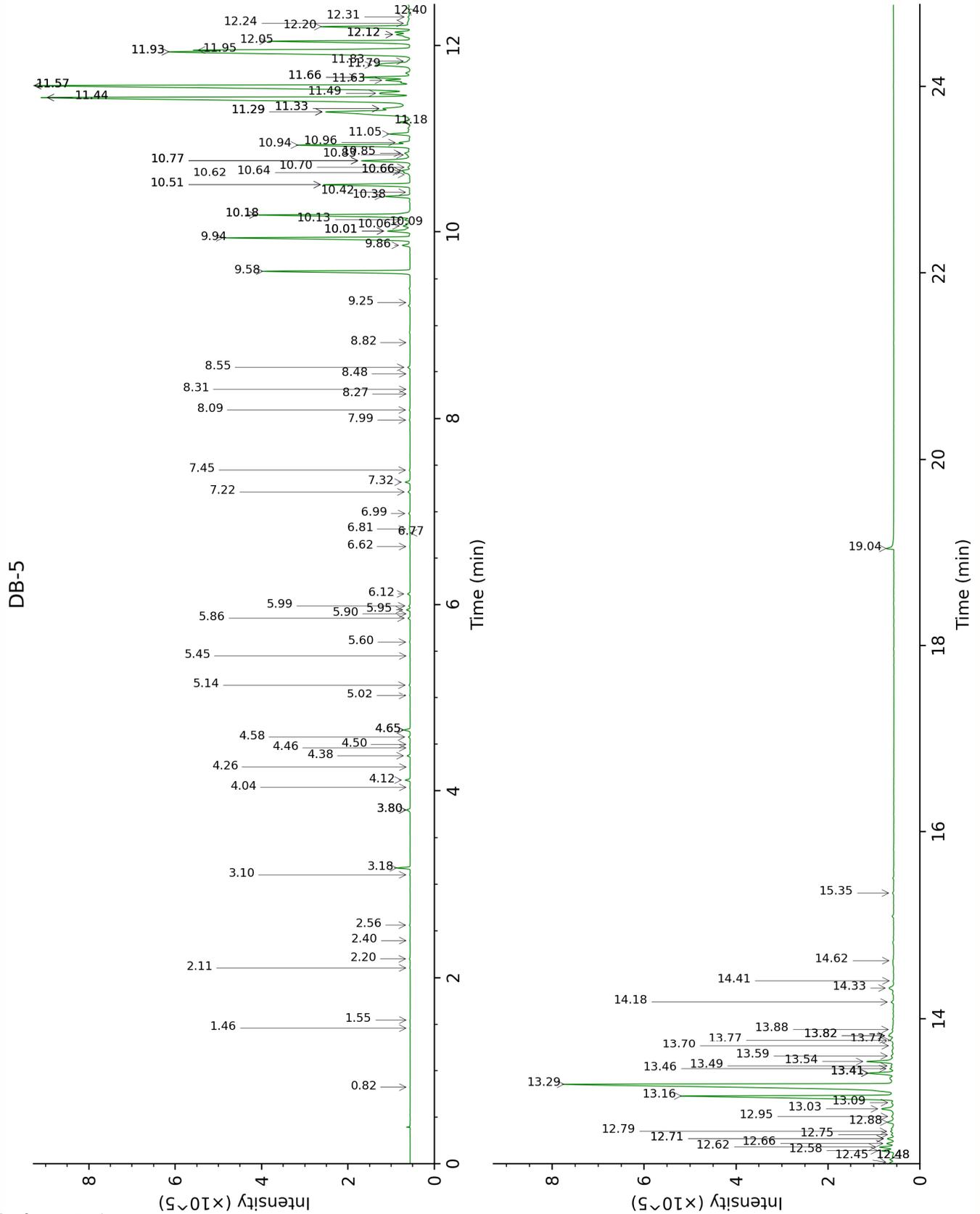
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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.





FULL ANALYSIS DATA

2-Ethylfuran	Column DB-WAX			Column DB-5		
	1.02	920.3	tr	0.82	702.5	tr
2,4-Dimethyl-3-pentanone	1.32	965.0	tr	1.46	792.4	tr
Octane	0.55	778.3	0.03	1.55	804.3	tr
Ethylbenzene	2.45*	1084.5	[0.02]	2.11	850.5	0.01
(3Z)-Hexenol	6.01	1348.7	0.03	2.20	858.4	0.03
Hexanol	5.64	1323.1	0.01	2.40	874.5	0.01
Styrene	4.07	1208.5	0.02	2.56	887.9	0.02
α -Thujene	1.56	1000.4	0.01	3.10	926.7	0.01
α -Pinene	1.50	992.3	0.23	3.18	931.6	0.22
β -Pinene	2.26	1066.8	0.07	3.80*	972.3	[0.08]
Sabinene	2.45*	1084.5	[0.02]	3.80*	972.3	[0.08]
6-Methyl-5-hepten-2-one	5.28	1294.1	0.01	4.04	988.2	0.01
Myrcene	3.06	1132.8	0.10	4.12	993.3	0.09
α -Phellandrene	2.96	1125.9	0.01	4.26	1002.4	0.01
(3Z)-Hexenyl acetate	5.06	1278.6	0.07	4.38	1010.1	0.06
α -Terpinene	3.14	1139.5	0.01	4.46	1015.4	0.01
Hexyl acetate	4.49*	1238.3	[0.02]	4.50	1017.7	0.01
<i>para</i> -Cymene	4.31	1225.3	0.04	4.58	1022.6	0.03
1,8-Cineole	3.50	1166.0	0.10	4.65*	1027.3	[0.13]
Limonene	3.38	1157.0	0.06	4.65*	1027.3	[0.13]
(E)- β -Ocimene	4.18	1216.6	0.02	5.02	1050.4	0.01
γ -Terpinene	4.01	1204.2	0.03	5.14	1057.7	0.03
Octanol	8.42	1524.9	0.01	5.45	1077.2	0.01
Terpinolene	4.49*	1238.3	[0.02]	5.60	1086.5	0.02
Linalool	8.29	1515.3	0.05	5.86	1102.4	0.04
Nonanal	6.10	1354.9	0.01	5.90	1105.3	0.01
Isoamyl isovalerate	4.90*	1267.2	[0.10]	5.95	1108.0	0.07
Amyl isovalerate	4.90*	1267.2	[0.10]	5.99	1110.8	0.03
3-Methyl-3-butenyl isovalerate	5.87	1338.9	0.05	6.12	1118.9	0.05
Prenyl isovalerate	6.50	1383.7	0.01	6.62	1151.2	0.01
Dimethyloctanedione isomer	7.03*	1421.9	[3.51]	6.77	1160.4	0.01
2,7-Dimethyl-3,5-octanedione	7.10	1427.2	0.03	6.81	1163.1	0.02
Terpinen-4-ol	8.80*	1554.0	[0.99]	6.98	1174.1	0.03
α -Terpineol	10.04*	1651.5	[0.24]	7.22	1188.8	0.05
2-Methylbutyl tiglate	7.15	1430.9	0.12	7.32	1195.5	0.11
3-Methyl-3-butenyl tiglate				7.45	1203.7	0.02
Benzylacetone	11.69	1788.1	0.03	7.98	1239.4	0.03

Prenyl tiglate	8.94	1565.3	0.04	8.09	1246.6	0.02
Geraniol	11.87	1804.4	0.01	8.26	1258.0	0.01
(2E)-Decenal	9.30	1592.1	0.02	8.31	1261.3	0.01
Geranial	10.40	1680.4	0.11	8.48	1272.3	0.01
Undec-(5Z)-en-2-one	9.17	1582.4	0.09	8.55	1277.1	0.05
2-Undecanone	8.86*	1559.0	[0.16]	8.82	1295.2	0.01
Methyl geranate	10.04*	1651.5	[0.24]	9.25	1324.7	0.01
α -Cubebene	7.03*	1421.9	[3.51]	9.58	1348.1	3.29
α -Ylangene	7.28	1440.1	0.18	9.86	1367.6	0.19
α -Copaene	7.41	1449.7	4.62	9.94	1373.2	4.31
Methyl (E)-cinnamate	14.04*	1999.8	[1.09]	10.01*	1378.3	[0.57]
β -Bourbonene	7.71	1472.1	0.08	10.01*	1378.3	[0.57]
<i>cis</i> - β -Elemene	8.54	1534.1	0.15	10.06	1382.2	0.17
Benzyl 2-methylbutyrate?	11.92	1808.1	0.07	10.09	1383.9	0.05
β -Cubebene	8.01	1493.6	0.13	10.13	1386.7	0.12
Benzyl isovalerate	12.08	1822.3	0.02	10.18*	1390.4	[3.60]
β -Elemene	8.67*†	1544.0	[2.66]	10.18*	1390.4	[3.60]
α -Gurjunene	7.85	1482.3	0.52	10.38	1404.3	0.52
Unknown EUGL V [m/z 119, 107 (86), 105 (85), 93 (78), 189 (66), 81 (65), 121 (64)... 204 (23)]				10.42	1407.6	0.02
β -Ylangene	8.33	1518.3	0.02	10.50*	1413.6	[1.89]
β -Caryophyllene	8.67*†	1544.0	[2.66]	10.50*	1413.6	[1.89]
γ -Maaliene	8.69*†	1545.6	[3.22]	10.62	1421.8	0.03
β -Copaene	8.59*	1538.1	[0.32]	10.64	1423.8	0.12
β -Gurjunene	8.59*	1538.1	[0.32]	10.66*	1425.2	[0.19]
<i>cis</i> -Thujopsene	8.90	1561.5	0.09	10.66*	1425.2	[0.19]
α -Maaliene	8.86*	1559.0	[0.16]	10.70	1428.0	0.05
Aromadendrene	8.80*	1554.0	[0.99]	10.77*	1433.2	[1.24]
<i>trans</i> - α -Bergamotene	8.69*†	1545.6	[3.22]	10.77*	1433.2	[1.24]
α -Guaiene	8.69*†	1545.6	[3.22]	10.77*	1433.2	[1.24]
Selina-5,11-diene	9.03	1571.6	0.04	10.83	1437.8	0.05
6,9-Guaiadiene	8.86*	1559.0	[0.16]	10.85	1439.1	0.14
<i>trans</i> -Muuro-la-3,5-diene	9.12	1579.1	2.70	10.94	1445.6	2.62
α -Humulene	9.53	1610.5	0.36	10.96	1447.6	0.21
allo-Aromadendrene	9.25	1588.5	0.47	11.05	1454.4	0.45
4,5-diepi-Aristolochene	9.68*	1622.9	[2.55]	11.18	1463.9	0.26
γ -Muuro-lene	9.84*	1635.8	[1.14]	11.29*	1472.0	[3.65]
<i>trans</i> -Cadina-1(6),4-diene	9.49	1607.9	1.33	11.29*	1472.0	[3.65]

Selina-4,11-diene	9.68*	1622.9	[2.55]	11.29*	1472.0	[3.65]
Germacrene D	10.04*	1651.5	[0.24]	11.33*	1474.6	[0.87]
α -Amorphene	9.84*	1635.8	[1.14]	11.33*	1474.6	[0.87]
allo-Aromadendr-9-ene	9.80	1632.5	0.16	11.44*	1483.4	[13.92]
β -Selinene	10.17*	1662.0	[14.43]	11.44*	1483.4	[13.92]
<i>trans</i> -Muurola-4(15),5-diene	10.08	1655.1	0.68	11.49	1486.8	0.93
α -Selinene	10.25	1668.5	13.95	11.57*	1492.8	[13.23]
Bicyclogermacrene	10.32	1674.2	0.23	11.57*	1492.8	[13.23]
Viridiflorene	9.90	1641.0	0.40	11.57*	1492.8	[13.23]
α -Muurolene	10.28	1671.4	0.49	11.63	1497.1	0.53
δ -Amorphene	10.17*	1662.0	[14.43]	11.66*	1499.5	[1.01]
δ -Guaiene	10.17*	1662.0	[14.43]	11.66*	1499.5	[1.01]
γ -Cadinene	10.64	1700.1	2.87	11.79	1509.5	1.30
Unknown EUGL VII [m/z 159, 145 (91), 131 (67), 105 (46), 202 (43)]	11.04	1733.6	0.15	11.83	1512.7	0.05
δ -Cadinene	10.69	1704.3	3.91	11.93*†	1520.6	[8.74]
<i>trans</i> -Calamenene	11.51	1773.4	8.27	11.93*†	1520.6	[8.74]
<i>cis</i> -Calamenene	11.45	1768.0	0.11	11.95*†	1522.0	[3.51]
<i>trans</i> -Cadina-1,4-diene	10.93	1724.7	3.33	12.05	1529.5	3.14
Unknown JUOX V [m/z 157, 143 (86), 200 (43), 142 (36), 141 (28), 128 (25)]	12.26	1838.6	0.26	12.12*	1535.0	[0.41]
α -Calacorene	12.36	1847.5	0.37	12.12*	1535.0	[0.41]
Flavesone				12.20	1541.7	1.99
Isocaryophyllene epoxide B	12.41	1851.7	0.02	12.24	1544.4	0.12
Germacrene B	11.37	1761.3	0.04	12.31	1549.8	0.06
Unknown MEAL III [m/z 161, 109 (98), 82 (93), 43 (72), 105 (68), 93 (59), 69 (56), 119 (55)... 222 (7)]	13.53	1952.6	0.05	12.40	1557.0	0.06
Palustrol	12.52	1861.0	0.11	12.45	1560.9	0.11
(<i>E</i>)-Nerolidol	14.04*	1999.8	[1.09]	12.48*	1563.7	[0.09]
β -Calacorene	12.95	1898.9	0.02	12.48*	1563.7	[0.09]
Spathulenol	14.65*†	2058.0	[1.49]	12.58	1571.1	0.27
Caryophyllene oxide	13.03	1906.3	0.30	12.62	1574.1	0.30
Globulol	14.17*†	2012.5	[5.14]	12.66	1577.1	0.17
Unknown LESC II				12.71*	1581.2	[0.16]

[m/z 161, 159 (64), 43 (58), 182 (53), 41 (48), 105 (40)... 252 (25)]						
Gleenol	13.83	1979.7	0.15	12.71*	1581.2	[0.16]
Viridiflorol	14.17*†	2012.5	[5.14]	12.75	1584.6	0.06
Cubeban-11-ol	13.94*	1990.5	[0.51]	12.79	1587.3	0.08
Ledol	13.62	1961.0	0.15	12.88	1595.1	0.17
Eudesm-5-en-11-ol	14.65*†	2058.0	[1.49]	12.95	1599.8	0.08
Unknown POBA VI [m/z 151, 41 (15), 81 (13), 111 (13), 91 (13)...]	14.47*†	2040.6	[2.07]	13.03	1606.4	0.37
Unknown MECA V [m/z 179, 161 (66), 119 (44), 95 (38), 105 (35)... 204 (24), 222 (1)]				13.09	1611.8	0.07
Isoleptospermone	14.10*†	2005.2	[1.39]	13.16	1617.7	5.90
Leptospermone	14.65*†	2058.0	[1.49]	13.29	1628.1	12.49
τ-Cadinol	15.88*†	2179.5	[1.25]	13.41*	1637.9	[0.61]
Cubenol	13.94*	1990.5	[0.51]	13.41*	1637.9	[0.61]
τ-Muurolol	15.88*†	2179.5	[1.25]	13.41*	1637.9	[0.61]
β-Eudesmol	14.65*†	2058.0	[1.49]	13.46	1641.8	0.10
α-Eudesmol	14.77*†	2069.1	[5.80]	13.49	1644.3	0.07
Selin-11-en-4α-ol	15.88*†	2179.5	[1.25]	13.54	1648.2	0.67
cis-Calamenen-10-ol	16.71	2265.2	0.21	13.59	1653.1	0.08
trans-Calamenen-10-ol	17.07*	2303.1	[0.13]	13.70	1662.1	0.05
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	17.07*	2303.1	[0.13]	13.77*	1667.5	[0.16]
Unknown LESC III [m/z 159, 118 (33), 91 (30), 131 (30)... 220? (4)]	16.51	2244.2	0.07	13.77*	1667.5	[0.16]
Unknown RHGR XIV [m/z 107, 91 (95), 93 (87), 79 (86), 105 (78), 41 (76), 95 (72)... 220 (18)]	17.07*	2303.1	[0.13]	13.82*	1671.6	[0.22]
Unknown LESC V [m/z 175, 91 (94), 105 (51), 218 (33), 104 (17), 176 (12)...]	16.54	2247.6	0.05	13.82*	1671.6	[0.22]
cis-14-nor-Muurolol-5-en-4-one?				13.88	1677.0	0.05

Unknown OCSA IV [m/z 133, 93 (97), 131 (85), 145 (83), 107 (69)...220]				14.18	1701.2	0.07
<i>trans</i> -14-nor-Cadina- 5-en-4-one	16.25	2217.1	0.11	14.33	1714.1	0.18
(2 <i>E</i> ,6 <i>E</i>)-Farnesol	17.07*	2303.1	[0.13]	14.41	1720.8	0.03
Unknown ZIOE I [m/z 43, 194 (68), 136 (63), 81 (63), 177 (56), 223 (51)... 238 (3)]	19.90	2622.5	0.01	14.62	1739.5	0.03
14-Hydroxy- <i>trans</i> - calamenene	19.46	2570.2	0.01	15.34	1802.1	0.04
Grandiflorone				19.04	2157.1	0.22
Total reported		96.93%			97.89%	

*: 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