

Date : February 26, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22B21-PTH04


Customer identification : Lemongrass - India - L80113206R

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 : Sylvain Mercier, M. Sc., Chimiste 2014-005

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: Yellow Liquid

Refractive index: 1.4868 ± 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-Methyl-3-buten-2-ol	0.03	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
(3Z)-Hexenol	0.01	Aliphatic alcohol
4-Heptanone	0.01	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	0.98	Aliphatic ketone
Myrcene	0.08	Monoterpene
6-Methyl-5-hepten-2-ol	0.06	Aliphatic alcohol
α-Phellandrene	0.01	Monoterpene
Octanal	0.07	Aliphatic aldehyde
α-Terpinene	tr	Monoterpene
para-Cymene	0.01	Monoterpene
Limonene	0.23	Monoterpene
1,8-Cineole	0.04	Monoterpenic ether
(Z)-β-Ocimene	0.33	Monoterpene
(E)-β-Ocimene	0.20	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.02	Aliphatic aldehyde
γ-Terpinene	0.01	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
4-Nonanone	0.78	Aliphatic ketone
Camphenilone	0.01	Normonoterpenic ketone
trans-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Terpinolene	0.05	Monoterpene
4-Nonanol	0.02	Aliphatic alcohol
Rosefuran	0.19	Monoterpenic ether
Linalool	0.88	Monoterpenic alcohol
cis-Chrysanthemal?	0.02	Monoterpenic aldehyde
(Z)-6-Methyl-3,5-heptadien-2-one	0.03	Aliphatic ketone
trans-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
Unknown	0.01	Unknown
Unknown	0.12	Unknown
Unknown	0.01	Unknown
trans-Chrysanthemal	0.27	Monoterpenic aldehyde
exo-Isocitral	0.04	Monoterpenic aldehyde
trans-Chrysanthemol	0.02	Monoterpenic alcohol
Citronellal	0.17	Monoterpenic aldehyde
Borneol	0.19	Monoterpenic alcohol

Isoneral	0.51	Monoterpenic aldehyde
α -Phellandren-8-ol	0.01	Monoterpenic alcohol
Unknown	0.05	Oxygenated monoterpene
Terpinen-4-ol	0.21*	Monoterpenic alcohol
Rosefuran oxide	0.21*	Monoterpenic ether
Isogeranial	0.72	Monoterpenic aldehyde
Unknown	0.02	Unknown
α -Terpineol	0.14	Monoterpenic alcohol
Myrtenal	0.02	Monoterpenic aldehyde
Unknown	0.05	Unknown
(4Z)-Decenal	0.01	Aliphatic aldehyde
<i>trans</i> -Isopiperitenol	0.03	Monoterpenic alcohol
Unknown	0.04	Oxygenated monoterpene
Decanal	0.14	Aliphatic aldehyde
<i>cis</i> -Isopiperitenol	0.03	Monoterpenic alcohol
2,3-Epoxyneral?	0.03	Monoterpenic aldehyde
Nerol	0.02	Monoterpenic alcohol
Citronellol	0.11	Monoterpenic alcohol
Neral	31.26	Monoterpenic aldehyde
(Z)-Isogeraniol	0.02	Monoterpenic alcohol
Piperitone	0.10	Monoterpenic ketone
Geraniol	5.49	Monoterpenic alcohol
Geranial	41.40	Monoterpenic aldehyde
Unknown	0.18	Oxygenated monoterpene
Geranyl formate	0.02	Monoterpenic ester
Methyl geranate	0.01	Monoterpenic ester
Unknown	0.02	Unknown
Neric acid	0.10	Monoterpenic acid
α -Cubebene	0.02	Sesquiterpene
Citronellyl acetate	0.12	Monoterpenic ester
Cyclosativene I	tr	Sesquiterpene
Cyclosativene II	0.08	Sesquiterpene
Neryl acetate	0.07	Monoterpenic ester
α -Ylangene	0.04	Sesquiterpene
Geranic acid	0.25	Aliphatic acid
α -Copaene	0.03	Sesquiterpene
β -Bourbonene	0.03	Sesquiterpene
1,5-diepi- β -Bourbonene	0.03	Sesquiterpene
Geranyl acetate	2.96	Monoterpenic ester
β -Cubebene	0.08	Sesquiterpene
β -Elemene	0.08	Sesquiterpene
Longifolene	0.02	Sesquiterpene
β -Caryophyllene	1.64	Sesquiterpene
β -Copaene	0.03	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.01	Sesquiterpene
6,9-Guaiadiene	0.02	Sesquiterpene
α -Humulene	0.18	Sesquiterpene
(E)-Isoeugenol	0.48	Phenylpropanoid
<i>cis</i> -Muurolo-4(15),5-diene	0.04	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.03	Sesquiterpene
Germacrene D	0.29	Sesquiterpene
epi-Cubebol	0.12	Sesquiterpenic alcohol

α-Murolene	0.09	Sesquiterpene
Methyl (E)-isoeugenol	0.01	Phenylpropanoid
δ-Amorphene	0.03	Sesquiterpene
γ-Cadinene	1.04	Sesquiterpene
Cubebol	0.29	Sesquiterpenic alcohol
δ-Cadinene	0.29	Sesquiterpene
10-epi-Cubebol?	0.06	Sesquiterpenic alcohol
trans-Cadina-1,4-diene	0.03	Sesquiterpene
(E)-γ-Bisabolene	0.09	Sesquiterpene
α-Cadinene	0.04	Sesquiterpene
Neryl butyrate	0.04	Monoterpenic ester
α-Elemol	0.07	Sesquiterpenic alcohol
Germacrene B	0.04	Sesquiterpene
Geranyl butyrate	0.08	Monoterpenic ester
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Caryophyllene oxide	0.40	Sesquiterpenic ether
Humulene epoxide II	0.04	Sesquiterpenic ether
10-epi-Cubebol	0.02	Sesquiterpenic alcohol
Selin-6-en-4α-ol isomer	0.01	Sesquiterpenic alcohol
1-epi-Cubebol	0.03	Sesquiterpenic alcohol
τ-Murolol	0.02	Sesquiterpenic alcohol
Cubebol	0.01	Sesquiterpenic alcohol
(2Z,6Z)-Farnesol	0.04	Sesquiterpenic alcohol
Farnesal isomer	0.01	Sesquiterpenic aldehyde
(2E,6Z)-Farnesal	0.01	Sesquiterpenic aldehyde
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
Neophytadiene	0.03	Diterpene
Phytone	0.01	Terpenic ketone
Geranyl caprylate	0.02	Monoterpenic ester
meta-Camphorene	0.01	Diterpene
Unknown	0.07	Unknown
Unknown	0.03	Unknown
Unknown	0.17	Unknown
Unknown	0.18	Unknown
Dicitral	0.08	Diterpenic aldehyde
Unknown	0.10	Unknown
Unknown	0.39	Unknown
Phytol isomer I	0.02	Diterpenic alcohol
Unknown	0.01	Unknown
Unknown	0.02	Unknown
Unknown	0.03	Unknown
Unknown	0.05	Unknown
Consolidated total	97.81%	

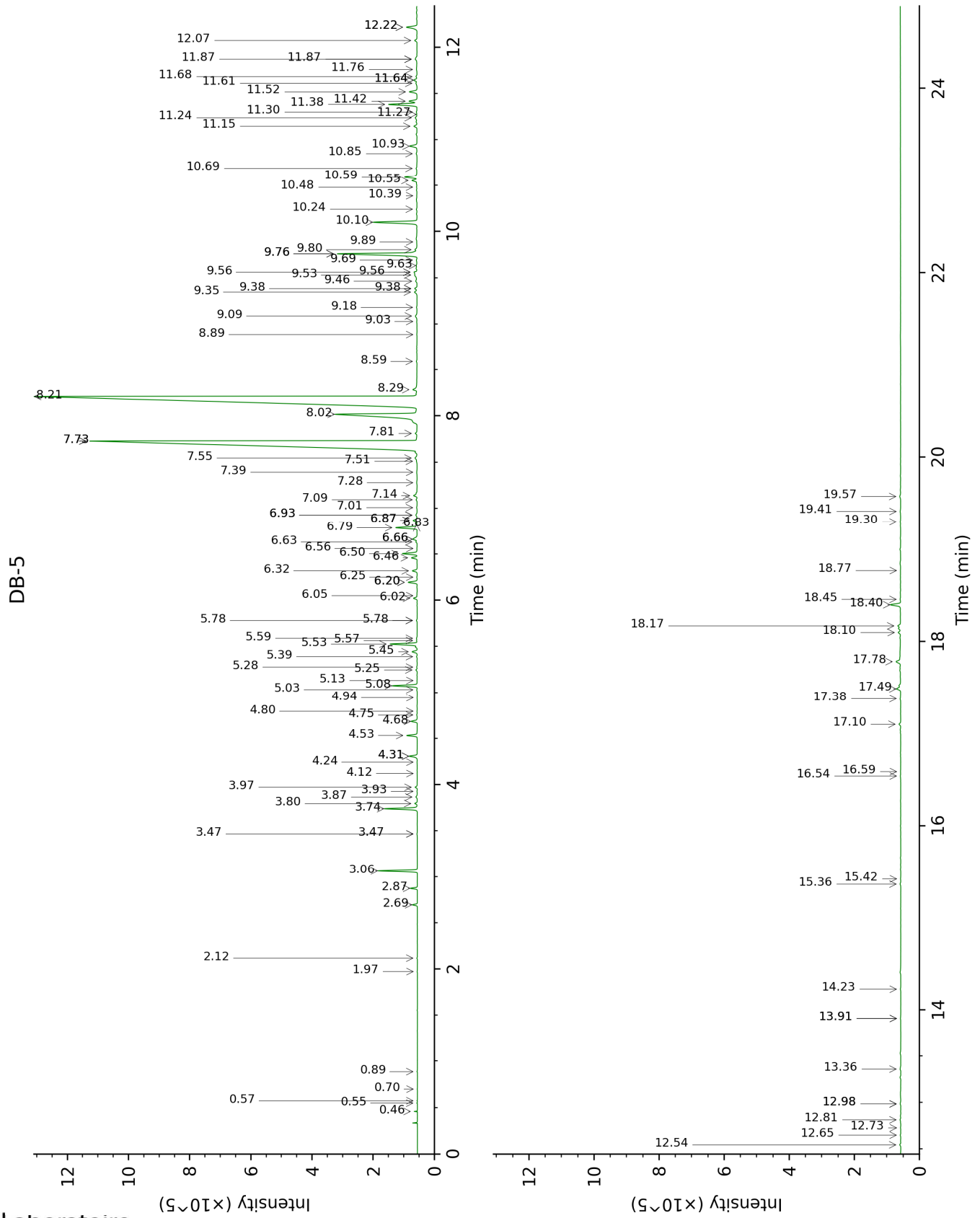
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

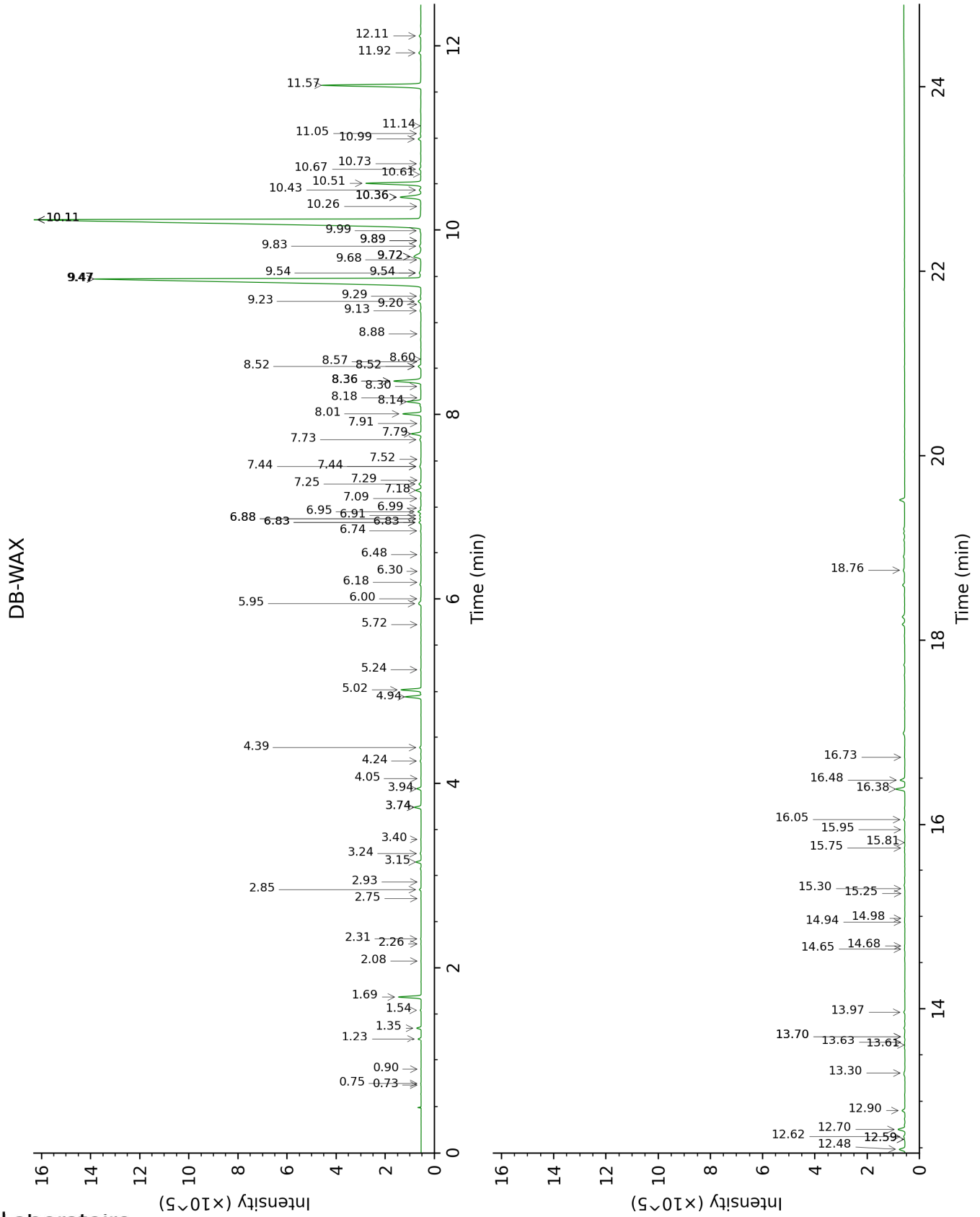
Note: no correction factor was applied

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-Methyl-3-buten-2-ol	0.46	605	0.03	1.54	1014	0.03
Isovaleral	0.55	640	0.01	0.75	888	0.01
2-Methylbutyral	0.57	650	tr	0.73	881	tr
2-Ethylfuran	0.70	700	tr	0.90	920	tr
Isoamyl alcohol	0.89	731	0.01	3.40	1177	0.01
(3Z)-Hexenol	1.97	858	0.01	5.72	1348	0.01
4-Heptanone	2.12	871	0.01	2.31	1090	0.02
Tricyclene	2.70	917	0.13	1.23	973	0.12
α-Pinene	2.87	929	0.18	1.35	992	0.18
Camphene	3.06	942	1.03	1.69	1028	1.01
β-Pinene	3.47*	970	0.02	2.08	1066	0.01
Sabinene	3.47*	970	[0.02]	2.26	1084	0.01
6-Methyl-5-hepten-2-one	3.74	988	0.98	5.02	1300	0.97
Myrcene	3.80	992	0.08	2.85	1134	0.08
6-Methyl-5-hepten-2-ol	3.87	997	0.06	6.88*	1432	0.09
α-Phellandrene	3.93	1001	0.01	2.75	1126	0.01
Octanal	3.97	1004	0.07	4.39	1252	0.07
α-Terpinene	4.12	1013	tr	2.93	1140	0.01
para-Cymene	4.24	1021	0.01	4.05	1228	0.01
Limonene	4.31*	1025	0.28	3.15	1158	0.23
1,8-Cineole	4.31*	1025	[0.28]	3.24	1165	0.04
(Z)-β-Ocimene	4.53	1039	0.33	3.74*	1205	0.33
(E)-β-Ocimene	4.68	1049	0.20	3.94	1220	0.19
2,6-Dimethyl-5-heptenal (melonal)	4.76	1053	0.02	5.24	1314	0.02
γ-Terpinene	4.80	1056	0.01	3.74*	1205	[0.33]
cis-Sabinene hydrate	4.94	1065	0.01	6.83*	1428	0.12
cis-Linalool oxide (fur.)	5.03	1071	0.02	6.48	1403	0.02
4-Nonanone	5.08	1074	0.78	4.94	1293	0.76
Camphenilone	5.13	1077	0.01	6.30	1390	0.01
trans-Linalool oxide (fur.)	5.25†	1084	0.07	6.83*	1428	[0.12]
Terpinolene	5.28†	1086	[0.07]	4.24	1242	0.05
4-Nonanol	5.39	1094	0.02			
Rosefuran	5.44	1097	0.19	5.95	1365	0.19
Linalool	5.53	1102	0.88	8.01	1517	0.88
cis-Chrysanthemal?	5.57	1105	0.02	6.00	1368	0.03
(Z)-6-Methyl-3,5-heptadien-2-one	5.59	1106	0.03	8.18	1530	0.02

<i>trans</i> -para-Mentha-2,8-dien-1-ol	5.78*	1118	0.02	8.88	1584	0.01
Unknown [m/z 81, 79 (19), 41 (12), 92 (8), 77 (8)...]	5.78*	1118	[0.02]	6.18	1381	0.01
Unknown [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	6.02	1134	0.12	6.83*	1428	[0.12]
Unknown [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	6.05	1136	0.01	7.52	1480	0.01
<i>trans</i> -Chrysanthemal exo-Isocitral	6.20*	1145	0.31	7.18	1455	0.27
	6.20*	1145	[0.31]	7.44*	1474	0.10
<i>trans</i> -Chrysanthemol	6.25	1149	0.02	9.54*	1637	0.17
Citronellal	6.32	1153	0.17	6.95	1438	0.16
Borneol	6.46	1162	0.19	9.72*	1651	0.66
Isoneral	6.50	1165	0.51	7.79	1500	0.51
α -Phellandren-8-ol	6.56	1168	0.01	10.11*	1684	41.59
Unknown [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	6.63	1173	0.05	9.54*	1637	[0.17]
Terpinen-4-ol	6.66*	1175	0.21	8.52*	1556	0.18
Rosefuran oxide	6.66*	1175	[0.21]	8.52*	1556	[0.18]
Isogeranial	6.79	1183	0.72	8.14	1527	0.74
Unknown [m/z 69, 41 (65), 109 (36), 67 (16), 84 (11), 43 (10), 55 (9)...]	6.83	1186	0.02			
α -Terpineol	6.87*	1188	0.16	9.72*	1651	[0.66]
Myrtenal	6.87*	1188	[0.16]	8.60	1562	0.02
Unknown [m/z 43, 81 (47), 67 (45), 69 944), 41 (42), 59 (40), 55 (39)...]	6.93*	1192	0.07	9.13	1604	0.05
(4Z)-Decenal	6.93*	1192	[0.07]			
<i>trans</i> -Isopiperitenol	7.01	1197	0.03	10.36*	1704	1.40
Unknown [m/z 84, 41 (83), 83 (79), 91 (76), 93	7.10	1203	0.04	10.11*	1684	[41.59]

(67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]						
Decanal	7.14	1206	0.14	7.25	1460	0.11
<i>cis</i> - Isopiperitenol	7.28	1215	0.03	10.26	1695	0.03
2,3-Epoxyneral?	7.39	1223	0.03			
Nerol	7.51	1231	0.02	10.99	1758	0.14
Citronellol	7.55	1233	0.11	10.67	1730	0.09
Neral	7.73*†	1245	31.65	9.47*	1632	31.38
(<i>Z</i>)-Isogeraniol	7.73*†	1245	[31.65]	11.14	1770	0.02
Piperitone	7.81†	1251	[31.65]	9.83	1660	0.10
Geraniol	8.02†	1265	46.89	11.57	1807	5.49
Geranial	8.21†	1278	[46.89]	10.11*	1684	[41.59]
Unknown [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	8.28	1283	0.18	12.90	1927	0.17
Geranyl formate	8.59	1303	0.02	9.89*	1665	0.03
Methyl geranate	8.89	1324	0.01	9.68	1648	0.02
Unknown [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	9.03	1334	0.02	12.62	1901	0.08
Neric acid	9.09	1338	0.10	16.06	2237	0.07
α-Cubebene	9.18	1345	0.02	6.74	1422	0.03
Citronellyl acetate	9.35	1357	0.12	9.47*	1632	[31.38]
Cyclosativene I	9.38*	1359	0.09	6.88*	1432	[0.09]
Cyclosativene II	9.38*	1359	[0.09]	6.91	1435	0.08
Neryl acetate	9.46	1365	0.07	10.11*	1684	[41.59]
α-Ylangene	9.53†	1370	0.28	6.99	1440	0.04
Geranic acid	9.56*†	1372	[0.28]	16.48	2282	0.25
α-Copaene	9.56*†	1372	[0.28]	7.10	1448	0.03
β-Bourbonene	9.63	1377	0.03	7.44*	1474	[0.10]
1,5-diepi-β- Bourbonene	9.69	1381	0.03	7.29	1463	0.01
Geranyl acetate	9.76*	1386	3.14	10.51	1716	2.96
β-Cubebene	9.76*	1386	[3.14]	7.73	1495	0.08
β-Elemene	9.80	1389	0.08	8.36*	1544	1.67
Longifolene	9.89	1395	0.02	7.90	1509	0.02
β- Caryophyllene	10.10	1410	1.64	8.36*	1544	[1.67]
β-Copaene	10.24	1421	0.03	8.30	1540	0.02
<i>trans</i> -α- Bergamotene	10.39	1432	0.01	8.36*	1544	[1.67]
6,9-Guaiadiene	10.48	1439	0.02	8.57	1560	0.02
α-Humulene	10.55	1444	0.18	9.23	1612	0.19
(<i>E</i>)-Isoeugenol	10.59	1447	0.48	16.38	2272	0.48

<i>cis</i> -Muurolo-4(15),5-diene	10.69	1454	0.04	9.29	1616	0.05
<i>trans</i> -Cadina-1(6),4-diene	10.85	1466	0.03	9.20	1609	0.02
Germacrene D	10.93	1472	0.29	9.72*	1651	[0.66]
epi-Cubebol	11.15	1488	0.12	11.92	1839	0.15
α -Muurolene	11.24	1495	0.09	10.00	1674	0.06
Methyl (<i>E</i>)-isoeugenol	11.27	1498	0.01	14.94	2123	0.02
δ -Amorphene	11.30	1500	0.03	9.89*	1665	[0.03]
γ -Cadinene	11.38	1506	1.04	10.36*	1704	[1.40]
Cubebol	11.42	1509	0.29	12.48	1889	0.32
δ -Cadinene	11.52	1517	0.29	10.36*	1704	[1.40]
10-epi-Cubebol?	11.61	1524	0.06	13.70*	2002	0.06
<i>trans</i> -Cadina-1,4-diene	11.64*	1527	0.12	10.61	1725	0.03
(<i>E</i>)- γ -Bisabolene	11.64*	1527	[0.12]	10.43	1710	0.09
α -Cadinene	11.68	1530	0.04	10.73	1735	0.04
Neryl butyrate	11.76	1536	0.04			
α -Elemol	11.87*	1545	0.11	13.97	2027	0.07
Germacrene B	11.87*	1545	[0.11]	11.05	1763	0.04
Geranyl butyrate	12.07	1560	0.08	12.11	1855	0.11
Caryophyllene oxide isomer	12.22*	1572	0.45	12.59*	1898	0.04
Caryophyllene oxide	12.22*	1572	[0.45]	12.70	1908	0.40
Humulene epoxide II	12.54	1598	0.04	13.30	1964	0.05
10-epi-Cubebol	12.65	1606	0.02	13.64	1995	0.02
Selin-6-en-4 α -ol isomer	12.73	1612	0.01	14.68	2097	0.02
1-epi-Cubebol	12.81	1620	0.03	13.70*	2002	[0.06]
τ -Muurolol	12.98*	1634	0.03	14.98	2127	0.02
Cubebol	12.98*	1634	[0.03]	13.60	1992	0.01
(2 <i>Z</i> ,6 <i>Z</i>)-Farnesol	13.36	1665	0.04	15.95	2225	0.02
Farnesal isomer	13.91*	1711	0.02			
(2 <i>E</i> ,6 <i>Z</i>)-Farnesal	13.91*	1711	[0.02]	15.25	2154	0.01
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	14.23	1738	0.02	15.75	2204	0.02
Neophytadiene	15.36	1838	0.03	12.59*	1898	[0.04]
Phytone	15.42	1844	0.01	14.65	2093	0.03
Geranyl caprylate	16.54	1947	0.02	15.81	2211	0.01
meta-Camphorene	16.59	1952	0.01	15.30	2159	0.01
Unknown [m/z 41, 69 (95), 109 (41), 95 (39), 55 (36), 121 (36)...]	17.10	2001	0.07			
Unknown [m/z 69, 41 (90), 95]	17.38	2028	0.03			

(49), 109 (43), 219 (43), 55 (30)...						
Unknown [m/z 69, 41 (94), 81 (42), 109 (39), 107 (33), 43 (31)...	17.49	2039	0.17			
Unknown [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53), 109 (50)... 235 (10)...	17.78	2069	0.18			
Dicitral	18.10	2100	0.08	16.73	2308	0.02
Unknown [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...	18.17	2107	0.10	18.76	2536	0.08
Unknown [m/z 69, 41 (38), 151 (36), 123 (34), 82 (24), 43 (23), 109 (21)...	18.40	2131	0.39			
Phytol isomer I	18.46	2137	0.02			
Unknown [m/z 94, 43 (85), 93 (81), 69 (76), 137 (76), 95 (60), 134 (51)...	18.77	2169	0.01			
Unknown [m/z 94, 43 (56), 123 (55), 69 (53), 95 (42), 79 (39)...	19.30	2225	0.02			
Unknown [m/z 93, 69 (79), 43 (70), 137 (53), 41 (41), 119 (37)... 289 (33)...	19.41	2238	0.03			
Unknown [m/z 123, 94 (100), 43 (86), 69 (75), 95 (47), 41 (47), 93 (45)...	19.57	2255	0.05			
Total identified		96.71%			96.47%	
Total reported		98.20%			96.87%	

*: 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)

