

Date : January 07, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21A05-PTH03

Customer identification : Manuka - MF0105911R

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 : Sylvain Mercier, M. Sc., Chimiste

Analysis date : January 06, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Light yellow liquid

Refractive index: 1.5029 ± 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
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2,4-Dimethyl-3-pentanone	0.01	Aliphatic ketone
(3Z)-Hexenol	0.01	Aliphatic alcohol
Styrene	0.01	Simple phenolic
Hashishene	tr	Monoterpene
α -Thujene	0.02	Monoterpene
α -Pinene	1.00	Monoterpene
Camphene	0.01	Monoterpene
β -Pinene	0.11	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	0.24	Monoterpene
(3Z)-Hexenyl acetate	0.04	Aliphatic ester
α -Terpinene	0.01	Monoterpene
Isoamyl isobutyrate	0.01	Aliphatic ester
para-Cymene	0.14	Monoterpene
Limonene	0.08	Monoterpene
1,8-Cineole	0.13	Monoterpenic ether
(E)- β -Ocimene	0.03	Monoterpene
γ -Terpinene	0.11	Monoterpene
Isoamyl butyrate	0.01	Aliphatic ester
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.03	Monoterpene
para-Cymenene	0.01	Monoterpene
<i>trans</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
Linalool	0.09	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
Isoamyl isovalerate	0.09	Aliphatic ester
Amyl isovalerate	0.04	Aliphatic ester
3-Methyl-3-butenyl 2-methylbutyrate	0.01	Aliphatic ester
3-Methyl-3-butenyl isovalerate	0.18	Aliphatic ester
<i>trans</i> -Pinocarveol	0.01	Monoterpenic alcohol
Prenyl 2-methylbutyrate	0.01	Aliphatic ester
Prenyl isovalerate	0.03	Aliphatic ester
Dimethyloctanedione isomer	0.01	β -Diketone
Terpinen-4-ol	0.04	Monoterpenic alcohol
α -Terpineol	0.04	Monoterpenic alcohol
2-Methylbutyl tiglate	0.09	Aliphatic ester
3-Methyl-3-butenyl tiglate	0.05	Aliphatic ester
Benzylacetone	0.02	Simple phenolic
Prenyl tiglate	0.06	Aliphatic ester
Geraniol	0.02	Monoterpenic alcohol
(2E)-Decenal	0.04	Aliphatic aldehyde
Undec-(5Z)-en-2-one	0.07	Aliphatic ketone
2-Undecanone	0.03	Aliphatic ketone

Methyl geranate	0.01	Monoterpenic ester
Bicycloelemene	0.01	Sesquiterpene
α -Cubebene	2.24	Sesquiterpene
α -Ylangene	0.26	Sesquiterpene
α -Copaene	4.56	Sesquiterpene
Methyl (<i>E</i>)-cinnamate	0.02	Phenylpropanoid ester
β -Bourbonene	0.04	Sesquiterpene
1,5-diepi- β -Bourbonene	0.01	Sesquiterpene
Benzyl 2-methylbutyrate?	0.04	Phenolic ester
β -Cubebene	0.15	Sesquiterpene
β -Elemene	0.85	Sesquiterpene
Benzyl isovalerate	0.03	Phenolic ester
α -Gurjunene	0.73	Sesquiterpene
Unknown	0.02	Sesquiterpene
β -Ylangene	0.08	Sesquiterpene
β -Caryophyllene	1.51	Sesquiterpene
γ -Maaliene	0.06	Sesquiterpene
β -Copaene	0.22	Sesquiterpene
α -Maaliene	0.10	Sesquiterpene
Aromadendrene	1.51	Sesquiterpene
α -Guaiene	0.08	Sesquiterpene
Selina-5,11-diene	0.07	Sesquiterpene
6,9-Guaiadiene	0.15	Sesquiterpene
<i>trans</i> -Muuro-la-3,5-diene	3.71	Sesquiterpene
α -Humulene	0.25	Sesquiterpene
allo-Aromadendrene	0.65	Sesquiterpene
4,5-diepi-Aristolochene	0.07	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	1.90	Sesquiterpene
Selina-4,11-diene	0.57	Sesquiterpene
γ -Muuro-lene	0.41	Sesquiterpene
α -Amorphene	0.87	Sesquiterpene
Germacrene D	0.36	Sesquiterpene
β -Selinene	3.86	Sesquiterpene
allo-Aromadendr-9-ene	0.22	Sesquiterpene
<i>trans</i> -Muuro-la-4(15),5-diene	0.75	Sesquiterpene
Eudesma-3,5,11-triene	0.04	Sesquiterpene
α -Selinene	3.52	Sesquiterpene
Viridiflorene	0.02	Sesquiterpene
Bicyclogermacrene	0.19	Sesquiterpene
α -Muuro-lene	0.70	Sesquiterpene
Germacrene A	0.47	Sesquiterpene
δ -Guaiene	0.06	Sesquiterpene
δ -Amorphene	0.04	Sesquiterpene
γ -Cadinene	0.73	Sesquiterpene
Unknown	0.26	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	0.73	Sesquiterpene
7-epi- α -Selinene	0.07	Sesquiterpene
δ -Cadinene	4.89	Sesquiterpene
<i>trans</i> -Calamenene	14.10	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	4.04	Sesquiterpene
Unknown	0.56	Sesquiterpene
α -Calacorene	0.67	Sesquiterpene

Flavesone	4.97	Norsesquiterpenic ketone
Isocaryophyllene epoxide B	0.21	Sesquiterpenic ether
Germacrene B	0.02	Sesquiterpene
Unknown	0.10	Oxygenated sesquiterpene
Palustrol	0.29	Sesquiterpenic alcohol
(E)-Nerolidol	0.16	Sesquiterpenic alcohol
Spathulenol	0.64	Sesquiterpenic alcohol
Caryophyllene oxide	0.60	Sesquiterpenic ether
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Globulol	0.39	Sesquiterpenic alcohol
Gleenol	0.30	Sesquiterpenic alcohol
Viridiflorol	0.18	Sesquiterpenic alcohol
Cubeban-11-ol	0.13	Sesquiterpenic alcohol
Ledol	0.40	Sesquiterpenic alcohol
Eudesm-5-en-11-ol	0.13	Sesquiterpenic alcohol
Unknown	0.04	Oxygenated sesquiterpene
Unknown	0.18	Oxygenated sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Isoleptospermone	5.29	Sesquiterpenic ketone
Leptospermone	16.00	Sesquiterpenic ketone
γ-Eudesmol	0.13	Sesquiterpenic alcohol
τ-Muurolol	0.20	Sesquiterpenic alcohol
τ-Cadinol	0.25	Sesquiterpenic alcohol
Cubenol	1.25	Sesquiterpenic alcohol
α-Muurolol	0.17	Sesquiterpenic alcohol
β-Eudesmol	0.27	Sesquiterpenic alcohol
α-Cadinol	0.10	Sesquiterpenic alcohol
α-Eudesmol	0.20	Sesquiterpenic alcohol
Selin-11-en-4α-ol	0.27	Sesquiterpenic alcohol
cis-Calamenen-10-ol	0.20	Sesquiterpenic alcohol
trans-Calamenen-10-ol	0.10	Sesquiterpenic alcohol
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.23	Oxygenated sesquiterpene
Unknown	0.18	Unknown
Unknown	0.02	Oxygenated sesquiterpene
cis-14-nor-Muurolol-5-en-4-one?	0.03	Norsesquiterpenic ketone
14-Hydroxy-trans-calamenene	0.08	Sesquiterpenic alcohol
Grandiflorone	0.69	Terpenophenolic
trans-14-nor-Cadina-5-en-4-one	0.12	Norsesquiterpenic ketone
Consolidated total	95.17%	

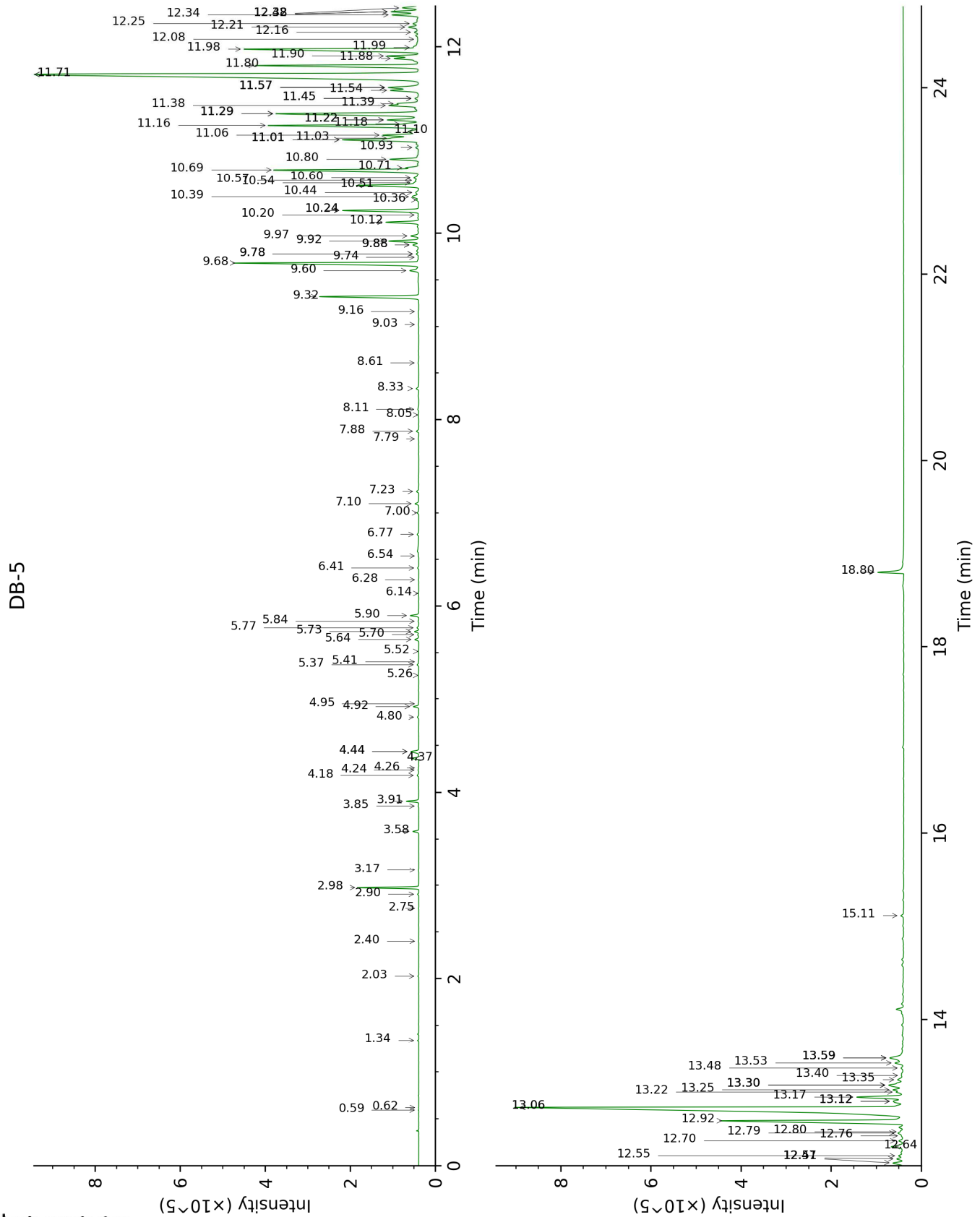
tr: The compound has been detected below 0.005% of total signal.

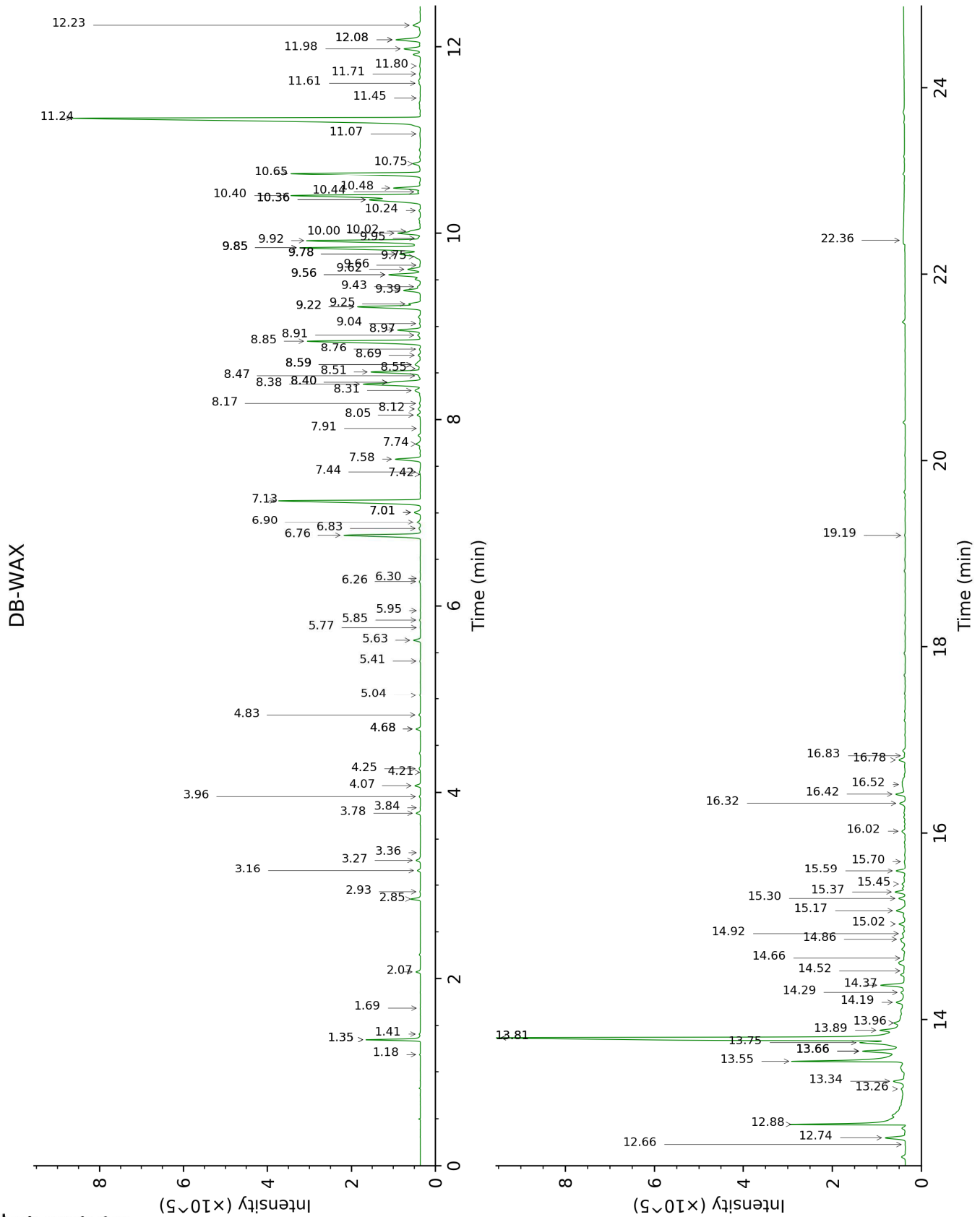
Note: no correction factor was applied

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	%
Isovaleral	0.59	639	tr			
2-Methylbutyral	0.62	651	tr			
2,4-Dimethyl-3-pentanone	1.34	796	0.01	1.18	962	0.01
(3Z)-Hexenol	2.03	858	0.01	5.77	1347	0.01
Styrene	2.40	889	0.01	3.84	1209	0.01
Hashishene	2.75	916	tr	1.35*	989	1.01
α -Thujene	2.90	925	0.02	1.41	998	0.03
α -Pinene	2.98	930	1.00	1.35*	989	[1.01]
Camphene	3.17	943	0.01	1.69	1025	0.01
β -Pinene	3.58	970	0.11	2.07	1064	0.10
6-Methyl-5-hepten-2-one	3.85	988	0.02	5.04	1298	0.02
Myrcene	3.91	992	0.24	2.85	1132	0.23
(3Z)-Hexenyl acetate	4.18	1010	0.04	4.83	1282	0.05
α -Terpinene	4.24	1013	0.01	2.93	1138	0.01
Isoamyl isobutyrate	4.26	1014	0.01	3.36	1172	tr
para-Cymene	4.36	1021	0.14	4.07	1226	0.15
Limonene	4.44*	1026	0.20	3.16	1156	0.08
1,8-Cineole	4.44*	1026	[0.20]	3.27	1165	0.13
(E)- β -Ocimene	4.80	1048	0.03	3.96	1218	0.03
γ -Terpinene	4.92	1056	0.11	3.78	1205	0.12
Isoamyl butyrate	4.95	1058	0.01	4.22	1237	0.01
Octanol	5.26	1077	0.02	8.17	1525	0.03
Terpinolene	5.37	1084	0.03	4.25	1240	0.05
para-Cymenene	5.40	1086	0.01	6.30	1385	tr
<i>trans</i> -Sabinene hydrate	5.52	1093	0.01	7.91	1504	0.01
Linalool	5.64	1101	0.09	8.05	1515	0.10
Nonanal	5.70	1104	0.02	5.85	1353	0.02
Isoamyl isovalerate	5.73	1107	0.09	4.68*	1271	0.12
Amyl isovalerate	5.77	1109	0.04	4.68*	1271	[0.12]
3-Methyl-3-butenyl 2-methylbutyrate	5.84	1114	0.01	5.41	1321	0.02
3-Methyl-3-butenyl isovalerate	5.90	1118	0.18	5.64	1337	0.18
<i>trans</i> -Pinocarveol	6.14	1133	0.01	9.22*	1606	1.91
Prenyl 2-methylbutyrate	6.28	1142	0.01	5.95	1360	0.01
Prenyl isovalerate	6.41	1150	0.03	6.26	1382	0.03
Dimethyloctanedione isomer	6.54	1158	0.01	6.83	1424	0.04
Terpinen-4-ol	6.77	1173	0.04	8.55	1554	0.03
α -Terpineol	7.00	1189	0.04	9.78*	1652	0.83
2-Methylbutyl tiglate	7.10	1195	0.09	6.90	1429	0.11
3-Methyl-3-butenyl tiglate	7.23	1204	0.05			
Benzylacetone	7.80	1242	0.02	11.45	1791	0.01

Prenyl tiglate	7.88	1247	0.06	8.76	1570	0.03
Geraniol	8.05	1259	0.02	11.61	1805	0.04
(2E)-Decenal	8.11	1263	0.04	9.04	1592	0.03
Undec-(5Z)-en-2-one	8.33	1278	0.07	8.91	1582	0.10
2-Undecanone	8.61	1297	0.03	8.59*	1557	0.26
Methyl geranate	9.03	1322	0.01	9.75	1649	0.14
Bicycloelemene	9.16	1332	0.01	7.01*	1437	0.20
α-Cubebene	9.32	1344	2.24	6.76	1419	2.24
α-Ylangene	9.60	1364	0.26	7.01*	1437	[0.20]
α-Copaene	9.68	1369	4.56	7.13	1446	4.58
Methyl (E)-cinnamate	9.74	1374	0.02	13.81*†	2004	16.59
β-Bourbonene	9.78*	1376	0.06	7.44	1469	0.04
1,5-diepi-β-Bourbonene	9.78*	1376	[0.06]	7.42	1467	0.01
Benzyl 2-methylbutyrate?	9.88*	1383	0.16	11.71	1814	0.04
β-Cubebene	9.88*	1383	[0.16]	7.74	1492	0.15
β-Elemene	9.92†	1386	0.88	8.40*†	1542	[2.43]
Benzyl isovalerate	9.97†	1390	[0.88]	11.80	1822	0.03
α-Gurjunene	10.12	1401	0.73	7.58	1480	0.75
Unknown [m/z 119, 107 (86), 105 (85), 93 (78), 189 (66), 81 (65), 121 (64)... 204 (23)]	10.20	1406	0.02			
β-Ylangene	10.24*	1410	1.73	8.12	1520	0.08
β-Caryophyllene	10.24*	1410	[1.73]	8.38†	1541	2.43
γ-Maaliene	10.36	1418	0.06	8.47	1548	0.04
β-Copaene	10.39	1421	0.22	8.31	1536	0.22
α-Maaliene	10.44	1424	0.10	8.59*	1557	[0.26]
Aromadendrene	10.51	1430	1.51	8.51	1551	1.49
α-Guaiene	10.54	1432	0.08	8.40*†	1542	[2.43]
Selina-5,11-diene	10.57	1434	0.07	8.69	1565	0.07
6,9-Guaiadiene	10.60	1436	0.15	8.59*	1557	[0.26]
trans-Muurola-3,5-diene	10.68	1443	3.71	8.85	1577	3.54
α-Humulene	10.71	1445	0.25	9.25	1608	0.31
allo-Aromadendrene	10.80	1452	0.65	8.97	1586	0.65
4,5-diepi-Aristolochene	10.93	1461	0.07	9.39†	1620	0.64
trans-Cadina-1(6),4-diene	11.01*	1468	2.03	9.22*	1606	[1.91]
Selina-4,11-diene	11.01*	1468	[2.03]	9.43†	1623	[0.64]
γ-Muurolole	11.02	1469	0.41	9.62	1638	0.40
α-Amorphene	11.06	1471	0.87	9.56*	1634	1.04
Germacrene D	11.10	1474	0.36	9.78*	1652	[0.83]
β-Selinene	11.16	1479	3.86	9.85*	1657	3.92
allo-Aromadendr-9-ene	11.18	1480	0.22	9.56*	1634	[1.04]
trans-Muurola-4(15),5-diene	11.22*	1483	0.80	9.85*	1657	[3.92]
Eudesma-3,5,11-triene	11.22*	1483	[0.80]	10.24	1689	0.04

α-Selinene	11.29*	1488	4.15	9.92	1663	3.52
Viridiflorene	11.29*	1488	[4.15]	9.66	1642	0.02
Bicyclogermacrene	11.29*	1488	[4.15]	10.02	1671	0.19
α-Muurolene	11.38†	1495	1.17	10.00	1670	0.70
Germacrene A	11.39†	1496	[1.17]	10.36*†	1699	6.09
δ-Guaiene	11.45*	1501	0.10	9.85*	1657	[3.92]
δ-Amorphene	11.45*	1501	[0.10]	9.95	1665	0.04
γ-Cadinene	11.54	1507	0.73	10.36*†	1699	[6.09]
Unknown [m/z 159, 145 (91), 131 (67), 105 (46), 202 (43)]	11.57*	1510	0.85	10.75	1732	0.26
(3E,6E)-α-Farnesene	11.57*	1510	[0.85]	10.48	1709	0.73
7-epi-α-Selinene	11.57*	1510	[0.85]	10.44	1706	0.07
δ-Cadinene	11.71*	1521	19.03	10.40†	1703	[6.09]
trans-Calamenene	11.71*	1521	[19.03]	11.24	1773	14.10
trans-Cadina-1,4-diene	11.80	1528	4.04	10.65	1723	4.05
Unknown [m/z 157, 143 (86), 200 (43), 142 (36), 141 (28), 128 (25)]	11.88	1534	0.56	11.98	1838	0.52
α-Calacorene	11.90	1536	0.67	12.08*	1846	0.83
Flavesone	11.98	1542	4.97	12.88	1918	4.58
Isocaryophyllene epoxide B	11.99	1544	0.21	12.08*	1846	[0.83]
Germacrene B	12.08	1550	0.02	11.07	1759	0.02
Unknown [m/z 161, 109 (98), 82 (93), 43 (72), 105 (68), 93 (59), 69 (56), 119 (55)... 222 (7)]	12.16	1556	0.10	13.26	1953	0.28
Palustrol	12.21	1561	0.29	12.23	1860	0.28
(E)-Nerolidol	12.25	1564	0.16	13.75†	1999	[7.17]
Spathulenol	12.34	1571	0.64	14.37	2058	0.82
Caryophyllene oxide	12.38*	1574	0.66	12.74	1905	0.60
Caryophyllene oxide isomer	12.38*	1574	[0.66]	12.66	1898	0.01
Globulol	12.42	1577	0.39	13.89†	2012	[16.59]
Gleenol	12.47	1581	0.30	13.55†	1980	7.17
Viridiflorol	12.51	1584	0.18	13.96†	2019	[16.59]
Cubeban-11-ol	12.55	1587	0.13	13.66*†	1990	[7.17]
Ledol	12.64	1595	0.40	13.34	1960	0.49
Eudesm-5-en-11-ol	12.70	1600	0.13	14.29	2051	0.21
Unknown [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	12.76	1604	0.04	14.52	2073	0.05
Unknown [m/z 151, 41 (15), 81 (13), 111 (13), 91 (13)...]	12.79	1606	0.18	14.19	2041	0.44
Unknown [m/z 179, 161 (66), 119 (44), 95	12.80	1607	0.07	14.66	2086	0.06

(38), 105 (35)... 204 (24), 222 (1)]						
Isoleptospermone	12.92	1617	5.29	13.66*†	1990	[7.17]
Leptospermone	13.06*	1629	17.87	13.81*†	2004	[16.59]
γ-Eudesmol	13.06*	1629	[17.87]	14.92	2112	0.13
τ-Muurolol	13.12*	1634	0.36	15.02	2122	0.20
τ-Cadinol	13.12*	1634	[0.36]	14.86	2106	0.25
Cubenol	13.17	1638	1.25	13.66*†	1990	[7.17]
α-Muurolol	13.22	1642	0.17	15.17	2136	0.36
β-Eudesmol	13.25	1644	0.27	15.37	2156	0.30
α-Cadinol	13.30*	1648	0.46	15.45	2165	0.10
α-Eudesmol	13.30*	1648	[0.46]	15.30	2150	0.20
Selin-11-en-4α-ol	13.30*	1648	[0.46]	15.59	2179	0.27
cis-Calamenen-10-ol	13.35	1653	0.20	16.42	2264	0.29
trans-Calamenen-10-ol	13.40	1657	0.10	16.78	2303	0.20
Unknown [m/z 159, 177 (59), 135 (57), 91 (47), 105 (47)... 220? (25)]	13.48	1663	0.08			
Unknown [m/z 159, 118 (33), 91 (30), 131 (30)... 220? (4)]	13.53	1668	0.23	16.32	2254	0.19
Unknown [m/z 175, 91 (94), 105 (51), 218 (33), 104 (17), 176 (12)...]	13.58*	1672	0.66	16.52	2275	0.18
Unknown [m/z 107, 91 (95), 93 (87), 79 (86), 105 (78), 41 (76), 95 (72)... 220 (18)]	13.58*	1672	[0.66]	16.83	2308	0.02
cis-14-nor-Muurolol-5-en-4-one?	13.58*	1672	[0.66]	15.70	2190	0.03
14-Hydroxy-trans-calamenene	15.11	1803	0.08	19.19	2571	0.03
Grandiflorone	18.80	2153	0.69	22.36	2967	0.55
trans-14-nor-Cadina-5-en-4-one				16.02	2223	0.12
Total identified		95.74%			93.17%	
Total reported		97.02%			95.17%	

*: 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