

Date : August 16, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22H09-PTH02


Customer identification : Lemongrass ORGANIC - India - L90111R

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 : Amélie Simard, Analyste

Analysis date : August 15, 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: 1.4854 ± 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
Ethanol	tr	Aliphatic alcohol
2-Methyl-3-buten-2-ol	0.03	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
Hexanal	0.01	Aliphatic aldehyde
(3Z)-Hexenol	0.01	Aliphatic alcohol
4-Heptanone	0.02	Aliphatic ketone
Hexanol	0.01	Aliphatic alcohol
Tricyclene	0.24	Monoterpene
α -Pinene	0.32	Monoterpene
Camphene	1.76	Monoterpene
β -Pinene	0.02	Monoterpene
Sabinene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	1.81	Aliphatic ketone
Myrcene	0.10	Monoterpene
6-Methyl-5-hepten-2-ol	0.06	Aliphatic alcohol
α -Phellandrene	0.02	Monoterpene
Octanal	0.07	Aliphatic aldehyde
Δ^3 -Carene	0.01	Monoterpene
α -Terpinene	0.01	Monoterpene
para-Cymene	0.04	Monoterpene
1,8-Cineole	0.06	Monoterpenic ether
Limonene	0.42	Monoterpene
Benzeneacetaldehyde	0.01	Simple phenolic
(Z)- β -Ocimene	0.33	Monoterpene
(E)- β -Ocimene	0.22	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.03	Aliphatic aldehyde
γ -Terpinene	0.02	Monoterpene
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
4-Nonanone	1.29	Aliphatic ketone
Camphenilone	0.03	Normonoterpenic ketone
trans-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Terpinolene	0.06	Monoterpene
4-Nonanol	0.04	Aliphatic alcohol
Rosefuran	0.21	Monoterpenic ether
Linalool	1.37	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	0.06	Monoterpenic alcohol
Unknown	0.19	Unknown
Unknown	0.02	Unknown
exo-Isocitral	0.08	Monoterpenic aldehyde
trans-Chrysanthemal	0.38	Monoterpenic aldehyde

Citronellal	0.27	Monoterpenic aldehyde
Borneol	0.18	Monoterpenic alcohol
Isoneral	0.60	Monoterpenic aldehyde
α -Phellandren-8-ol	0.02	Monoterpenic alcohol
Rosefuran oxide	0.13*	Monoterpenic ether
Terpinen-4-ol	0.13*	Monoterpenic alcohol
Unknown	0.19	Oxygenated monoterpene
Isogeranial	0.86	Monoterpenic aldehyde
α -Terpineol	0.18	Monoterpenic alcohol
Myrtenal	0.02	Monoterpenic aldehyde
Unknown	0.07	Unknown
(4Z)-Decenal	0.01	Aliphatic aldehyde
γ -Terpineol	0.02	Monoterpenic alcohol
<i>trans</i> -Isopiperitenol	0.05	Monoterpenic alcohol
Unknown	0.11	Oxygenated monoterpene
Decanal	0.13	Aliphatic aldehyde
<i>cis</i> -Isopiperitenol	0.03	Monoterpenic alcohol
2,3-Epoxyneral?	0.03	Monoterpenic aldehyde
Nerol	0.12	Monoterpenic alcohol
Citronellol	0.12	Monoterpenic alcohol
Neral	29.45	Monoterpenic aldehyde
(Z)-Isogeraniol	0.03	Monoterpenic alcohol
Piperitone	0.08	Monoterpenic ketone
Geraniol	5.02	Monoterpenic alcohol
Geranial	39.33	Monoterpenic aldehyde
Unknown	0.23	Oxygenated monoterpene
Bornyl acetate	0.01	Monoterpenic ester
2-Undecanone	0.01	Aliphatic ketone
Geranyl formate	0.04	Monoterpenic ester
Methyl geranate	0.01	Monoterpenic ester
Unknown	0.01	Unknown
Neric acid	0.10	Monoterpenic acid
α -Cubebene	0.02	Sesquiterpene
Citronellyl acetate	0.02	Monoterpenic ester
Cyclosativene I	0.05	Sesquiterpene
Cyclosativene II	0.07	Sesquiterpene
Neryl acetate	0.09	Monoterpenic ester
Geranic acid	0.34	Aliphatic acid
α -Ylangene	0.05	Sesquiterpene
α -Copaene	0.01	Sesquiterpene
β -Bourbonene	0.02	Sesquiterpene
1,5-diepi- β -Bourbonene	0.03	Sesquiterpene
Geranyl acetate	3.68	Monoterpenic ester
β -Cubebene	0.03	Sesquiterpene
β -Elemene	0.09	Sesquiterpene
Longifolene	0.01	Sesquiterpene
β -Caryophyllene	1.27	Sesquiterpene
β -Copaene	0.02	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.03	Sesquiterpene
6,9-Guaiadiene	0.02	Sesquiterpene
(E)-Isoeugenol	0.37	Phenylpropanoid
α -Humulene	0.15	Sesquiterpene

<i>cis</i> -Muurolo-4(15),5-diene	0.05	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.05	Sesquiterpene
γ -Muurolole	0.01	Sesquiterpene
Germacrene D	0.15	Sesquiterpene
γ -Amorphene	0.04	Sesquiterpene
epi-Cubebol	0.09	Sesquiterpenic alcohol
α -Muurolole	0.09	Sesquiterpene
δ -Amorphene	0.04	Sesquiterpene
Cubebol	0.13	Sesquiterpenic alcohol
γ -Cadinene	0.99	Sesquiterpene
δ -Cadinene	0.38	Sesquiterpene
10-epi-Cubebol?	0.03	Sesquiterpenic alcohol
(<i>E</i>)- γ -Bisabolene	0.22	Sesquiterpene
α -Cadinene	0.06	Sesquiterpene
Neryl butyrate	0.02	Monoterpenic ester
α -Elemol	0.07	Sesquiterpenic alcohol
Germacrene B	0.03	Sesquiterpene
Geranyl butyrate	0.12	Monoterpenic ester
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Caryophyllene oxide	0.50	Sesquiterpenic ether
Humulene epoxide II	0.05	Sesquiterpenic ether
10-epi-Cubebol	0.03	Sesquiterpenic alcohol
Selin-6-en-4 α -ol isomer	0.01	Sesquiterpenic alcohol
1-epi-Cubebol	0.06	Sesquiterpenic alcohol
Cubebol	0.03	Sesquiterpenic alcohol
τ -Cadinol	0.01	Sesquiterpenic alcohol
τ -Muurolol	0.02	Sesquiterpenic alcohol
β -Eudesmol	0.03	Sesquiterpenic alcohol
α -Eudesmol	0.02	Sesquiterpenic alcohol
(2 <i>Z</i> ,6 <i>Z</i>)-Farnesol	0.04	Sesquiterpenic alcohol
Farnesal isomer	0.01	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	0.02	Sesquiterpenic aldehyde
Neophytadiene	0.03	Diterpene
Phytone	0.02	Terpenic ketone
meta-Camphorene	0.03	Diterpene
para-Camphorene	0.04	Diterpene
Unknown	0.04	Unknown
Octadecanal	0.02	Aliphatic aldehyde
Unknown	0.05	Unknown
Unknown	0.18	Unknown
Unknown	0.02	Unknown
Unknown	0.20	Unknown
Dicitral	0.09	Diterpenic aldehyde
Unknown	0.11	Unknown
Phytol	0.06	Diterpenic alcohol
Unknown	0.36	Unknown
Phytol isomer I	0.01	Diterpenic alcohol
Unknown	0.01	Unknown
Unknown	0.04	Unknown
Unknown	0.06	Unknown
Consolidated total	98.11%	

*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered

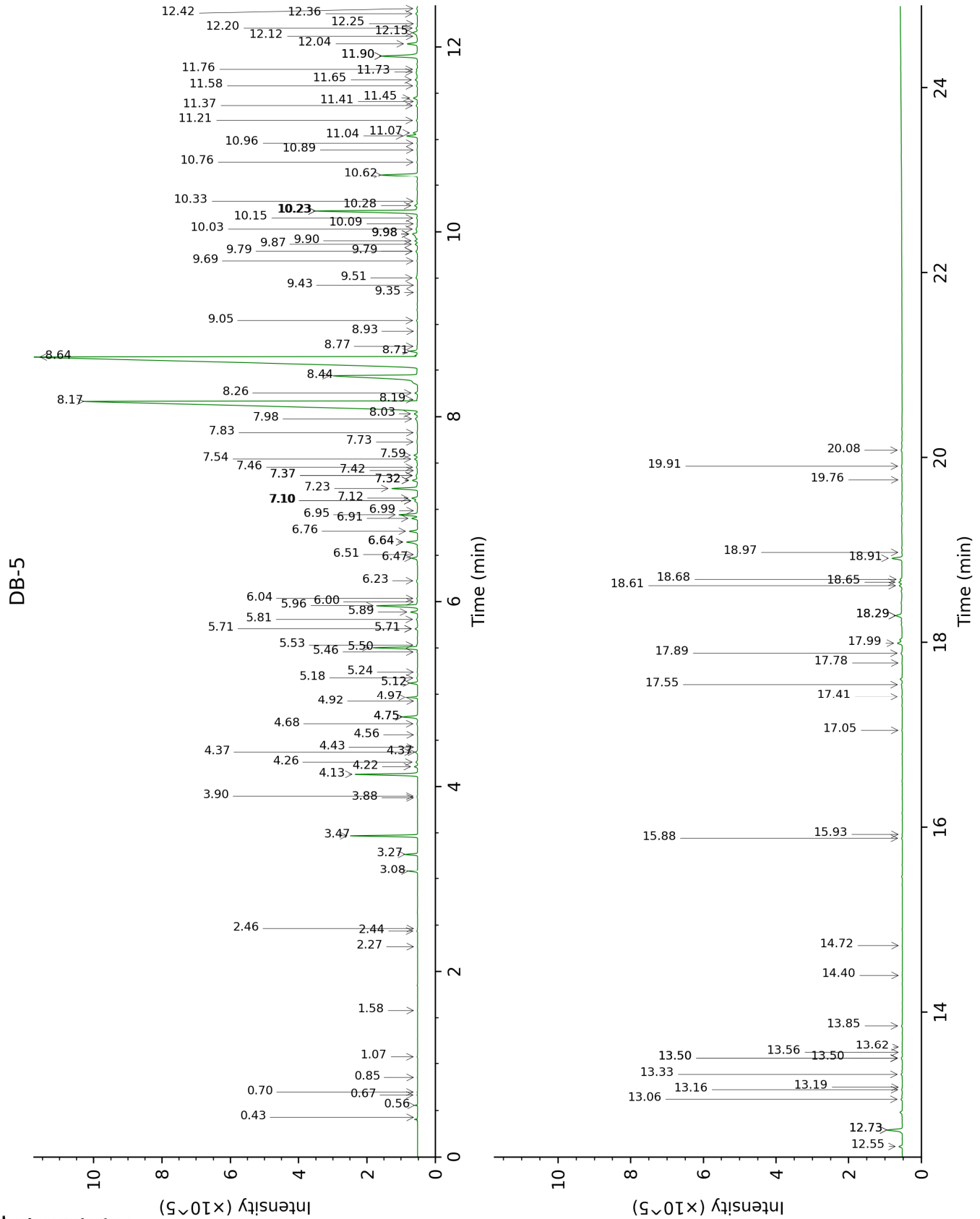
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

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	%
Ethanol	0.43	510	tr	0.77	906	tr
2-Methyl-3-buten-2-ol	0.56	607	0.03	1.44	1013	0.03
Isovaleral	0.67	643	0.01	0.71	885	0.01
2-Methylbutyral	0.70	653	0.01	0.69	879	0.01
2-Ethylfuran	0.85	703	tr	0.85	920	0.01
Isoamyl alcohol	1.08	733	0.01	3.24	1174	0.03
Hexanal	1.58	801	0.01	1.75	1043	tr
(3Z)-Hexenol	2.27	858	0.01	5.55	1342	0.01
4-Heptanone	2.44	871	0.02	2.20	1088	0.03
Hexanol	2.46	873	0.01	5.21	1317	0.02
Tricyclene	3.08	920	0.24	1.18	974	0.22
α-Pinene	3.27	932	0.32	1.30	993	0.31
Camphene	3.47	945	1.76	1.62	1030	1.74
β-Pinene	3.88†	972	0.03	1.99	1067	0.02
Sabinene	3.90†	973	[0.03]	2.16	1084	0.01
6-Methyl-5-hepten-2-one	4.13	988	1.81	4.86	1296	1.72
Myrcene	4.22	994	0.10	2.74	1134	0.09
6-Methyl-5-hepten-2-ol	4.26	997	0.06	6.72	1429	0.01
α-Phellandrene	4.37*	1004	0.08	2.65	1127	0.02
Octanal	4.37*	1004	[0.08]	4.24	1250	0.07
Δ3-Carene	4.43	1007	0.01			
α-Terpinene	4.56	1016	0.01	2.82	1140	0.01
para-Cymene	4.68	1023	0.04	3.92	1226	0.03
1,8-Cineole	4.75*	1028	0.49	3.13	1165	0.06
Limonene	4.75*	1028	[0.49]	3.05	1158	0.42
Benzeneacetaldehyde	4.92	1038	0.01	8.56	1570	0.02
(Z)-β-Ocimene	4.97	1041	0.33	3.62	1204	0.33
(E)-β-Ocimene	5.12	1051	0.22	3.82	1219	0.21
2,6-Dimethyl-5-heptenal (melonal)	5.18	1054	0.03	5.08	1307	0.03
γ-Terpinene	5.24	1058	0.02	3.65	1206	0.02
cis-Linalool oxide (fur.)	5.46	1072	0.02	6.31	1398	0.02
4-Nonanone	5.50	1074	1.29	4.80	1292	1.30
Camphenilone	5.53	1076	0.03	6.23	1392	0.01
trans-Linalool oxide (fur.)	5.71*	1087	0.08	6.67*	1424	0.21
Terpinolene	5.71*	1087	[0.08]	4.12	1241	0.06
4-Nonanol	5.81	1093	0.04			
Rosefuran	5.89	1098	0.21	5.79	1360	0.22
Linalool	5.96	1103	1.37	7.84	1514	1.27
cis-Chrysanthemal?	6.00	1105	0.02	5.85	1364	0.04
(Z)-6-Methyl-3,5-heptadien-2-one	6.04	1108	0.03	8.02	1528	0.02

<i>trans</i> -para-Mentha-2,8-dien-1-ol	6.23	1120	0.06	8.70	1582	0.06
Unknown [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	6.47	1135	0.19	6.67*	1424	[0.21]
Unknown [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	6.51	1138	0.02	7.37	1478	0.03
exo-Isocitral	6.64*	1146	0.41	7.27	1470	0.08
<i>trans</i> -Chrysanthemal	6.64*	1146	[0.41]	7.02	1451	0.38
Citronellal	6.76	1154	0.27	6.79*	1434	0.32
Borneol	6.91	1163	0.18	9.54*	1650	0.36
Isoneral	6.94	1166	0.60	7.63	1497	0.58
α-Phellandren-8-ol	6.99	1168	0.02	9.94*	1683	39.42
Rosefuran oxide	7.10*	1175	0.13	8.34*	1553	0.13
Terpinen-4-ol	7.10*	1175	[0.13]	8.34*	1553	[0.13]
Unknown [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	7.12	1177	0.19	9.36	1635	0.19
Isogeranial	7.23	1184	0.86	7.97	1524	0.88
α-Terpineol	7.32*	1189	0.19	9.54*	1650	[0.36]
Myrtenal	7.32*	1189	[0.19]	8.47	1563	0.02
Unknown [m/z 43, 81 (47), 67 (45), 69 944), 41 (42), 59 (40), 55 (39)...]	7.37*	1192	0.09	8.95	1602	0.07
(4Z)-Decenal	7.37*	1192	[0.09]	7.56	1492	0.01
γ-Terpineol	7.42	1196	0.02	9.65*	1659	0.15
<i>trans</i> -Isopiperitenol	7.46	1198	0.05	10.14	1699	0.05
Unknown [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]	7.54	1204	0.11	9.94*	1683	[39.42]
Decanal	7.59	1206	0.13	7.10	1458	0.11
<i>cis</i> -Isopiperitenol	7.73	1216	0.03	10.08	1694	0.02
2,3-Epoxyneral?	7.83	1223	0.03			
Nerol	7.98	1233	0.12	10.81	1757	0.14
Citronellol	8.03	1236	0.12	10.50	1730	0.18
Neral	8.17	1245	29.45	9.30*	1630	29.42
(Z)-Isogeraniol	8.19	1246	0.03	10.91	1765	0.05
Piperitone	8.26	1251	0.08	9.65*	1659	[0.15]
Geraniol	8.44	1264	5.02	11.40	1807	5.19
Geranial	8.64	1277	39.33	9.94*	1683	[39.42]
Unknown [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	8.71	1281	0.23	12.71	1926	0.25
Bornyl acetate	8.77	1285	0.01	8.06	1531	0.01
2-Undecanone	8.93	1296	0.01	8.37	1556	0.01
Geranyl formate	9.05	1304	0.04	9.73	1665	0.03

Methyl geranate	9.35	1325	0.01	9.50	1646	0.01
Unknown [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	9.43	1331	0.01	12.40	1898	0.03
Neric acid	9.50	1336	0.10	15.88	2237	0.09
α-Cubebene	9.69	1349	0.02	6.61	1420	0.01
Citronellyl acetate	9.79*	1356	0.07	9.30*	1630	[29.42]
Cyclosativene I	9.79*	1356	[0.07]	6.79*	1434	[0.32]
Cyclosativene II	9.87	1362	0.07	6.83	1437	0.08
Neryl acetate	9.90	1364	0.09	9.94*	1683	[39.42]
Geranic acid	9.98*†	1370	0.39	16.31	2282	0.34
α-Ylangene	9.98*†	1370	[0.39]	6.91	1443	0.05
α-Copaene	10.03†	1373	[0.39]	6.98	1448	0.01
β-Bourbonene	10.09	1377	0.02	7.33	1475	0.03
1,5-diepi-β-Bourbonene	10.15	1382	0.03	7.18	1464	0.01
Geranyl acetate	10.23*	1387	3.68	10.34	1716	3.68
β-Cubebene	10.23*	1387	[3.68]	7.60	1495	0.03
β-Elemene	10.28	1391	0.09	8.25*	1546	1.29
Longifolene	10.33	1394	0.01	7.78	1509	0.01
β-Caryophyllene	10.62	1415	1.27	8.25*	1546	[1.29]
β-Copaene	10.76	1426	0.02	8.22	1543	0.03
trans-α-Bergamotene	10.89	1435	0.03	8.25*	1546	[1.29]
6,9-Guaiadiene	10.96	1441	0.02	8.44	1561	0.02
(E)-Isoeugenol	11.04	1447	0.37	16.18	2268	0.38
α-Humulene	11.08	1449	0.15	9.11	1614	0.18
cis-Muurolo-4(15),5-diene	11.21	1459	0.05	9.18	1620	0.04
trans-Cadina-1(6),4-diene	11.37	1471	0.05	9.05	1610	0.02
γ-Muurolole	11.41	1474	0.01	9.41	1639	0.04
Germacrene D	11.45	1477	0.15	9.60	1655	0.15
γ-Amorphene	11.58	1487	0.04	9.65*	1659	[0.15]
epi-Cubebol	11.65	1492	0.09	11.76	1840	0.07
α-Muurolole	11.73	1498	0.09	9.94*	1683	[39.42]
δ-Amorphene	11.76	1500	0.04	9.79	1670	0.04
Cubebol	11.90*	1511	1.42	12.32	1890	0.13
γ-Cadinene	11.90*	1511	[1.42]	10.22*	1706	1.60
δ-Cadinene	12.04	1521	0.38	10.22*	1706	[1.60]
10-epi-Cubebol?	12.12	1528	0.03	13.53*	2003	0.07
(E)-γ-Bisabolene	12.15	1531	0.22	10.22*	1706	[1.60]
α-Cadinene	12.20	1534	0.06	10.60	1738	0.04
Neryl butyrate	12.25	1538	0.02			
α-Elemol	12.36	1547	0.07	13.79	2028	0.05
Germacrene B	12.42	1551	0.03	10.96	1769	0.02
Geranyl butyrate	12.56	1562	0.12	11.95	1856	0.11
Caryophyllene oxide isomer	12.73*	1576	0.56	12.45	1902	0.06
Caryophyllene oxide	12.73*	1576	[0.56]	12.53	1909	0.50
Humulene epoxide II	13.06	1602	0.05	13.08	1961	0.03
10-epi-Cubebol	13.16	1610	0.03	13.47	1996	0.03

Selin-6-en-4 α -ol isomer	13.19	1612	0.01	14.51	2097	0.02
1-epi-Cubenol	13.33	1624	0.06	13.53*	2003	[0.07]
Cubenol	13.50*	1638	0.06	13.44	1994	0.03
τ -Cadinol	13.50*	1638	[0.06]	14.64	2110	0.01
τ -Muurolol	13.50*	1638	[0.06]	14.80	2126	0.02
β -Eudesmol	13.56	1643	0.03	15.13	2160	0.03
α -Eudesmol	13.62	1648	0.02	15.07	2154	0.01
(2Z,6Z)-Farnesol	13.85	1667	0.04	15.79	2227	0.04
Farnesal isomer	14.40	1712	0.01			
(2E,6E)-Farnesal	14.72	1740	0.02	15.55*	2203	0.04
Neophytadiene	15.88	1843	0.03			
Phytone	15.93	1846	0.02	14.48	2095	0.02
meta-Camphorene	17.05	1950	0.03	15.16	2163	0.01
para-Camphorene	17.41	1985	0.04	15.55*	2203	[0.04]
Unknown [m/z 41, 69 (95), 109 (41), 95 (39), 55 (36), 121 (36)...]	17.55	1998	0.04			
Octadecanal	17.78	2021	0.02	16.54	2306	0.03
Unknown [m/z 69, 41 (90), 95 (49), 109 (43), 219 (43), 55 (30)...]	17.89	2031	0.05			
Unknown [m/z 69, 41 (94), 81 (42), 109 (39), 107 (33), 43 (31)...]	17.99	2042	0.18			
Unknown [m/z 57, 85 (55), 163 (47), 41 (44), 120 (35), 202 (30), 145 (25)... 219 (17), 304 (t)]	18.29*	2071	0.22	18.73*	2550	0.12
Unknown [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53), 109 (50)... 235 (10)...]	18.29*	2071	[0.22]			
Dicitral	18.61	2103	0.09	16.56	2309	0.02
Unknown [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...]	18.65	2107	0.11	18.73*	2550	[0.12]
Phytol	18.68	2110	0.06	18.98	2579	0.07
Unknown [m/z 69, 41 (38), 151 (36), 123 (34), 82 (24), 43 (23), 109 (21)...]	18.91	2134	0.36	19.34	2622	0.30
Phytol isomer I	18.97	2140	0.01			
Unknown [m/z 94, 43 (56), 123 (55), 69 (53), 95 (42), 79 (39)...]	19.76	2223	0.01			
Unknown [m/z 93, 69 (79), 43 (70), 137 (53), 41 (41), 119 (37)... 289 (33)...]	19.91	2239	0.04			
Unknown [m/z 123, 94 (100), 43 (86), 69	20.08	2257	0.06			

(75), 95 (47), 41 (47), 93 (45)...		
Total identified	96.73%	95.98%
Total reported	98.32%	96.85%

*: 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