

Date : June 01, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23E25-PTH02

Customer identification : Manuka - Australia - MF0108R

Type : Essential oil

Source : *Leptospermum scoparium*

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 : June 01, 2023

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Light yellow liquid

Refractive index: 1.5031 ± 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
2,4-Dimethyl-3-pentanone	0.01	Aliphatic ketone
(3Z)-Hexenol	0.03	Aliphatic alcohol
Styrene	0.03	Simple phenolic
Hashishene	tr	Monoterpene
α -Thujene	tr	Monoterpene
α -Pinene	0.83	Monoterpene
Camphene	0.01	Monoterpene
β -Pinene	0.19	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.11	Monoterpene
(3Z)-Hexenyl acetate	0.13	Aliphatic ester
α -Terpinene	0.01	Monoterpene
Isoamyl isobutyrate	0.02	Aliphatic ester
para-Cymene	0.04	Monoterpene
Limonene	0.08	Monoterpene
1,8-Cineole	0.07	Monoterpenic ether
(E)- β -Ocimene	0.01	Monoterpene
γ -Terpinene	0.02	Monoterpene
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.03	Monoterpene
Linalool	0.08	Monoterpenic alcohol
Isoamyl isovalerate	0.08	Aliphatic ester
Amyl isovalerate	0.04	Aliphatic ester
3-Methyl-3-butenyl isovalerate	0.07	Aliphatic ester
Prenyl isovalerate	0.02	Aliphatic ester
Dimethyloctanedione isomer	0.02	β -Diketone
2,7-Dimethyl-3,5-octanedione	0.04	β -Diketone
Terpinen-4-ol	0.03	Monoterpenic alcohol
α -Terpineol	0.07	Monoterpenic alcohol
2-Methylbutyl tiglate	0.15	Aliphatic ester
3-Methyl-3-butenyl tiglate	0.03	Aliphatic ester
Benzylacetone	0.04	Simple phenolic
Prenyl tiglate	0.03	Aliphatic ester
(2E)-Decenal	0.01	Aliphatic aldehyde
Geranial	0.02	Monoterpenic aldehyde
Undec-(5Z)-en-2-one	0.05	Aliphatic ketone
Bicycloelemene	0.02	Sesquiterpene
α -Cubebene	2.22	Sesquiterpene
Longicyclene	0.02	Sesquiterpene
α -Ylangene	0.31	Sesquiterpene
α -Copaene	4.13	Sesquiterpene
Modhephene	0.02	Sesquiterpene
Methyl (E)-cinnamate	0.40	Phenylpropanoid ester
β -Bourbonene	0.02	Sesquiterpene
cis- β -Elemene	0.10	Sesquiterpene

Benzyl 2-methylbutyrate?	0.07	Phenolic ester
β-Cubebene	0.06	Sesquiterpene
β-Elemene	2.92	Sesquiterpene
Benzyl isovalerate	0.03	Phenolic ester
α-Gurjunene	0.49	Sesquiterpene
Unknown	0.02	Sesquiterpene
β-Caryophyllene	1.64	Sesquiterpene
β-Ylangene	0.03	Sesquiterpene
γ-Maaliene	0.04	Sesquiterpene
β-Gurjunene	0.08	Sesquiterpene
α-Maaliene	tr	Sesquiterpene
α-Guaiene	0.27	Sesquiterpene
Aromadendrene	1.06	Sesquiterpene
Selina-5,11-diene	0.24	Sesquiterpene
6,9-Guaiadiene	0.09	Sesquiterpene
<i>trans</i> -Muuroala-3,5-diene	1.43	Sesquiterpene
α-Humulene	0.23	Sesquiterpene
allo-Aromadendrene	0.49	Sesquiterpene
4,5-diepi-Aristolochene	0.27	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	1.23	Sesquiterpene
Selina-4,11-diene	0.81	Sesquiterpene
γ-Murolene	1.23	Sesquiterpene
Germacrene D	0.67	Sesquiterpene
allo-Aromadendr-9-ene	0.35	Sesquiterpene
β-Selinene	13.85	Sesquiterpene
Eudesma-3,5,11-triene	0.65	Sesquiterpene
<i>trans</i> -Muuroala-4(15),5-diene	0.12	Sesquiterpene
Viridiflorene	0.40	Sesquiterpene
α-Selinene	12.12	Sesquiterpene
α-Murolene	0.23	Sesquiterpene
Germacrene A	0.58	Sesquiterpene
δ-Amorphene	0.29	Sesquiterpene
δ-Guaiene	0.15	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i>)-α-Farnesene	0.19	Sesquiterpene
γ-Cadinene	0.88	Sesquiterpene
Unknown	0.15	Sesquiterpene
<i>trans</i> -Calamenene	11.12	Sesquiterpene
δ-Cadinene	3.77	Sesquiterpene
<i>cis</i> -Calamenene	0.17	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	2.75	Sesquiterpene
Unknown	0.32	Sesquiterpene
α-Calacorene	0.50	Sesquiterpene
Flavesone	3.42	Norsesquiterpenic ketone
Palustrol	0.15	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.09	Sesquiterpenic alcohol
Spathulenol	0.28	Sesquiterpenic alcohol
Caryophyllene oxide	0.36	Sesquiterpenic ether
Globulol	0.21	Sesquiterpenic alcohol
Gleenol	0.19	Sesquiterpenic alcohol
Viridiflorol	0.07	Sesquiterpenic alcohol
Cubeban-11-ol	0.09	Sesquiterpenic alcohol
Ledol	0.20	Sesquiterpenic alcohol

Unknown	0.36	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Isoleptospermone	6.10	Sesquiterpenic ketone
Leptospermone	10.82	Sesquiterpenic ketone
τ -Cadinol	0.10	Sesquiterpenic alcohol
Cubenol	0.37	Sesquiterpenic alcohol
τ -Muurolol	0.17	Sesquiterpenic alcohol
β -Eudesmol	0.18	Sesquiterpenic alcohol
Selin-11-en-4 α -ol	0.70*	Sesquiterpenic alcohol
α -Cadinol	0.70*	Sesquiterpenic alcohol
α -Eudesmol	0.70*	Sesquiterpenic alcohol
<i>cis</i> -Calamenen-10-ol	0.15	Sesquiterpenic alcohol
<i>trans</i> -Calamenen-10-ol	0.05	Sesquiterpenic alcohol
Unknown	0.27	Oxygenated sesquiterpene
Unknown	0.22	Unknown
<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
5-Hydroxy- <i>cis</i> -calamenene?	0.03	Sesquiterpenic alcohol
14-Hydroxy- <i>trans</i> -calamenene	0.08	Sesquiterpenic alcohol
Grandiflorone	0.12	Terpenophenolic
Consolidated total	96.72%	

*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered [xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

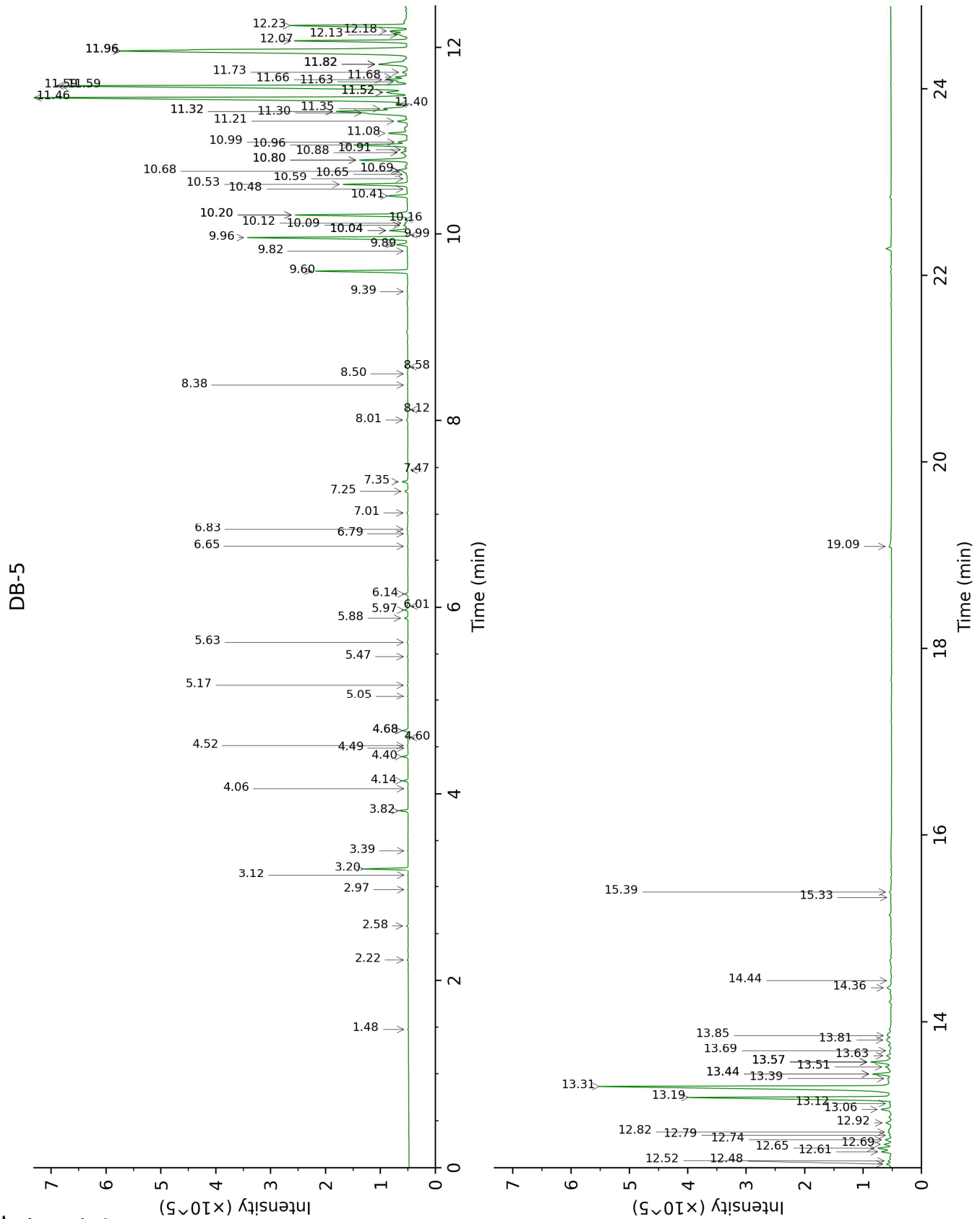
tr: The compound has been detected below 0.005% of total signal.

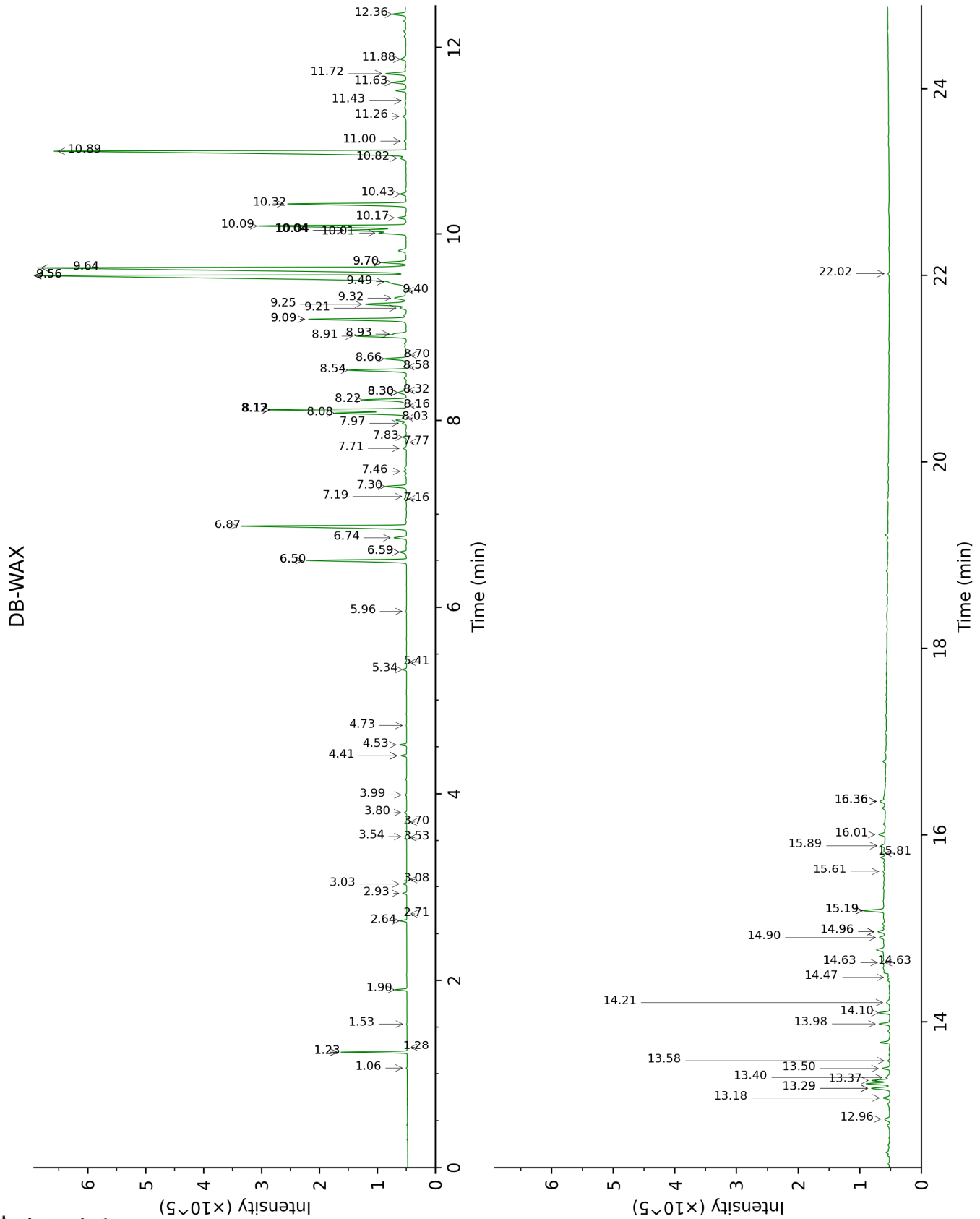
Note: no correction factor was applied

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	%
2,4-Dimethyl-3-pentanone	1.48	791	0.01	1.06	964	0.01
(3Z)-Hexenol	2.22	857	0.03	5.41	1345	0.03
Styrene	2.58	886	0.03	3.53	1209	0.02
Hashishene	2.97	916	tr	1.23*	993	0.88
α -Thujene	3.12	926	tr	1.28	1003	tr
α -Pinene	3.20	930	0.83	1.23*	993	[0.88]
Camphene	3.39	943	0.01	1.54	1029	0.01
β -Pinene	3.82	971	0.19	1.90	1067	0.19
6-Methyl-5-hepten-2-one	4.06	987	0.01	4.73	1302	0.01
Myrcene	4.14	992	0.11	2.64	1135	0.12
(3Z)-Hexenyl acetate	4.40	1009	0.13	4.52	1286	0.13
α -Terpinene	4.49	1015	0.01	2.71	1141	tr
Isoamyl isobutyrate	4.52	1016	0.02	3.08	1172	0.01
para-Cymene	4.60	1022	0.04	3.80	1230	0.05
Limonene	4.68*	1026	0.13	2.93	1159	0.08
1,8-Cineole	4.68*	1026	[0.13]	3.03	1168	0.07
(E)- β -Ocimene	5.05	1050	0.01	3.70	1222	0.02
γ -Terpinene	5.17	1057	0.02	3.54	1210	0.04
Octanol	5.47	1076	0.02	7.82	1526	0.08
Terpinolene	5.63	1086	0.03	3.99	1244	0.03
Linalool	5.88	1102	0.08	7.70	1517	0.07
Isoamyl isovalerate	5.97	1107	0.08	4.41*	1277	0.11
Amyl isovalerate	6.01	1110	0.04	4.41*	1277	[0.11]
3-Methyl-3-butenyl isovalerate	6.14	1118	0.07	5.34	1339	0.08
Prenyl isovalerate	6.65	1151	0.02	5.96	1385	0.02
Dimethyloctanedione isomer	6.79	1159	0.02	6.50*	1425	2.34
2,7-Dimethyl-3,5-octanedione	6.83	1162	0.04	6.59*	1432	0.18
Terpinen-4-ol	7.02	1174	0.03	8.16	1553	0.03
α -Terpineol	7.25	1188	0.07	9.40	1652	0.10
2-Methylbutyl tiglate	7.35	1195	0.15	6.59*	1432	[0.18]
3-Methyl-3-butenyl tiglate	7.47	1203	0.03			
Benzylacetone	8.01	1238	0.04	11.00	1788	0.05
Prenyl tiglate	8.12	1246	0.03	8.32†	1566	[0.36]
(2E)-Decenal	8.38	1263	0.01	8.70	1595	0.01
Geranial	8.50	1271	0.02	9.70*	1677	0.57
Undec-(5Z)-en-2-one	8.58	1276	0.05	8.58	1586	0.07
Bicycloelemene	9.39	1332	0.02			
α -Cubebene	9.60	1347	2.22	6.50*	1425	[2.34]
Longicyclene	9.82	1362	0.02			
α -Ylangene	9.89	1367	0.31	6.74	1444	0.29
α -Copaene	9.96	1372	4.13	6.87	1453	4.42
Modhephene	9.99	1374	0.02	7.16	1476	0.07

Methyl (<i>E</i>)-cinnamate	10.04*	1378	0.50	13.37	2004	0.40
β-Bourbonene	10.04*	1378	[0.50]	7.19	1478	0.02
<i>cis</i> -β-Elemene	10.09	1382	0.10	7.97	1538	0.09
Benzyl 2-methylbutyrate?	10.12	1383	0.07	11.26	1811	0.09
β-Cubebene	10.16	1386	0.06	7.46	1498	0.06
β-Elemene	10.20*	1390	2.95	8.12*	1549	3.23
Benzyl isovalerate	10.20*	1390	[2.95]	11.43	1826	0.03
α-Gurjunene	10.41	1404	0.49	7.30	1486	0.49
Unknown [m/z 119, 107 (86), 105 (85), 93 (78), 189 (66), 81 (65), 121 (64)... 204 (23)]	10.48	1409	0.02			
β-Caryophyllene	10.53	1413	1.64	8.08	1546	1.71
β-Ylangene	10.59	1418	0.03	7.77	1522	0.02
γ-Maaliene	10.65	1422	0.04	8.12*	1549	[3.23]
β-Gurjunene	10.68†	1424	0.32	8.03	1542	0.08
α-Maaliene	10.69†	1425	[0.32]	8.30*†	1564	0.36
α-Guaiene	10.80*	1433	1.44	8.12*	1549	[3.23]
Aromadendrene	10.80*	1433	[1.44]	8.22	1558	1.06
Selina-5,11-diene	10.88	1439	0.24	8.30*†	1564	[0.36]
6,9-Guaiadiene	10.91	1441	0.09	8.30*†	1564	[0.36]
<i>trans</i> -Muuro-la-3,5-diene	10.96	1445	1.43	8.54	1583	1.38
α-Humulene	10.99	1447	0.23	8.93	1614	0.24
allo-Aromadendrene	11.08	1454	0.49	8.66	1592	0.54
4,5-diepi-Aristolochene	11.21	1464	0.27	9.09*	1627	2.34
<i>trans</i> -Cadina-1(6),4-diene	11.30†	1470	3.27	8.91	1612	1.23
Selina-4,11-diene	11.32*†	1471	[3.27]	9.09*	1627	[2.34]
γ-Muuro-lene	11.32*†	1471	[3.27]	9.25	1640	1.23
Germacrene D	11.35	1474	0.67	9.49	1660	0.60
allo-Aromadendr-9-ene	11.40	1477	0.35	9.21	1637	0.15
β-Selinene	11.46	1482	13.85	9.56*	1665	14.20
Eudesma-3,5,11-triene	11.52*	1487	0.76	10.01	1703	0.65
<i>trans</i> -Muuro-la-4(15),5-diene	11.52*	1487	[0.76]	9.56*	1665	[14.20]
Viridiflorene	11.59*	1492	12.52	9.32	1646	0.40
α-Selinene	11.59*	1492	[12.52]	9.64*	1672	13.29
α-Muuro-lene	11.63	1495	0.23	9.70*	1677	[0.57]
Germacrene A	11.66	1497	0.58	10.04*	1705	1.46
δ-Amorphene	11.68	1499	0.29	9.64*	1672	[13.29]
δ-Guaiene	11.74	1502	0.15	9.56*	1665	[14.20]
(3 <i>E</i> ,6 <i>E</i>)-α-Farnesene	11.82*†	1509	1.30	10.17	1717	0.19
γ-Cadinene	11.82*†	1509	[1.30]	10.04*	1705	[1.46]
Unknown [m/z 159, 145 (91), 131 (67), 105 (46), 202 (43)]	11.82*†	1509	[1.30]	10.43	1738	0.15
<i>trans</i> -Calamenene	11.96*	1520	15.03	10.89	1779	11.12

δ-Cadinene	11.96*	1520	[15.03]	10.09	1709	3.77
cis-Calamenene	11.96*	1520	[15.03]	10.82	1772	0.17
trans-Cadina-1,4-diene	12.07	1529	2.75	10.32	1729	2.87
Unknown [m/z 157, 143 (86), 200 (43), 142 (36), 141 (28), 128 (25)]	12.13†	1534	0.92	11.63	1843	0.32
α-Calacorene	12.18†	1537	[0.92]	11.72	1852	0.50
Flavesone	12.23	1542	3.42			
Palustrol	12.48	1561	0.15	11.88	1866	0.16
(E)-Nerolidol	12.52	1564	0.09	13.40	2007	0.13
Spathulenol	12.61	1571	0.28	13.98	2064	0.26
Caryophyllene oxide	12.65	1574	0.36	12.36	1909	0.34
Globulol	12.69	1577	0.21	13.50	2016	0.18
Gleenol	12.74	1581	0.19	13.18	1987	0.17
Viridiflorol	12.79	1585	0.07	13.58	2024	0.05
Cubeban-11-ol	12.82	1588	0.09	13.29*	1996	0.46
Ledol	12.92	1595	0.20	12.96	1966	0.19
Unknown [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	13.06	1607	0.36	14.10	2075	0.26
Unknown [m/z 179, 161 (66), 119 (44), 95 (38), 105 (35)... 204 (24), 222 (1)]	13.12	1612	0.07	14.21	2086	0.13
Isoleptospermone	13.19	1617	6.10	14.96*†	2162	[19.14]
Leptospermone	13.31	1627	10.82	14.63*†	2128	19.14
τ-Cadinol	13.39	1634	0.10	14.48	2112	0.05
Cubenol	13.44*	1638	0.55	13.29*	1996	[0.46]
τ-Muurolol	13.44*	1638	[0.55]	14.63*†	2128	[19.14]
β-Eudesmol	13.51	1644	0.18	14.96*†	2162	[19.14]
Selin-11-en-4α-ol	13.57*	1648	0.70	15.19*†	2185	[19.14]
α-Cadinol	13.57*	1648	[0.70]	15.19*†	2185	[19.14]
α-Eudesmol	13.57*	1648	[0.70]	14.90†	2155	[19.14]
cis-Calamenen-10-ol	13.63	1654	0.15	16.01†	2271	[19.14]
trans-Calamenen-10-ol	13.68	1658	0.05	16.36*†	2308	[19.14]
Unknown [m/z 159, 118 (33), 91 (30), 131 (30)... 220? (4)]	13.81	1668	0.27	15.81†	2250	[19.14]
Unknown [m/z 175, 91 (94), 105 (51), 218 (33), 104 (17), 176 (12)...]	13.85	1672	0.22	15.89†	2258	[19.14]
trans-14-nor-Cadina-5-en-4-one	14.36	1714	0.18	15.61†	2228	[19.14]
(2E,6E)-Farnesol	14.44	1721	0.03	16.36*†	2308	[19.14]
5-Hydroxy-cis-calamenene?	15.33	1798	0.03			

14-Hydroxy- <i>trans</i> -calamenene	15.39	1803	0.08			
Grandiflorone	19.09	2159	0.12	22.02	2992	0.03
Total identified		95.41%			95.31%	
Total reported		97.26%			96.17%	

*: 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