

Date : September 30, 2019

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 19I23-PTH03-1-SCC

Customer identification : Manuka - Australia - MF0103811R

Type : Essential oil

Source : *Leptospermum scoparium*

Customer : Plant Therapy

ANALYSIS

Method: PC-PA-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 : Sylvain Mercier, M. Sc., Chimiste

Analysis date : September 26, 2019

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Light yellow viscous liquid

Refractive index: 1.5029 ± 0.0003 (20 °C)

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	%	Classe
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
2,4-Dimethyl-3-pentanone	0.01	Aliphatic ketone
Hexanal	tr	Aliphatic aldehyde
Octane	0.01	Alkane
(2E)-Hexenal	0.01	Aliphatic aldehyde
Ethylbenzene	0.02	Simple phenolic
(3Z)-Hexenol	0.02	Aliphatic alcohol
Styrene	0.01	Simple phenolic
α -Thujene	0.02	Monoterpene
α -Pinene	0.98	Monoterpene
Camphene	0.01	Monoterpene
α -Fenchene	tr	Monoterpene
β -Pinene	0.11	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
2-Pentylfuran	0.01	Furan
Myrcene	0.24	Monoterpene
Octanal	0.01	Aliphatic aldehyde
(3Z)-Hexenyl acetate	0.04	Aliphatic ester
α -Terpinene	0.01	Monoterpene
Isoamyl isobutyrate	tr	Aliphatic ester
para-Cymene	0.14	Monoterpene
Limonene	0.09	Monoterpene
1,8-Cineole	0.14	Monoterpenic ether
(E)- β -Ocimene	0.03	Monoterpene
γ -Terpinene	0.11	Monoterpene
Unknown	0.01	Oxygenated monoterpene
Octanol	0.03	Aliphatic alcohol
Terpinolene	0.04	Monoterpene
Linalool	0.07	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
2-Methylbutyl 2-methylbutyrate	0.02	Aliphatic ester
Isoamyl isovalerate	0.08	Aliphatic ester
Amyl isovalerate	0.04	Aliphatic ester
3-Methyl-3-butenyl 2-methylbutyrate	0.02	Aliphatic ester
3-Methyl-3-butenyl isovalerate	0.18	Aliphatic ester
Prenyl 2-methylbutyrate	0.01	Aliphatic ester
Prenyl isovalerate	0.03	Aliphatic ester
Dimethyloctanedione isomer	0.03	β -Diketone
2,7-Dimethyl-3,5-octanedione	0.07	β -Diketone
Terpinen-4-ol	0.04	Monoterpenic alcohol
α -Terpineol	0.05	Monoterpenic alcohol
2-Methylbutyl tiglate	0.09	Aliphatic ester
3-Methyl-3-butenyl tiglate	0.06	Aliphatic ester
Benzylacetone	0.03	Simple phenolic
Prenyl tiglate	0.06	Aliphatic ester

Geraniol	0.02	Monoterpenic alcohol
(2E)-Decenal	0.02	Aliphatic aldehyde
Geranial	0.01	Monoterpenic aldehyde
Undec-(5Z)-en-2-one	0.07	Aliphatic ketone
Bicycloelemene	0.01	Sesquiterpene
α -Cubebene	2.23	Sesquiterpene
Longicyclene	0.01	Sesquiterpene
α -Ylangene	0.22	Sesquiterpene
α -Copaene	4.48	Sesquiterpene
Modhephene	0.04	Sesquiterpene
Methyl (E)-cinnamate	0.07	Phenylpropanoid ester
β -Bourbonene	0.02	Sesquiterpene
1,5-diepi- β -Bourbonene	0.03	Sesquiterpene
cis- β -Elemene	0.03	Sesquiterpene
Benzyl 2-methylbutyrate?	0.08	Phenolic ester
β -Cubebene	0.14	Sesquiterpene
β -Elemene	0.85	Sesquiterpene
Benzyl isovalerate	0.02	Phenolic ester
α -Gurjunene	0.73	Sesquiterpene
Unknown	0.04	Sesquiterpene
β -Caryophyllene	1.63	Sesquiterpene
β -Ylangene	0.09	Sesquiterpene
γ -Maaliene	0.02	Sesquiterpene
β -Gurjunene	0.04	Sesquiterpene
β -Copaene	0.02	Sesquiterpene
cis-Thujopsene	0.02	Sesquiterpene
α -Maaliene	0.22	Sesquiterpene
Aromadendrene	0.08	Sesquiterpene
Selina-5,11-diene	0.07	Sesquiterpene
α -Guaiene	1.53*	Sesquiterpene
trans- α -Bergamotene	[1.53]*	Sesquiterpene
6,9-Guaiadiene	0.10	Sesquiterpene
trans-Muurolo-3,5-diene	3.61	Sesquiterpene
α -Humulene	0.22	Sesquiterpene
allo-Aromadendrene	0.66	Sesquiterpene
4,5-diepi-Aristolochene	0.08	Sesquiterpene
Selina-4,11-diene	0.08	Sesquiterpene
trans-Cadina-1(6),4-diene	2.04	Sesquiterpene
γ -Muurolole	1.15	Sesquiterpene
Germacrene D	0.31	Sesquiterpene
β -Selinene	3.89	Sesquiterpene
allo-Aromadendr-9-ene	0.17	Sesquiterpene
trans-Muurolo-4(15),5-diene	0.34	Sesquiterpene
Eudesma-3,5,11-triene	0.04	Sesquiterpene
α -Selinene	3.51	Sesquiterpene
epi-Cubebol	0.14	Sesquiterpenic alcohol
Bicyclogermacrene	0.21	Sesquiterpene
Viridiflorene	0.44	Sesquiterpene
α -Muurolole	0.79	Sesquiterpene
δ -Amorphene	0.27	Sesquiterpene
δ -Guaiene	0.10	Sesquiterpene
γ -Cadinene	0.38	Sesquiterpene

(3E,6E)- α -Farnesene	0.73	Sesquiterpene
7-epi- α -Selinene	0.10	Sesquiterpene
Unknown	0.16	Sesquiterpene
δ -Cadinene	6.35	Sesquiterpene
<i>trans</i> -Calamenene	15.37	Sesquiterpene
<i>cis</i> -Calamenene?	0.23	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	3.99	Sesquiterpene
α -Cadinene	0.07	Sesquiterpene
Unknown	0.40	Sesquiterpene
α -Calacorene	0.86	Sesquiterpene
Isocaryophyllene epoxide B	0.06	Sesquiterpenic ether
Flavesone	5.04	Norsesquiterpenic ketone
Unknown	0.11	Oxygenated sesquiterpene
Palustrol	0.30	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.22	Sesquiterpenic alcohol
Spathulenol	0.66	Sesquiterpenic alcohol
Caryophyllene oxide	0.68	Sesquiterpenic ether
Globulol	0.38	Sesquiterpenic alcohol
Unknown	0.05	Terpenic ketone
Gleenol	0.25	Sesquiterpenic alcohol
Viridiflorol	0.15	Sesquiterpenic alcohol
Cubeban-11-ol	0.14	Sesquiterpenic alcohol
Ledol	0.38	Sesquiterpenic alcohol
Eudesm-5-en-11-ol analog	0.14	Sesquiterpenic alcohol
Unknown	0.29	Oxygenated sesquiterpene
Unknown	0.13	Oxygenated sesquiterpene
Isoleptospermone	5.32	Sesquiterpenic ketone
Leptospermone	17.78	Sesquiterpenic ketone
Cubenol	0.36	Sesquiterpenic alcohol
τ -Muurolol	1.25*	Sesquiterpenic alcohol
τ -Cadinol	[1.25]*	Sesquiterpenic alcohol
β -Eudesmol	0.16	Sesquiterpenic alcohol
α -Eudesmol	0.27	Sesquiterpenic alcohol
α -Cadinol	0.63	Sesquiterpenic alcohol
Selin-11-en-4 α -ol	0.20	Sesquiterpenic alcohol
<i>cis</i> -Calamenen-10-ol	0.10	Sesquiterpenic alcohol
<i>trans</i> -Calamenen-10-ol	0.09	Sesquiterpenic alcohol
Unknown	0.44	Oxygenated sesquiterpene
Cadalene	0.21	Sesquiterpene
Unknown	0.31	Unknown
<i>trans</i> -14-nor-Cadina-5-en-4-one	0.26	Norsesquiterpenic ketone
(2E,6E)-Farnesol	0.08	Sesquiterpenic alcohol
14-Hydroxy- <i>trans</i> -calamenene	0.02	Sesquiterpenic alcohol
5-Hydroxy- <i>cis</i> -calamenene?	0.06	Sesquiterpenic alcohol
Grandiflorone	0.55	Terpenophenolic
Consolidated total	99.73%	

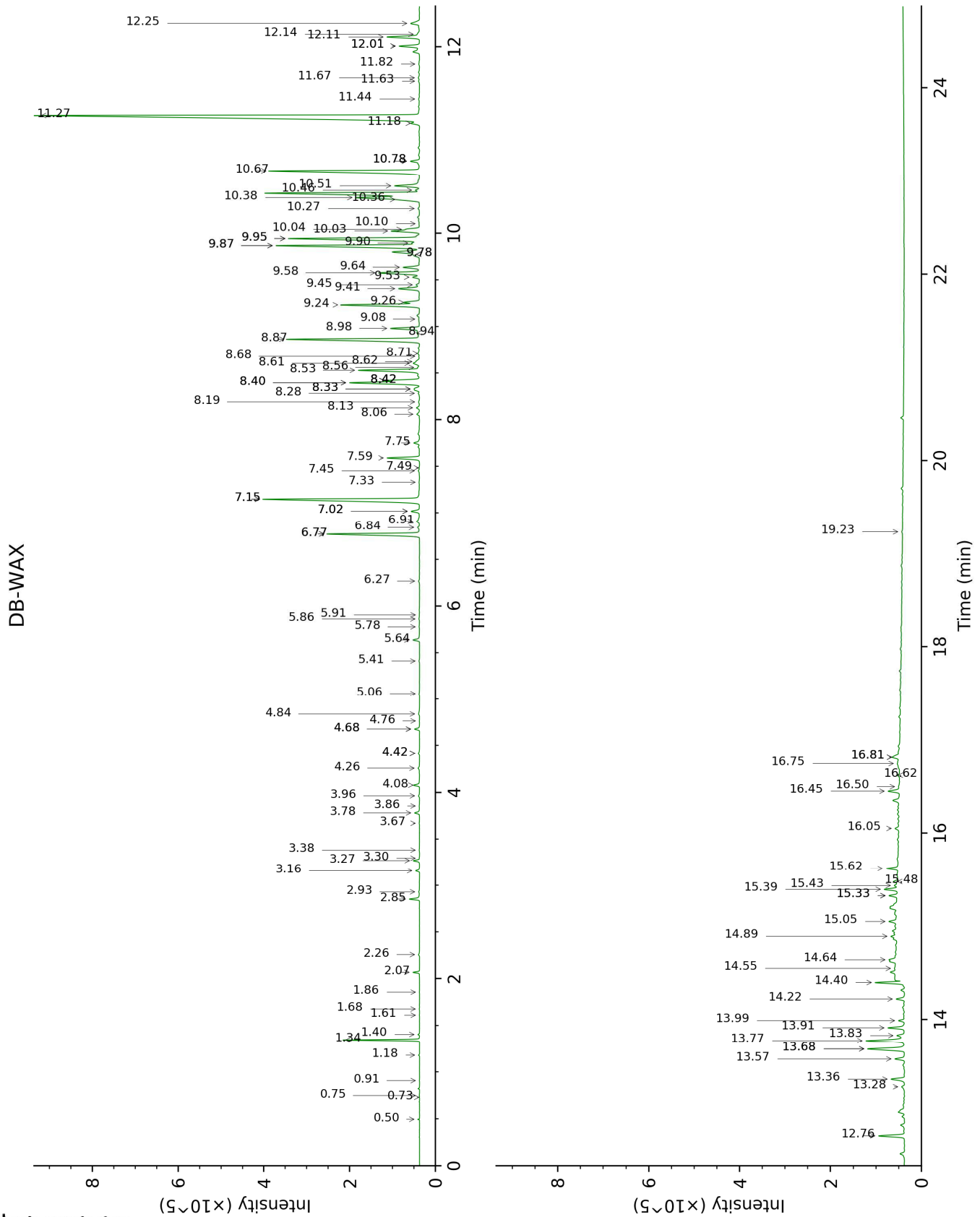
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

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.

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isovaleral	0.60	641	tr	0.75	888	tr
2-Methylbutyral	0.62	651	tr	0.73	882	tr
2-Ethylfuran	0.74	694	tr	0.91	922	tr
2,4-Dimethyl-3-pentanone	1.38	792	0.01	1.18	965	0.01
Hexanal	1.43	800	tr	1.86	1045	tr
Octane	1.46	803	0.01	0.50	788	0.01
(2E)-Hexenal	2.00	849	0.01	3.38	1175	0.01
Ethylbenzene	2.07	855	0.02	2.26	1084	0.04
(3Z)-Hexenol	2.10	856	0.02	5.78	1350	0.02
Styrene	2.44	884	0.01	3.86	1210	0.01
α-Thujene	2.99	924	0.02	1.40	1001	0.03
α-Pinene	3.06	929	0.98	1.34	992	1.11
Camphene	3.25*	942	0.01	1.68	1028	0.01
α-Fenchene	3.25*	942	[0.01]	1.61	1021	tr
β-Pinene	3.67	969	0.11	2.07	1066	0.12
6-Methyl-5-hepten-2-one	3.91	985	0.02	5.06	1298	0.02
2-Pentylfuran	3.99*	990	0.23	3.67	1197	0.01
Myrcene	3.99*	990	[0.23]	2.85	1134	0.24
Octanal	4.13	1000	0.01	4.42*	1251	0.04
(3Z)-Hexenyl acetate	4.25	1008	0.04	4.84	1282	0.05
α-Terpinene	4.33	1012	0.01	2.93	1140	0.03
Isoamyl isobutyrate	4.34	1013	tr	3.30	1168	0.01
para-Cymene	4.44	1020	0.14	4.08	1226	0.15
Limonene	4.52*	1025	0.20	3.16	1157	0.09
1,8-Cineole	4.52*	1025	[0.20]	3.27	1166	0.14
(E)-β-Ocimene	4.89	1048	0.03	3.96	1218	0.03
γ-Terpinene	5.00	1055	0.11	3.78	1205	0.12
Unknown [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	5.18	1066	0.01	4.76	1276	0.01
Octanol	5.30	1074	0.03	8.19	1528	0.04
Terpinolene	5.46	1084	0.04	4.26	1240	0.05
Linalool	5.71	1100	0.07	8.06	1518	0.08
Nonanal	5.73	1101	0.02	5.86	1356	0.03
2-Methylbutyl 2-methylbutyrate	5.76	1103	0.02	4.42*	1251	[0.04]
Isoamyl isovalerate	5.82	1107	0.08	4.68*	1270	0.13
Amyl isovalerate	5.86	1110	0.04	4.68*	1270	[0.13]
3-Methyl-3-butenyl 2-methylbutyrate	5.93	1114	0.02	5.41	1323	0.02
3-Methyl-3-butenyl isovalerate	5.98	1118	0.18	5.64	1340	0.18
Prenyl 2-methylbutyrate	6.36	1143	0.01	5.91	1360	0.01
Prenyl isovalerate	6.49	1151	0.03	6.27	1386	0.03

Dimethyloctanedione isomer	6.62	1159	0.03	6.77*	1422	2.46
2,7-Dimethyl-3,5-octanedione	6.67	1163	0.07	6.84	1427	0.07
Terpinen-4-ol	6.83	1174	0.04	8.56	1556	0.04
α -Terpineol	7.06	1188	0.05	9.78*†	1653	1.06
2-Methylbutyl tiglate	7.19	1197	0.09	6.91	1432	0.11
3-Methyl-3-butenyl tiglate	7.31	1205	0.06			
Benzylacetone	7.82	1241	0.03	11.44	1792	0.03
Prenyl tiglate	7.95	1250	0.06			
Geraniol	8.10	1259	0.02	11.63	1808	0.03
(2E)-Decenal	8.16	1263	0.02	9.08	1597	0.05
Geranial	8.33	1274	0.01	10.10	1679	0.02
Undec-(5Z)-en-2-one	8.41	1279	0.07	8.94	1586	0.10
Bicycloelemene	9.22	1334	0.01	7.02*	1440	0.26
α -Cubebene	9.44	1350	2.23	6.77*	1422	[2.46]
Longicyclene	9.60	1361	0.01	7.15*	1450	5.04
α -Ylangene	9.72	1369	0.22	7.02*	1440	[0.26]
α -Copaene	9.80*	1375	4.53	7.15*	1450	[5.04]
Modhephene	9.80*	1375	[4.53]	7.45	1472	0.04
Methyl (E)-cinnamate	9.85	1378	0.07	13.83	2007	0.25
β -Bourbonene	9.90*	1382	0.07	7.49	1475	0.02
1,5-diepi- β -Bourbonene	9.90*	1382	[0.07]	7.33	1464	0.03
<i>cis</i> - β -Elemene	9.90*	1382	[0.07]	8.28	1535	0.03
Benzyl 2-methylbutyrate?	9.93	1384	0.08	11.67	1811	0.04
β -Cubebene	9.99	1388	0.14	7.75	1494	0.17
β -Elemene	10.03*	1391	0.87	8.42*†	1546	[2.67]
Benzyl isovalerate	10.03*	1391	[0.87]	11.82	1824	0.02
α -Gurjunene	10.24	1406	0.73	7.59	1483	0.82
Unknown [m/z 119, 107 (86), 105 (85), 93 (78), 189 (66), 81 (65), 121 (64)... 204 (23)]	10.28	1409	0.04			
β -Caryophyllene	10.36*	1414	1.72	8.40*†	1544	2.67
β -Ylangene	10.36*	1414	[1.72]	8.13	1523	0.09
γ -Maaliene	10.42	1419	0.02	8.42*†	1546	[2.67]
β -Gurjunene	10.47	1423	0.04	8.33*	1539	0.24
β -Copaene	10.50*†	1425	0.26	8.33*	1539	[0.24]
<i>cis</i> -Thujopsene	10.50*†	1425	[0.26]	8.68	1566	0.02
α -Maaliene	10.52†	1426	[0.26]	8.60	1560	0.22
Aromadendrene	10.56	1429	0.08	8.53	1554	1.62
Selina-5,11-diene	10.62*	1434	1.59	8.71	1568	0.07
α -Guaiene	10.62*	1434	[1.59]	8.40*†	1544	[2.67]
<i>trans</i> - α -Bergamotene	10.62*	1434	[1.59]	8.42*†	1546	[2.67]
6,9-Guaiadiene	10.71	1441	0.10	8.62	1561	0.09
<i>trans</i> -Muurola-3,5-diene	10.80	1447	3.61	8.87	1580	3.88
α -Humulene	10.82	1448	0.22	9.26	1611	0.38
allo-Aromadendrene	10.91	1455	0.66	8.98	1589	0.74

4,5-diepi-Aristolochene	11.04	1464	0.08	9.45	1626	0.11
Selina-4,11-diene	11.09	1468	0.08	9.41	1623	0.59
<i>trans</i> -Cadina-1(6),4-diene	11.12†	1471	3.36	9.24	1609	2.04
γ-Muurolene	11.17†	1474	[3.36]	9.58	1637	1.15
Germacrene D	11.21	1477	0.31	9.78*†	1653	[1.06]
β-Selinene	11.27	1482	3.89	9.87*	1660	4.23
allo-Aromadendr-9-ene	11.29	1483	0.17	9.53	1633	0.18
<i>trans</i> -Muurola-4(15),5-diene	11.33*	1486	0.81	9.87*	1660	[4.23]
Eudesma-3,5,11-triene	11.33*	1486	[0.81]	10.27	1692	0.04
α-Selinene	11.40*	1491	4.11	9.94*	1666	3.77
epi-Cubebol	11.40*	1491	[4.11]	12.01*	1841	0.54
Bicyclogermacrene	11.40*	1491	[4.11]	10.04	1674	0.21
Viridiflorene	11.40*	1491	[4.11]	9.64	1642	0.44
α-Muurolene	11.49	1498	0.79	10.03	1673	0.80
δ-Amorphene	11.50	1499	0.27	9.94*	1666	[3.77]
δ-Guaiene	11.56	1504	0.10	9.90	1662	0.15
γ-Cadinene	11.64*†	1510	1.54	10.36	1700	0.38
(3 <i>E</i> ,6 <i>E</i>)-α-Farnesene	11.64*†	1510	[1.54]	10.51	1712	0.73
7-epi-α-Selinene	11.68*†	1512	[1.54]	10.46	1709	0.10
Unknown [m/z 159, 145 (91), 131 (67), 105 (46), 202 (43)]	11.68*†	1512	[1.54]	10.78*	1735	0.23
δ-Cadinene	11.80*†	1522	19.05	10.38	1702	6.35
<i>trans</i> -Calamenene	11.80*†	1522	[19.05]	11.27	1777	15.37
<i>cis</i> -Calamenene?	11.81†	1523	[19.05]	11.18	1770	0.23
<i>trans</i> -Cadina-1,4-diene	11.91	1530	3.99	10.67	1726	4.43
α-Cadinene	11.94	1532	0.07	10.78*	1735	[0.23]
Unknown [m/z 157, 143 (86), 200 (43), 142 (36), 141 (28), 128 (25)]	11.98*†	1536	1.25	12.01*	1841	[0.54]
α-Calacorene	11.98*†	1536	[1.25]	12.11	1850	0.86
Isocaryophyllene epoxide B	12.08*	1543	5.09	12.14	1852	0.06
Flavesone	12.08*	1543	[5.09]			
Unknown [m/z 161, 109 (98), 82 (93), 43 (72), 105 (68), 93 (59), 69 (56), 119 (55)... 222 (7)]	12.25	1557	0.11	13.28	1955	0.10
Palustrol	12.31	1561	0.30	12.25	1862	0.31
(<i>E</i>)-Nerolidol	12.34	1564	0.22	13.77	2001	1.09
Spathulenol	12.43	1571	0.66	14.40	2061	0.72
Caryophyllene oxide	12.48	1574	0.68	12.76	1908	0.66
Globulol	12.51	1577	0.38	13.91	2015	0.43
Unknown [m/z 161,	12.56*	1581	0.30			

159 (64), 43 (58), 182 (53), 41 (48), 105 (40)... 252 (25)						
Gleenol	12.56*	1581	[0.30]	13.58	1983	0.25
Viridiflorol	12.60	1584	0.15	13.99	2022	0.14
Cubeban-11-ol	12.63	1587	0.14	13.68*	1993	1.12
Ledol	12.74	1595	0.38	13.36	1963	0.38
Eudesm-5-en-11-ol analog	12.80	1600	0.14	14.22	2044	0.22
Unknown [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	12.87	1605	0.29	14.55†	2076	25.24
Unknown [m/z 179, 161 (66), 119 (44), 95 (38), 105 (35)... 204 (24), 222 (1)]	12.94	1612	0.13	14.64†	2085	[25.24]
Isoleptospermone	13.02	1618	5.32	16.05†	2226	[25.24]
Leptospermone	13.16	1629	17.78	15.33*†	2153	[25.24]
Cubenol	13.21	1633	0.36	13.68*	1993	[1.12]
τ-Muurolol	13.27*	1638	1.25	15.05†	2125	[25.24]
τ-Cadinol	13.27*	1638	[1.25]	14.89†	2109	[25.24]
β-Eudesmol	13.32	1642	0.16	15.40†	2160	[25.24]
α-Eudesmol	13.33	1644	0.27	15.33*†	2153	[25.24]
α-Cadinol	13.38	1647	0.63	15.48†	2168	[25.24]
Selin-11-en-4α-ol	13.43	1652	0.20	15.62†	2182	[25.24]
cis-Calamenen-10-ol	13.49	1656	0.10	16.45†	2268	[25.24]
trans-Calamenen-10-ol	13.56	1662	0.09	16.81*†	2306	[25.24]
Unknown [m/z 159, 118 (33), 91 (30), 131 (30)... 220? (4)]	13.62	1667	0.44	16.50†	2273	[25.24]
Cadalene	13.66	1670	0.21	15.43†	2164	[25.24]
Unknown [m/z 175, 91 (94), 105 (51), 218 (33), 104 (17), 176 (12)...]	13.68	1672	0.31	16.75†	2299	[25.24]
trans-14-nor-Cadina-5-en-4-one	14.18	1714	0.26	16.62†	2286	[25.24]
(2E,6E)-Farnesol	14.26	1720	0.08	16.81*†	2306	[25.24]
14-Hydroxy-trans-calamenene	15.16*	1799	0.08	19.23	2577	0.02
5-Hydroxy-cis-calamenene?	15.16*	1799	[0.08]			
Grandiflorone	18.88	2158	0.55			
Total identified		96.00%			71.95%	
Total reported		97.33%			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

