

Date : February 28, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22B14-PTH03

Customer identification : Manuka - Australia - MF01062011R

Type : Essential oil

Source : *Leptospermum scoparium* ct. Triketones

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 : Seydou Ka, Ph. D.

Analysis date : February 25, 2022

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: 1.5018 ± 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-Ethylfuran	0.01	Furan
2,4-Dimethyl-3-pentanone	0.02	Aliphatic ketone
Octane	0.04	Alkane
Ethylbenzene	0.01	Simple phenolic
(3Z)-Hexenol	0.01	Aliphatic alcohol
Styrene	tr	Simple phenolic
Hashishene	0.01	Monoterpene
α -Thujene	0.02	Monoterpene
α -Pinene	1.33	Monoterpene
α -Fenchene	tr	Monoterpene
Camphene	tr	Monoterpene
Sabinene	0.01	Monoterpene
β -Pinene	0.18	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
2-Pentylfuran	0.02	Furan
Myrcene	0.38	Monoterpene
α -Phellandrene	0.01	Monoterpene
Octanal	0.01	Aliphatic aldehyde
(3Z)-Hexenyl acetate	0.01	Aliphatic ester
α -Terpinene	0.02	Monoterpene
Isoamyl isobutyrate	0.01	Aliphatic ester
para-Cymene	0.13	Monoterpene
Limonene	0.11	Monoterpene
1,8-Cineole	0.20	Monoterpenic ether
(Z)- β -Ocimene	tr	Monoterpene
(E)- β -Ocimene	0.04	Monoterpene
γ -Terpinene	0.12	Monoterpene
Unknown	0.01	Oxygenated monoterpene
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.05	Monoterpene
Linalool	0.09	Monoterpenic alcohol
Nonanal	0.04	Aliphatic aldehyde
Isoamyl isovalerate	0.09	Aliphatic ester
Amyl isovalerate	0.04	Aliphatic ester
3-Methyl-3-butenyl 2-methylbutyrate	0.02	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	0.03	β -Diketone
2,7-Dimethyl-3,5-octanedione	0.06	β -Diketone
Terpinen-4-ol	0.05	Monoterpenic alcohol
α -Terpineol	0.05	Monoterpenic alcohol
2-Methylbutyl tiglate	0.10	Aliphatic ester

3-Methyl-3-butenyl tiglate	0.04	Aliphatic ester
Benzylacetone	0.01	Simple phenolic
Prenyl tiglate	0.05	Aliphatic ester
Geraniol	0.02	Monoterpenic alcohol
(2E)-Decenal	0.05	Aliphatic aldehyde
Undec-(5Z)-en-2-one	0.05	Aliphatic ketone
α -Cubebene	3.55	Sesquiterpene
Longicyclene	0.02	Sesquiterpene
α -Ylangene	0.25	Sesquiterpene
α -Copaene	5.04	Sesquiterpene
Modhephene	0.02	Sesquiterpene
Methyl (E)-cinnamate	0.02	Phenylpropanoid ester
α -Isocomene	0.03	Sesquiterpene
β -Bourbonene	0.04	Sesquiterpene
1,5-diepi- β -Bourbonene	0.06	Sesquiterpene
Benzyl 2-methylbutyrate?	0.18	Phenolic ester
β -Cubebene	0.15	Sesquiterpene
β -Elemene	0.75	Sesquiterpene
Benzyl isovalerate	0.26	Phenolic ester
α -Gurjunene	0.96	Sesquiterpene
Unknown	0.02	Sesquiterpene
β -Caryophyllene	2.55	Sesquiterpene
β -Ylangene	0.02	Sesquiterpene
γ -Maaliene	0.05	Sesquiterpene
β -Gurjunene	0.25	Sesquiterpene
β -Copaene	tr	Sesquiterpene
α -Maaliene	0.07	Sesquiterpene
Aromadendrene	1.44	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.21*	Sesquiterpene
α -Guaiene	0.21*	Sesquiterpene
Selina-5,11-diene	0.01	Sesquiterpene
6,9-Guaiadiene	0.12	Sesquiterpene
<i>trans</i> -Muurolo-3,5-diene	5.50	Sesquiterpene
α -Humulene	0.33	Sesquiterpene
allo-Aromadendrene	0.66	Sesquiterpene
4,5-diepi-Aristolochene	0.09	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	3.75	Sesquiterpene
Selina-4,11-diene	0.83	Sesquiterpene
γ -Muurolole	1.06	Sesquiterpene
α -Amorphene	0.61	Sesquiterpene
Germacrene D	0.16	Sesquiterpene
allo-Aromadendr-9-ene	0.18	Sesquiterpene
β -Selinene	4.52	Sesquiterpene
<i>trans</i> -Muurolo-4(15),5-diene	1.08	Sesquiterpene
Viridiflorene	0.01	Sesquiterpene
epi-Cubebol	0.14	Sesquiterpenic alcohol
α -Selinene	4.89	Sesquiterpene
Bicyclogermacrene	0.31	Sesquiterpene
α -Muurolole	0.73	Sesquiterpene
δ -Amorphene	0.54	Sesquiterpene
δ -Guaiene	0.12	Sesquiterpene
(3E,6E)- α -Farnesene	1.14	Sesquiterpene

γ-Cadinene	0.86	Sesquiterpene
δ-Cadinene	5.69	Sesquiterpene
cis-Calamenene	11.09	Sesquiterpene
trans-Cadina-1,4-diene	5.33	Sesquiterpene
α-Cadinene	0.08	Sesquiterpene
Unknown	0.40	Sesquiterpene
α-Calacorene	0.46	Sesquiterpene
Flavesone	5.12	Norsesquiterpenic ketone
Germacrene B	0.02	Sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Palustrol	0.19	Sesquiterpenic alcohol
(E)-Nerolidol	0.10	Sesquiterpenic alcohol
Spathulenol	0.43	Sesquiterpenic alcohol
Caryophyllene oxide	0.41	Sesquiterpenic ether
Globulol	0.25*	Sesquiterpenic alcohol
Gleenol	0.25*	Sesquiterpenic alcohol
Unknown	0.18	Terpenic ketone
Viridiflorol	0.09	Sesquiterpenic alcohol
Cubeban-11-ol	0.08	Sesquiterpenic alcohol
Ledol	0.23	Sesquiterpenic alcohol
Humulene epoxide II	0.07	Sesquiterpenic ether
Unknown	0.10	Oxygenated sesquiterpene
Unknown	0.09	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
Isoleptospermone	4.01	Sesquiterpenic ketone
Unknown	0.01	Oxygenated sesquiterpene
1-epi-Cubenol	0.62	Sesquiterpenic alcohol
Leptospermone	12.82	Sesquiterpenic ketone
τ-Cadinol	0.18	Sesquiterpenic alcohol
τ-Muurolol	0.02	Sesquiterpenic alcohol
Jinkoh-eremol	1.02*	Sesquiterpenic alcohol
Cubenol	1.02*	Sesquiterpenic alcohol
α-Muurolol	1.02*	Sesquiterpenic alcohol
β-Eudesmol	0.27	Sesquiterpenic alcohol
α-Cadinol	0.02	Sesquiterpenic alcohol
Selin-11-en-4α-ol	0.24	Sesquiterpenic alcohol
α-Eudesmol	0.10	Sesquiterpenic alcohol
cis-Calamenen-10-ol	0.07	Sesquiterpenic alcohol
trans-Calamenen-10-ol	0.01	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.01	Unknown
Unknown	0.12	Oxygenated sesquiterpene
Unknown	0.29	Oxygenated sesquiterpene
Unknown	0.02	Lignan
trans-14-nor-Cadina-5-en-4-one	0.18	Norsesquiterpenic ketone
14-Hydroxy-trans-calamenene	0.02	Sesquiterpenic alcohol
5-Hydroxy-cis-calamenene?	0.01	Sesquiterpenic alcohol
Grandiflorone	0.40	Terpenophenolic
Consolidated total	98.19%	

*: 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

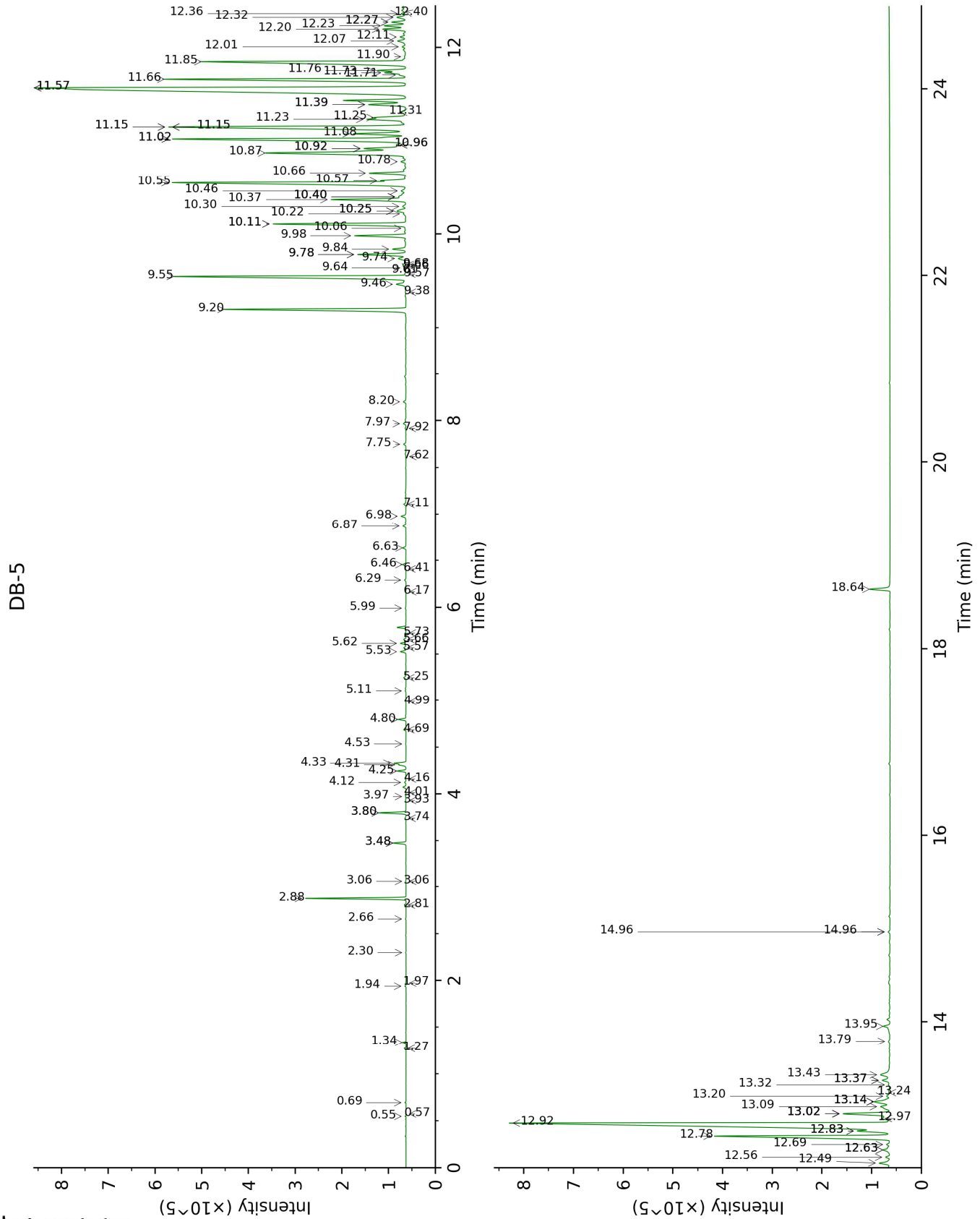
tr: The compound has been detected below 0.005% of total signal.

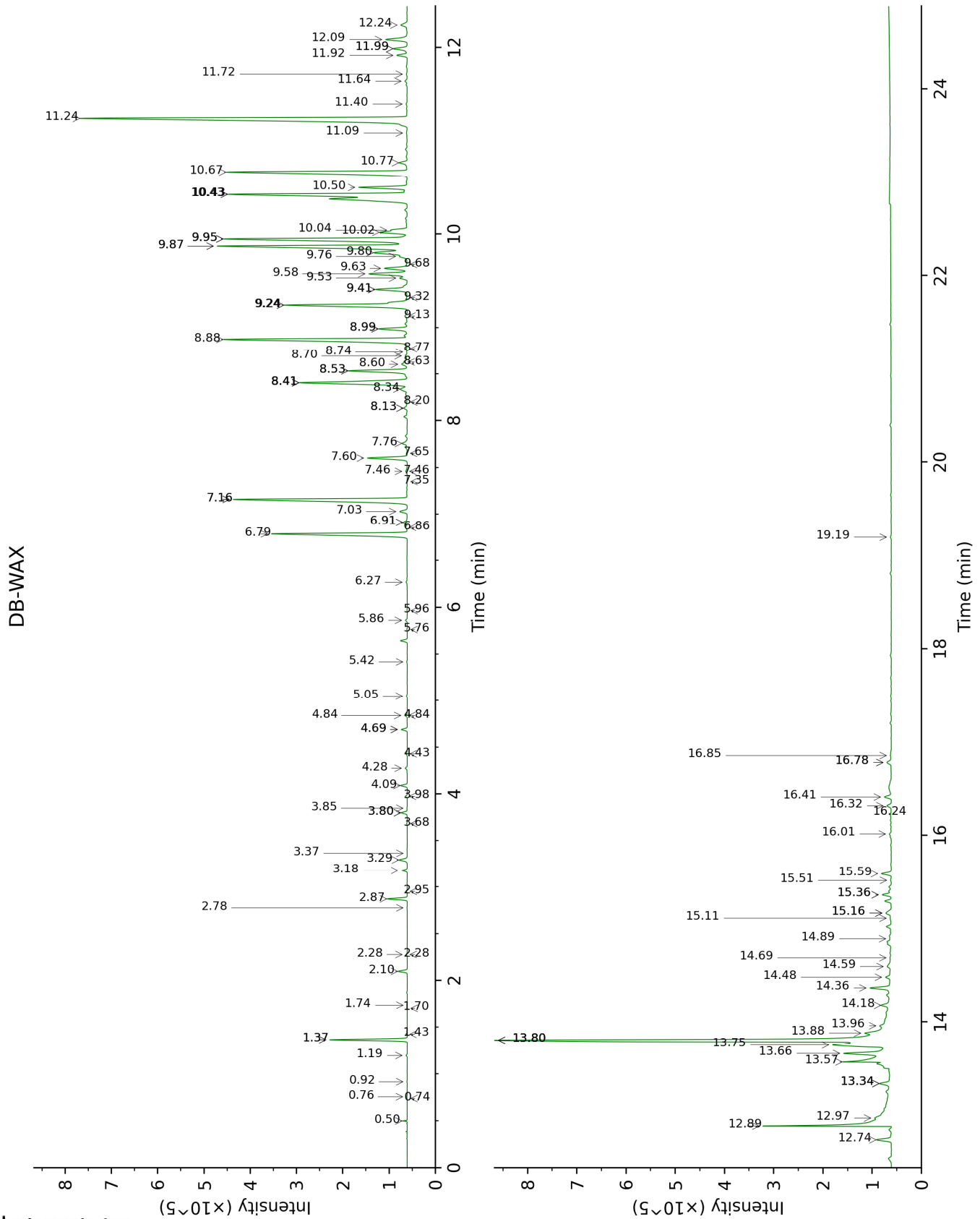
Note: no correction factor was applied

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	0.55	641	tr	0.76	884	0.01
2-Methylbutyral	0.57	651	tr	0.74	878	tr
2-Ethylfuran	0.69	698	0.01	0.92	917	tr
2,4-Dimethyl-3-pentanone	1.27	792	0.02	1.19	962	0.02
Octane	1.34	802	0.04	0.50	785	0.03
Ethylbenzene	1.94	856	0.01	2.28*	1082	0.02
(3Z)-Hexenol	1.97	859	0.01	5.76	1344	0.01
Styrene	2.30	887	tr	3.85	1208	0.01
Hashishene	2.66	915	0.01	1.37*	989	1.38
α-Thujene	2.81	925	0.02	1.43	998	0.03
α-Pinene	2.88	930	1.33	1.37*	989	[1.38]
α-Fenchene	3.06*	943	0.01	1.70	1025	tr
Camphene	3.06*	943	[0.01]	1.74	1028	tr
Sabinene	3.48*	971	0.19	2.28*	1082	[0.02]
β-Pinene	3.48*	971	[0.19]	2.10	1064	0.18
6-Methyl-5-hepten-2-one	3.74	989	0.02	5.05	1298	0.02
2-Pentylfuran	3.80*	993	0.39	3.68	1196	0.02
Myrcene	3.80*	993	[0.39]	2.87	1132	0.38
α-Phellandrene	3.93	1002	0.01	2.78	1124	tr
Octanal	3.97	1004	0.01	4.43	1251	0.03
(3Z)-Hexenyl acetate	4.01	1007	0.01	4.84*	1282	0.05
α-Terpinene	4.12	1014	0.02	2.95	1138	0.02
Isoamyl isobutyrate	4.16	1016	0.01	3.37	1171	tr
para-Cymene	4.24	1022	0.13	4.09	1226	0.13
Limonene	4.31†	1026	0.29	3.18	1156	0.11
1,8-Cineole	4.33†	1027	[0.29]	3.29	1165	0.20
(Z)-β-Ocimene	4.53	1040	tr	3.80*	1205	0.13
(E)-β-Ocimene	4.69	1050	0.04	3.98	1218	0.04
γ-Terpinene	4.80	1057	0.12	3.80*	1205	[0.13]
Unknown [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	4.99	1069	0.01	4.84*	1282	[0.05]
Octanol	5.11	1076	0.01	8.20	1525	0.02
Terpinolene	5.25	1085	0.05	4.28	1240	0.04
Linalool	5.53	1103	0.09	8.13*	1520	0.11
Nonanal	5.57	1106	0.04	5.86	1352	0.03
Isoamyl isovalerate	5.62	1109	0.09	4.69*	1271	0.12
Amyl isovalerate	5.66	1111	0.04	4.69*	1271	[0.12]
3-Methyl-3-butenyl 2-methylbutyrate	5.73	1116	0.02	5.42	1320	0.01
trans-Pinocarveol	5.99	1133	0.01	9.24*	1606	3.77
Prenyl 2-methylbutyrate	6.17	1144	0.01	5.96	1359	0.01
Prenyl isovalerate	6.29	1152	0.03	6.27	1381	0.02

Dimethyloctanedione isomer	6.41	1160	0.03	6.86	1424	0.05
2,7-Dimethyl-3,5-octanedione	6.46	1163	0.06	6.91*	1428	0.11
Terpinen-4-ol	6.64	1174	0.05	8.63	1558	0.07
α-Terpineol	6.87	1190	0.05	9.80	1652	1.12
2-Methylbutyl tiglate	6.98	1196	0.10	6.91*	1428	[0.11]
3-Methyl-3-butenyl tiglate	7.11	1205	0.04			
Benzylacetone	7.62	1239	0.01	11.40	1785	0.03
Prenyl tiglate	7.75	1248	0.05	8.77	1570	0.03
Geraniol	7.92	1259	0.02	11.64	1806	0.05
(2E)-Decenal	7.97	1263	0.05	9.13	1597	0.07
Undec-(5Z)-en-2-one	8.20	1278	0.05	8.99*	1586	0.70
α-Cubebene	9.20	1347	3.55	6.79	1419	3.64
Longicyclene	9.38	1360	0.02	7.16*	1447	5.24
α-Ylangene	9.46	1366	0.25	7.03	1437	0.20
α-Copaene	9.55	1372	5.04	7.16*	1447	[5.24]
Modhephene	9.57	1374	0.02	7.46*	1469	0.05
Methyl (E)-cinnamate	9.61	1376	0.02	13.80*†	2002	[18.08]
α-Isocomene	9.64	1378	0.03	7.65	1483	0.02
β-Bourbonene	9.66	1380	0.04	7.46*	1469	[0.05]
1,5-diepi-β-Bourbonene	9.68	1381	0.06	7.35	1461	0.01
Benzyl 2-methylbutyrate?	9.74	1386	0.18	11.72	1813	0.02
β-Cubebene	9.78*	1389	0.89	7.76	1491	0.15
β-Elemene	9.78*	1389	[0.89]	8.41*	1541	3.56
Benzyl isovalerate	9.84	1393	0.26	11.92	1831	0.25
α-Gurjunene	9.98	1403	0.96	7.60	1479	0.98
Unknown [m/z 119, 107 (86), 105 (85), 93 (78), 189 (66), 81 (65), 121 (64)... 204 (23)]	10.06	1409	0.02			
β-Caryophyllene	10.11*	1412	2.56	8.41*	1541	[3.56]
β-Ylangene	10.11*	1412	[2.56]	8.13*	1520	[0.11]
γ-Maaliene	10.22	1420	0.05	8.53*	1551	1.59
β-Gurjunene	10.25*	1422	0.24	8.34	1536	0.25
β-Copaene	10.25*	1422	[0.24]	8.41*	1541	[3.56]
α-Maaliene	10.30	1426	0.07	8.70	1564	0.06
Aromadendrene	10.37	1432	1.44	8.53*	1551	[1.59]
trans-α-Bergamotene	10.40*	1434	0.23	8.41*	1541	[3.56]
α-Guaiene	10.40*	1434	[0.23]	8.41*	1541	[3.56]
Selina-5,11-diene	10.40*	1434	[0.23]	8.74	1567	0.01
6,9-Guaiadiene	10.46	1439	0.12	8.60	1556	0.18
trans-Muurola-3,5-diene	10.55	1445	5.50	8.88	1578	5.44
α-Humulene	10.57	1447	0.33	9.32	1613	0.02
allo-Aromadendrene	10.66	1453	0.66	8.99*	1586	[0.70]
4,5-diepi-Aristolochene	10.78	1462	0.09	9.41*	1620	0.92

<i>trans</i> -Cadina-1(6),4-diene	10.87†	1469	4.94	9.24*	1606	[3.77]
Selina-4,11-diene	10.92*†	1473	[4.94]	9.41*	1620	[0.92]
γ-Muurolene	10.92*†	1473	[4.94]	9.58	1634	1.06
α-Amorphene	10.96*†	1476	5.82	9.64	1638	0.61
Germacrene D	10.96*†	1476	[5.82]	9.76	1649	0.16
allo-Aromadendr-9-ene	11.02*†	1480	[5.82]	9.53	1630	0.18
β-Selinene	11.02*†	1480	[5.82]	9.87*	1658	5.60
<i>trans</i> -Muurola-4(15),5-diene	11.08	1485	1.08	9.87*	1658	[5.60]
Viridiflorene	11.15*	1490	6.16	9.68	1642	0.01
epi-Cubebol	11.15*	1490	[6.16]	11.99*†	1837	1.00
α-Selinene	11.15*	1490	[6.16]	9.95*	1664	5.55
Bicyclogermacrene	11.15*	1490	[6.16]	10.04	1671	0.31
α-Muurolene	11.23†	1496	1.27	10.02	1670	0.73
δ-Amorphene	11.25†	1498	[1.27]	9.95*	1664	[5.55]
δ-Guaiene	11.31	1502	0.12	9.95*	1664	[5.55]
(3E,6E)-α-Farnesene	11.39*†	1508	2.00	10.50	1709	1.14
γ-Cadinene	11.39*†	1508	[2.00]	10.43*	1703	5.07
δ-Cadinene	11.57*†	1522	22.10	10.43*	1703	[5.07]
<i>cis</i> -Calamenene	11.57*†	1522	[22.10]	11.24	1772	11.09
<i>trans</i> -Cadina-1,4-diene	11.66†	1530	[22.10]	10.67	1723	5.33
α-Cadinene	11.71	1533	0.08	10.77	1732	0.22
Unknown [m/z 157, 143 (86), 200 (43), 142 (36), 141 (28), 128 (25)]	11.73	1535	0.40	11.99*†	1837	[1.00]
α-Calacorene	11.76	1537	0.46	12.09†	1846	[1.00]
Flavesone	11.85	1544	5.12	12.89†	1918	4.79
Germacrene B	11.90	1548	0.02	11.09	1759	0.02
Unknown [m/z 161, 109 (98), 82 (93), 43 (72), 105 (68), 93 (59), 69 (56), 119 (55)... 222 (7)]	12.01	1557	0.06	13.34*†	1959	[4.79]
Palustrol	12.07	1562	0.19	12.24	1859	0.20
(E)-Nerolidol	12.11	1565	0.10	13.80*†	2002	[18.08]
Spathulenol	12.20	1572	0.43	14.36	2056	0.47
Caryophyllene oxide	12.23	1574	0.41	12.74	1904	0.38
Globulol	12.27*	1578	0.25	13.88†	2010	[18.08]
Gleenol	12.27*	1578	[0.25]	13.57†	1980	[18.08]
Unknown [m/z 161, 159 (64), 43 (58), 182 (53), 41 (48), 105 (40)... 252 (25)]	12.32	1582	0.18			
Viridiflorol	12.36	1585	0.09	13.96†	2018	[18.08]
Cubeban-11-ol	12.40	1587	0.08	13.75†	1998	[18.08]
Ledol	12.49	1595	0.23	13.34*†	1959	[4.79]
Humulene epoxide II	12.56	1600	0.07	13.34*†	1959	[4.79]

Unknown [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	12.63*	1606	0.19	14.48	2068	0.10
Unknown [m/z 151, 41 (15), 81 (13), 111 (13), 91 (13)...]	12.63*	1606	[0.19]	14.18†	2039	18.08
Unknown [m/z 179, 161 (66), 119 (44), 95 (38), 105 (35)... 204 (24), 222 (1)]	12.69	1611	0.06	14.59	2078	0.12
Isoleptospermone	12.78	1618	4.01	12.97†	1926	[4.79]
Unknown [m/z 161, 43 (74), 105 (57), 121 (45), 81 (43)... 204 (31)...]	12.83*	1623	0.63	14.68	2088	0.01
1-epi-Cubenol	12.83*	1623	[0.63]	13.80*†	2002	[18.08]
Leptospermone	12.92	1630	12.82	13.80*†	2002	[18.08]
τ-Cadinol	12.97	1634	0.18	14.89	2108	0.02
τ-Muurolol	13.02*	1638	1.04	15.11	2130	0.02
Jinkoh-eremol	13.02*	1638	[1.04]	15.16*	2135	0.20
Cubenol	13.02*	1638	[1.04]	13.66†	1989	[18.08]
α-Muurolol	13.02*	1638	[1.04]	15.16*	2135	[0.20]
β-Eudesmol	13.09	1644	0.27	15.36*†	2155	0.37
α-Cadinol	13.14*	1648	0.46	15.51	2170	0.02
Selin-11-en-4α-ol	13.14*	1648	[0.46]	15.58	2177	0.24
α-Eudesmol	13.14*	1648	[0.46]	15.36*†	2155	[0.37]
cis-Calamenen-10-ol	13.20	1653	0.07	16.41	2262	0.16
trans-Calamenen-10-ol	13.24	1656	0.01	16.78*	2301	0.12
Unknown [m/z 159, 177 (59), 135 (57), 91 (47), 105 (47)... 220? (25)]	13.32	1663	0.02			
Unknown [m/z 175, 91 (94), 105 (51), 218 (33), 104 (17), 176 (12)...]	13.37*	1667	0.18	16.24	2244	0.01
Unknown [m/z 159, 118 (33), 91 (30), 131 (30)... 220? (4)]	13.37*	1667	[0.18]	16.32	2253	0.12
Unknown [m/z 107, 91 (95), 93 (87), 79 (86), 105 (78), 41 (76), 95 (72)... 220 (18)]	13.43	1672	0.29	16.78*	2301	[0.12]
Unknown [m/z 133, 93 (97), 131 (85), 145 (83), 107 (69)...220]	13.79	1702	0.02	16.85	2309	0.01
trans-14-nor-Cadina-5-en-4-one	13.95	1716	0.18	16.01	2221	0.04
14-Hydroxy-trans-calamenene	14.96*	1804	0.03	19.19	2570	0.02

5-Hydroxy- <i>cis</i> -calamenene?	14.96*	1804	[0.03]	
Grandiflorone	18.64	2158	0.40	
Total identified		97.72%		94.97%
Total reported		98.78%		95.34%

*: 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