

Date : May 20, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20118-PTH11


Customer identification : Lemongrass - India - L80109201R

Type : Essential oil

Source : *Cymbopogon flexuosus*

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 : Fanny Charlier, B. Sc., chimiste à l'entraînement

Analysis date : September 21, 2020

Checked and approved by :

Sylvain Mercier, M. Sc., chimiste 2014-005

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia. This report is digitally signed, it is only considered valid if the digital signature is intact. The results only describe the samples that were submitted to the assays.

This report is an update of the version first issued on September 21, 2020 to correct a mistake in the lot number.

PHYSICOCHEMICAL DATA

Physical aspect: Light yellow liquid

Refractive index: 1.4855 ± 0.0003 (20 °C; method PC-MAT-016)

ISO 4718:2004 - OIL OF LEMONGRASS

Compound	Min. %	Max. %	Observed %	Complies?
Geraniol	1.5	8.0	5.8	Yes
Geranyl acetate	0.5	6.0	2.4	Yes
Geranial	35.0	47.0	42.2	Yes
Neral	25.0	35.0	31.5	Yes
β-Caryophyllene	0.2	3.5	1.2	Yes
6-Methyl-5-hepten-2-one	0.1	2.0	0.8	Yes
Limonene	0.5	3.5	0.2	No
Refractive index	1.4830	1.4890	1.4855	Yes

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
Isobutyral	tr	Aliphatic aldehyde
Methacrolein	tr	Aliphatic aldehyde
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Hexanal	0.01	Aliphatic aldehyde
(3Z)-Hexenol	0.01	Aliphatic alcohol
4-Heptanone	0.02	Aliphatic ketone
Tricyclene	0.13	Monoterpene
α -Pinene	0.18	Monoterpene
Camphene	1.03	Monoterpene
β -Pinene	0.01	Monoterpene
Sabinene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	0.82	Aliphatic ketone
Myrcene	0.07	Monoterpene
6-Methyl-5-hepten-2-ol	0.07	Aliphatic alcohol
α -Phellandrene	0.01	Monoterpene
Octanal	0.08	Aliphatic aldehyde
Δ^3 -Carene	0.01	Monoterpene
α -Terpinene	0.01	Monoterpene
para-Cymene	0.01	Monoterpene
Limonene	0.24	Monoterpene
1,8-Cineole	tr	Monoterpenic ether
β -Phellandrene	0.03	Monoterpene
(Z)- β -Ocimene	0.31	Monoterpene
(E)- β -Ocimene	0.19	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.02	Aliphatic aldehyde
γ -Terpinene	0.01	Monoterpene
cis-Linalool oxide (fur.)	0.01	Monoterpenic alcohol
4-Nonanone	1.04	Aliphatic ketone
Camphenilone	0.01	Normonoterpenic ketone
Terpinolene	0.04	Monoterpene
trans-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
4-Nonanol	0.02	Aliphatic alcohol
Perillene	0.05	Monoterpenic ether
Rosefuran	0.13	Monoterpenic ether
Linalool	0.93	Monoterpenic alcohol
cis-Chrysanthamal?	0.03	Monoterpenic aldehyde
(Z)-6-Methyl-3,5-heptadien-2-one	0.01	Aliphatic ketone
trans-para-Mentha-2,8-dien-1-ol	0.03	Monoterpenic alcohol
Unknown	0.12	Unknown
Unknown	0.02	Unknown
trans-Chrysanthamal	0.27	Monoterpenic aldehyde
exo-Isocitral	0.15	Monoterpenic aldehyde

Citronellal	0.21	Monoterpenic aldehyde
Isoneral	0.11	Monoterpenic aldehyde
α -Phellandren-8-ol	0.99	Monoterpenic alcohol
Borneol	0.02	Monoterpenic alcohol
Rosefuran oxide	0.13	Monoterpenic ether
Terpinen-4-ol	0.01	Monoterpenic alcohol
Unknown	0.05	Oxygenated monoterpene
Isogeranial	1.49	Monoterpenic aldehyde
Unknown	0.04	Unknown
α -Terpineol	0.15	Monoterpenic alcohol
Myrtenal	0.02	Monoterpenic aldehyde
Unknown	0.06	Unknown
Myrtenol	tr	Monoterpenic alcohol
<i>trans</i> -Isopiperitenol	0.02	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
Decanal	0.15	Aliphatic aldehyde
<i>cis</i> -Isopiperitenol	0.05	Monoterpenic alcohol
2,3-Epoxyneral?	0.05	Monoterpenic aldehyde
Nerol	0.03	Monoterpenic alcohol
Citronellol	0.09	Monoterpenic alcohol
Neral	31.46	Monoterpenic aldehyde
Piperitone	0.06	Monoterpenic ketone
Geraniol	5.83	Monoterpenic alcohol
Geranial	42.15	Monoterpenic aldehyde
Unknown	0.12	Oxygenated monoterpene
Bornyl acetate	0.02	Monoterpenic ester
Isobornyl acetate	0.02	Monoterpenic ester
Geranyl formate	0.05	Monoterpenic ester
Unknown	0.03	Unknown
Neric acid	0.07	Monoterpenic acid
α -Cubebene	0.01	Sesquiterpene
Citronellyl acetate	0.14	Monoterpenic ester
Cyclosativene II	0.08	Sesquiterpene
Geranic acid	0.07	Aliphatic acid
α -Copaene	0.05	Sesquiterpene
β -Bourbonene	0.01	Sesquiterpene
1,5-diepi- β -Bourbonene	0.01	Sesquiterpene
Geranyl acetate	2.39	Monoterpenic ester
β -Cubebene	0.07	Sesquiterpene
β -Elemene	0.11	Sesquiterpene
β -Longipinene	0.03	Sesquiterpene
β -Caryophyllene	1.21	Sesquiterpene
β -Copaene	0.02	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.02	Sesquiterpene
α -Humulene	0.14	Sesquiterpene
(<i>E</i>)-Isoeugenol	0.26	Phenylpropanoid
<i>cis</i> -Muurolo-4(15),5-diene	0.05	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.04	Sesquiterpene
Germacrene D	0.20	Sesquiterpene
γ -Amorphene	0.03	Sesquiterpene
epi-Cubebol	0.09	Sesquiterpenic alcohol
α -Muurolole	0.08	Sesquiterpene

γ-Cadinene	1.06	Sesquiterpene
Cubebol	0.22	Sesquiterpenic alcohol
δ-Cadinene	0.25	Sesquiterpene
10-epi-Cubebol?	0.02	Sesquiterpenic alcohol
(E)-γ-Bisabolene	0.09	Sesquiterpene
Neryl butyrate	0.05	Monoterpenic ester
(E)-α-Bisabolene	0.02	Sesquiterpene
α-Elemol	0.04	Sesquiterpenic alcohol
Germacrene B	0.03	Sesquiterpene
Geranyl butyrate	0.11	Monoterpenic ester
Caryophyllene oxide	0.36	Sesquiterpenic ether
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Humulene epoxide II	0.04	Sesquiterpenic ether
Selin-6-en-4α-ol isomer	0.03	Sesquiterpenic alcohol
1-epi-Cubebol	0.03	Sesquiterpenic alcohol
Cubebol	0.03	Sesquiterpenic alcohol
β-Eudesmol	0.01	Sesquiterpenic alcohol
α-Eudesmol	0.01	Sesquiterpenic alcohol
Farnesal isomer	0.01	Sesquiterpenic aldehyde
(2E,6E)-Farnesal	0.01	Sesquiterpenic aldehyde
Neophytadiene	0.04	Diterpene
Phytone	0.02	Terpenic ketone
meta-Camphorene	0.02	Diterpene
Unknown	0.01	Unknown
Unknown	0.05	Unknown
Dicitral	0.05	Diterpenic aldehyde
Phytol	0.05	Diterpenic alcohol
Unknown	0.01	Unknown
Phytol isomer	0.05	Diterpenic alcohol
Unknown	0.03	Unknown
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Unknown	0.02	Unknown
Consolidated total	97.66%	

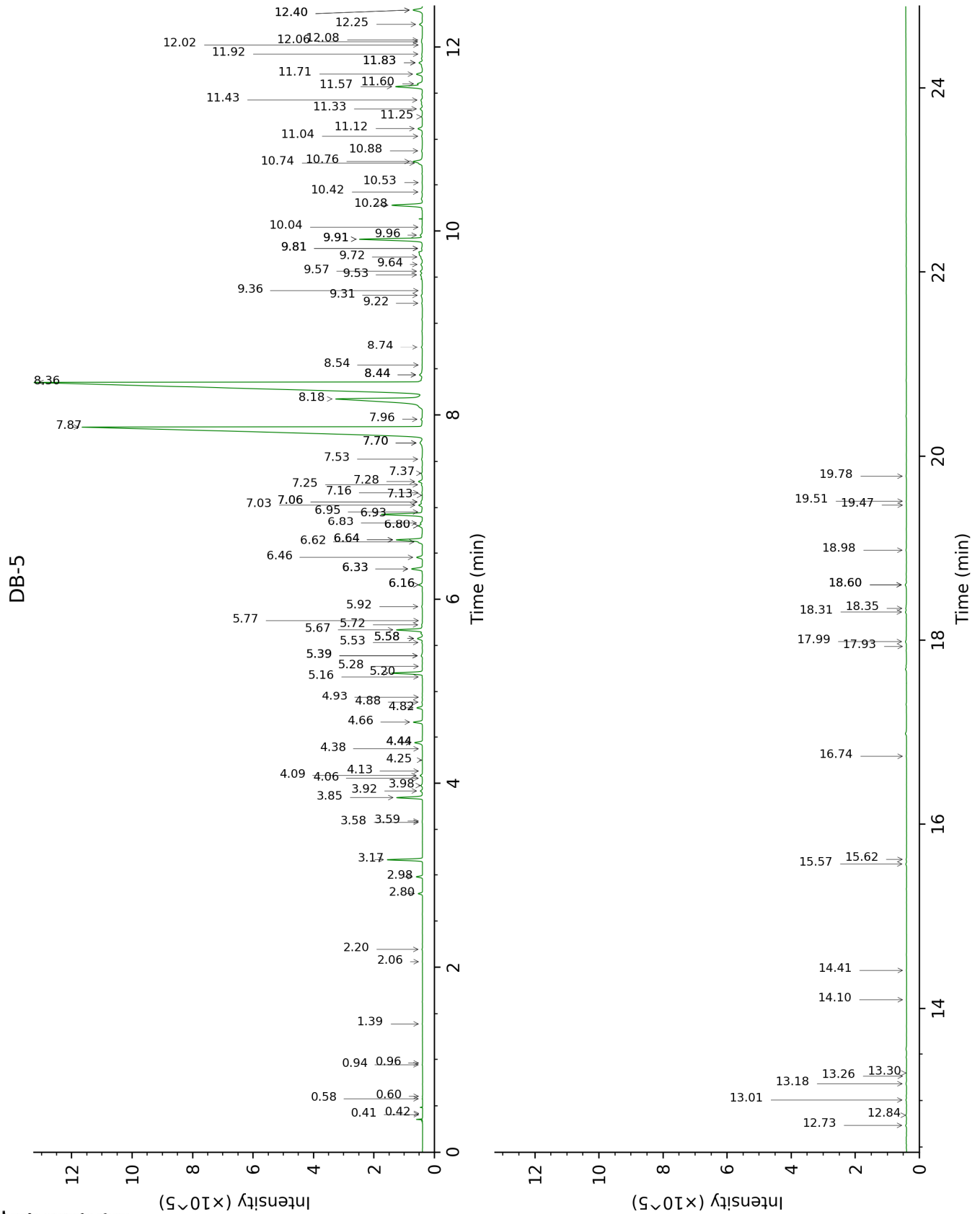
tr: The compound has been detected below 0.005% of total signal.

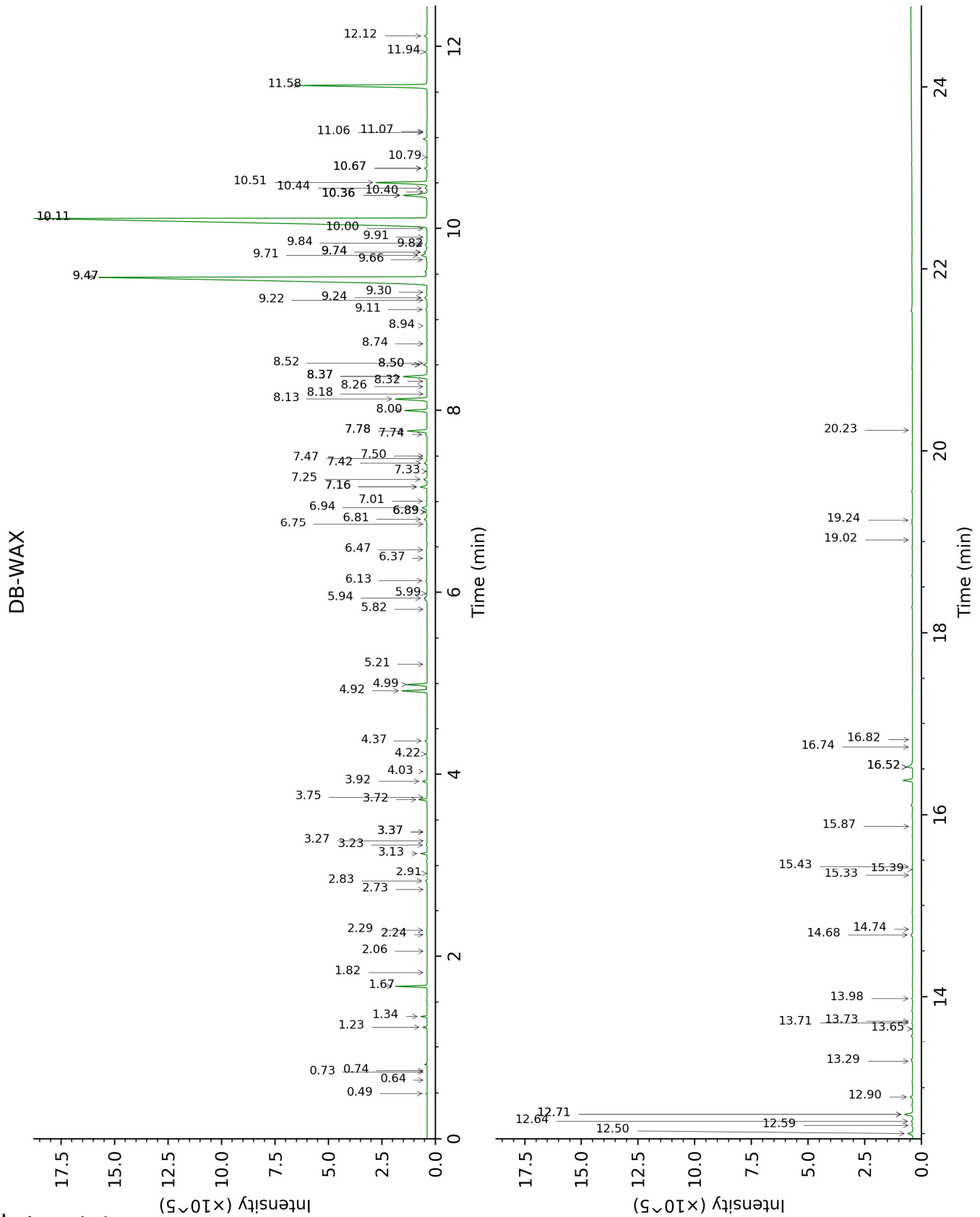
Note: no correction factor was applied

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	%
Isobutylal	0.41	533	tr	0.49	778	0.02
Methacrolein	0.42	545	tr	0.64	843	0.01
Isovaleral	0.58	639	tr	0.74	881	tr
2-Methylbutylal	0.60	650	tr	0.73	875	tr
Isoamyl alcohol	0.94	733	0.01	3.37*	1173	0.01
2-Methylbutanol	0.96	736	tr	3.37*	1173	[0.01]
Hexanal	1.39	800	0.01	1.82	1040	0.01
(3Z)-Hexenol	2.06	859	0.01	5.82	1349	0.01
4-Heptanone	2.20	870	0.02	2.29	1086	0.02
Tricyclene	2.80	917	0.13	1.22	970	0.12
α-Pinene	2.98	930	0.18	1.34	989	0.17
Camphene	3.18	942	1.03	1.67	1025	1.02
β-Pinene	3.58†	969	0.02	2.06	1064	0.01
Sabinene	3.59†	970	[0.02]	2.24	1081	0.01
6-Methyl-5-hepten-2-one	3.85	987	0.82	4.99	1292	0.81
Myrcene	3.92	992	0.07	2.83	1131	0.06
6-Methyl-5-hepten-2-ol	3.98	996	0.07	6.89*	1428	0.07
α-Phellandrene	4.06	1001	0.01	2.73	1123	0.01
Octanal	4.09	1003	0.08	4.37	1247	0.08
Δ ³ -Carene	4.13	1006	0.01			
α-Terpinene	4.25	1014	0.01	2.91	1137	0.01
para-Cymene	4.38	1021	0.01	4.03	1223	0.01
Limonene	4.44*	1025	0.28	3.13	1155	0.24
1,8-Cineole	4.44*	1025	[0.28]	3.27	1166	tr
β-Phellandrene	4.44*	1025	[0.28]	3.23	1162	0.03
(Z)-β-Ocimene	4.66	1039	0.31	3.72	1200	0.29
(E)-β-Ocimene	4.82	1049	0.19	3.92	1215	0.18
2,6-Dimethyl-5-heptenal (melonal)	4.88	1053	0.02	5.21	1306	0.02
γ-Terpinene	4.93	1056	0.01	3.75	1202	0.01
cis-Linalool oxide (fur.)	5.16	1070	0.01	6.47	1396	0.01
4-Nonanone	5.20	1073	1.04	4.92	1287	1.06
Camphenilone	5.28	1078	0.01	6.37	1390	0.01
Terpinolene	5.39*	1085	0.06	4.22	1236	0.04
trans-Linalool oxide (fur.)	5.39*	1085	[0.06]	6.89*	1428	[0.07]
4-Nonanol	5.53	1094	0.02			
Perillene	5.58*	1096	0.22	6.13	1372	0.05
Rosefuran	5.58*	1096	[0.22]	5.94	1358	0.13
Linalool	5.67	1102	0.93	8.00	1511	0.91
cis-Chrysanthemal?	5.72	1106	0.03	5.99	1362	0.02
(Z)-6-Methyl-	5.77	1109	0.01	8.18	1526	0.02

3,5-heptadien-2-one						
<i>trans</i> -para-Mentha-2,8-dien-1-ol	5.92	1118	0.03	8.94	1584	0.02
Unknown [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	6.16*†	1133	0.16	6.81	1422	0.12
Unknown [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	6.16*†	1133	[0.16]	7.47	1472	0.02
<i>trans</i> -Chrysanthemal	6.33*	1144	0.42	7.16*	1448	0.32
exo-Isocitral	6.33*	1144	[0.42]	7.42	1468	0.15
Citronellal	6.46	1152	0.21	6.94	1431	0.27
Isoneral	6.62	1163	0.11	7.78*	1494	0.88
α-Phellandren-8-ol	6.64*	1164	1.01	10.11*	1679	41.85
Borneol	6.64*	1164	[1.01]	9.74*	1649	0.17
Rosefuran oxide	6.80*†	1174	0.26	8.50*	1550	0.16
Terpinen-4-ol	6.80*†	1174	[0.26]	8.52	1552	0.01
Unknown [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	6.83†	1176	[0.26]	9.66	1642	0.05
Isogeranial	6.93	1182	1.49	8.13	1521	1.50
Unknown [m/z 69, 41 (65), 109 (36), 67 (16), 84 (11), 43 (10), 55 (9)...]	6.95	1184	0.04			
α-Terpineol	7.03	1189	0.15	9.74*	1649	[0.17]
Myrtenal	7.06*	1191	0.07	8.74	1569	0.02
Unknown [m/z 43, 81 (47), 67 (45), 69 944), 41 (42), 59 (40), 55 (39)...]	7.06*	1191	[0.07]	9.11	1598	0.06
Myrtenol	7.13	1196	tr	10.79	1736	tr
<i>trans</i> -Isopiperitenol	7.16	1197	0.02	10.40	1703	0.01
Unknown [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]	7.25	1203	0.03			

Decanal	7.28	1205	0.15	7.25	1454	0.14
<i>cis</i> -Isopiperitenol	7.37	1211	0.05	10.36*	1700	1.36
2,3-Epoxyneral?	7.52	1221	0.05			
Nerol	7.70*	1233	0.18	11.06	1759	0.03
Citronellol	7.70*	1233	[0.18]	10.67*	1725	0.11
Neral	7.87	1244	31.46	9.47*	1627	31.20
Piperitone	7.96	1250	0.06	9.82	1656	0.09
Geraniol	8.18	1265	5.83	11.58	1803	6.29
Geranial	8.36	1277	42.15	10.11*	1679	[41.85]
Unknown [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	8.44*	1282	0.19	12.90	1921	0.12
Bornyl acetate	8.44*	1282	[0.19]	8.26	1532	0.02
Isobornyl acetate	8.54	1289	0.02	8.32	1536	0.02
Geranyl formate	8.74	1302	0.05	9.91	1662	0.02
Unknown [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	9.22	1335	0.03	12.71*	1904	0.39
Neric acid	9.31	1341	0.07	16.52*	2275	0.34
α -Cubebene	9.36	1345	0.01	6.75	1417	0.01
Citronellyl acetate	9.53	1357	0.14	9.47*	1627	[31.20]
Cyclosativene II	9.57	1360	0.08	7.01	1437	0.04
Geranic acid	9.64	1365	0.07	16.82	2307	0.01
α -Copaene	9.72	1370	0.05	7.16*	1448	[0.32]
β -Bourbonene	9.81*	1377	0.04	7.50	1474	0.01
1,5-diepi- β -Bourbonene	9.81*	1377	[0.04]	7.33	1461	0.01
Geranyl acetate	9.91*	1384	2.42	10.50	1712	2.39
β -Cubebene	9.91*	1384	[2.42]	7.74	1491	0.07
β -Elemene	9.96	1387	0.11	8.37*	1540	1.23
β -Longipinene	10.04	1393	0.03	7.78*	1494	[0.88]
β -Caryophyllene	10.28	1410	1.21	8.37*	1540	[1.23]
β -Copaene	10.42	1421	0.02	8.37*	1540	[1.23]
<i>trans</i> - α -Bergamotene	10.53	1429	0.02	8.50*	1550	[0.16]
α -Humulene	10.74†	1445	0.53	9.24	1608	0.14
(<i>E</i>)-Isoeugenol	10.76†	1446	[0.53]	16.52*	2275	[0.34]
<i>cis</i> -Muurola-4(15),5-diene	10.88	1455	0.05	9.30	1613	0.04
<i>trans</i> -Cadina-1(6),4-diene	11.04	1467	0.04	9.22	1606	0.02
Germacrene D	11.12	1473	0.20	9.71	1646	0.33
γ -Amorphene	11.25	1482	0.03	9.84	1657	0.03
epi-Cubebol	11.33	1489	0.09	11.94	1835	0.09
α -Muurolene	11.43	1496	0.08	10.00	1670	0.02

γ-Cadinene	11.57†	1507	1.28	10.36*	1700	[1.36]
Cubebol	11.60†	1509	[1.28]	12.50	1885	0.22
δ-Cadinene	11.71	1518	0.25	10.36*	1700	[1.36]
10-epi-Cubebol?	11.83*	1527	0.19	13.73	1998	0.02
(E)-γ-Bisabolene	11.83*	1527	[0.19]	10.44	1706	0.09
Neryl butyrate	11.92	1535	0.05			
(E)-α-Bisabolene	12.02	1542	0.02	10.67*	1725	[0.11]
α-Elemol	12.06	1545	0.04	13.98	2022	0.04
Germacrene B	12.08	1547	0.03	11.07	1760	0.02
Geranyl butyrate	12.25	1560	0.11	12.12	1851	0.13
Caryophyllene oxide	12.40*	1572	0.43	12.71*	1904	[0.39]
Caryophyllene oxide isomer	12.40*	1572	[0.43]	12.64	1896	0.06
Humulene epoxide II	12.73	1598	0.04	13.29	1957	0.02
Selin-6-en-4α-ol isomer	12.84	1607	0.03	14.74	2094	0.01
1-epi-Cubebol	13.01	1621	0.03	13.71	1996	0.04
Cubebol	13.18	1635	0.03	13.65	1990	0.02
β-Eudesmol	13.26	1642	0.01	15.43	2164	0.02
α-Eudesmol	13.30	1645	0.01	15.33	2153	0.03
Farnesal isomer	14.10	1711	0.01			
(2E,6E)-Farnesal	14.41	1739	0.01	15.87	2208	0.01
Neophytadiene	15.57	1842	0.04	12.59	1892	0.04
Phytone	15.62	1846	0.02	14.68	2088	0.11
meta-Camphorene	16.74	1950	0.02	15.39	2160	0.01
Unknown [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53), 109 (50)... 235 (10)...]	17.93	2068	0.01			
Unknown [m/z 57, 85 (55), 163 (47), 41 (44), 120 (35), 202 (30), 145 (25)... 219 (17), 304 (t)]	17.99	2073	0.05	19.02	2550	0.02
Dicitral	18.31	2105	0.05	16.74	2298	0.02
Phytol	18.35	2109	0.05	19.24	2575	0.03
Unknown [m/z 69, 41 (38), 151 (36), 123 (34), 82 (24), 43 (23), 109 (21)...]	18.60*	2136	0.06	20.23	2692	0.01
Phytol isomer	18.60*	2136	[0.06]			
Unknown [m/z 94, 43 (85), 93	18.98	2175	0.03			

(81), 69 (76), 137 (76), 95 (60), 134 (51)...				
Unknown [m/z 94, 43 (56), 123 (55), 69 (53), 95 (42), 79 (39)...	19.47	2228	0.01	
Unknown [m/z 93, 69 (79), 43 (70), 137 (53), 41 (41), 119 (37)... 289 (33)...	19.51	2233	0.01	
Unknown [m/z 123, 94 (100), 43 (86), 69 (75), 95 (47), 41 (47), 93 (45)...	19.78	2262	0.02	
Total identified		97.88%		96.22%
Total reported		98.11%		96.62%

*: 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