

Date : September 04, 2020

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20H26-PTH12


Customer identification : Palmarosa - P1010795R

Type : Essential oil

Source : *Cymbopogon martini*

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 : September 01, 2020

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: 1.4735 ± 0.0003 (20 °C; method PC-MAT-016)

NFT 75-234:2011 - OIL OF PALMAROSA

Compound	Min. %	Max. %	Observed %	Complies?
Geranyl caproate	0.4	0.8	0.9	No
(2E,6E)-Farnesol	0.2	1.5	1.1	Yes
Nerol	0.2	0.5	0.2	Yes
Geranial	0.2	0.6	0.3	Yes
Neral		0.5	0.2	Yes
β-Caryophyllene	0.7	2.5	1.9	Yes
Geranyl acetate	7	16	7	Yes
Geraniol	72	86	80	Yes
Linalool	1.0	5.5	2.5	Yes
(E)-β-Ocimene	0.5	3.0	1.6	Yes
(Z)-β-Ocimene	0.2	0.6	0.4	Yes
Limonene		1.3	0.1	Yes
Myrcene		0.5	0.2	Yes
Refractive index	1.4700	1.4780	1.4735	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
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
Isoamyl alcohol	0.02	Aliphatic alcohol
(3Z)-Hexenol	tr	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
Isoamyl acetate	0.01	Aliphatic ester
Unknown	0.01	Unknown
2-Heptanone	0.01	Aliphatic ketone
Hashishene	tr	Monoterpene
Tricyclene	tr	Monoterpene
α -Pinene	tr	Monoterpene
6-Methyl-5-hepten-2-one	0.05	Aliphatic ketone
Myrcene	0.18	Monoterpene
<i>trans</i> -Dehydroxylinalool oxide	0.03	Monoterpenic ether
α -Phellandrene	0.01	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.03	Monoterpenic ether
para-Cymene	tr	Monoterpene
Limonene	0.10	Monoterpene
(Z)- β -Ocimene	0.41	Monoterpene
(E)- β -Ocimene	1.62	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.02	Aliphatic aldehyde
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.02	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Rosefuran	0.01	Monoterpenic ether
Linalool	2.54	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
Camphor	0.01	Monoterpenic ketone
Citronellal	0.02	Monoterpenic aldehyde
Terpinen-4-ol	0.01	Monoterpenic alcohol
Menthol	0.01	Monoterpenic alcohol
α -Terpineol	0.02	Monoterpenic alcohol
Decanal	0.01	Aliphatic aldehyde
Nerol	0.17	Monoterpenic alcohol
Citronellol	0.02	Monoterpenic alcohol
2,3-Epoxygeranial?	0.01	Monoterpenic aldehyde
Neral	0.16	Monoterpenic aldehyde
Isoamyl hexanoate	0.01	Aliphatic ester
Geraniol	79.56	Monoterpenic alcohol
Geranial	0.35	Monoterpenic aldehyde
Geranyl formate	0.09	Monoterpenic ester
2,3-Epoxygeraniol?	0.04	Oxygenated monoterpene

Neryl acetate	0.01	Monoterpenic ester
Unknown	0.03	Unknown
Geranic acid	0.03	Aliphatic acid
Geranyl acetate	7.34	Monoterpenic ester
β -Elemene	0.11	Sesquiterpene
β -Caryophyllene	1.89	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.01*	Sesquiterpene
α -Guaiene	[0.01]*	Sesquiterpene
α -Humulene	0.12	Sesquiterpene
Unknown	0.10	Sesquiterpene
Germacrene D	0.03	Sesquiterpene
β -Selinene	0.01	Sesquiterpene
Valencene	0.06	Sesquiterpene
α -Elemol	0.01	Sesquiterpenic alcohol
Unknown	0.01	Unknown
Geranyl butyrate	0.19	Monoterpenic ester
(<i>E</i>)-Nerolidol	0.14	Sesquiterpenic alcohol
Caryophyllene oxide	0.20	Sesquiterpenic ether
Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
Humulene epoxide II	0.01	Sesquiterpenic ether
Geranyl isovalerate	0.01	Monoterpenic ester
Caryophylladienol II	0.02	Sesquiterpenic alcohol
Precocene II	0.01	Chromane
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5 β -ol	0.01	Sesquiterpenic alcohol
(2 <i>E</i> ,6 <i>E</i>)-Farnesol	1.10	Sesquiterpenic alcohol
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	0.01	Sesquiterpenic aldehyde
Geranyl caproate	0.94	Monoterpenic ester
(2 <i>E</i> ,6 <i>E</i>)-Farnesyl acetate	0.12	Sesquiterpenic ester
Phytone	0.03	Terpenic ketone
Geranyl caprylate	0.23	Monoterpenic ester
Unknown	0.02	Unknown
Unknown	0.02	Unknown
Consolidated total	98.50%	

*: 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

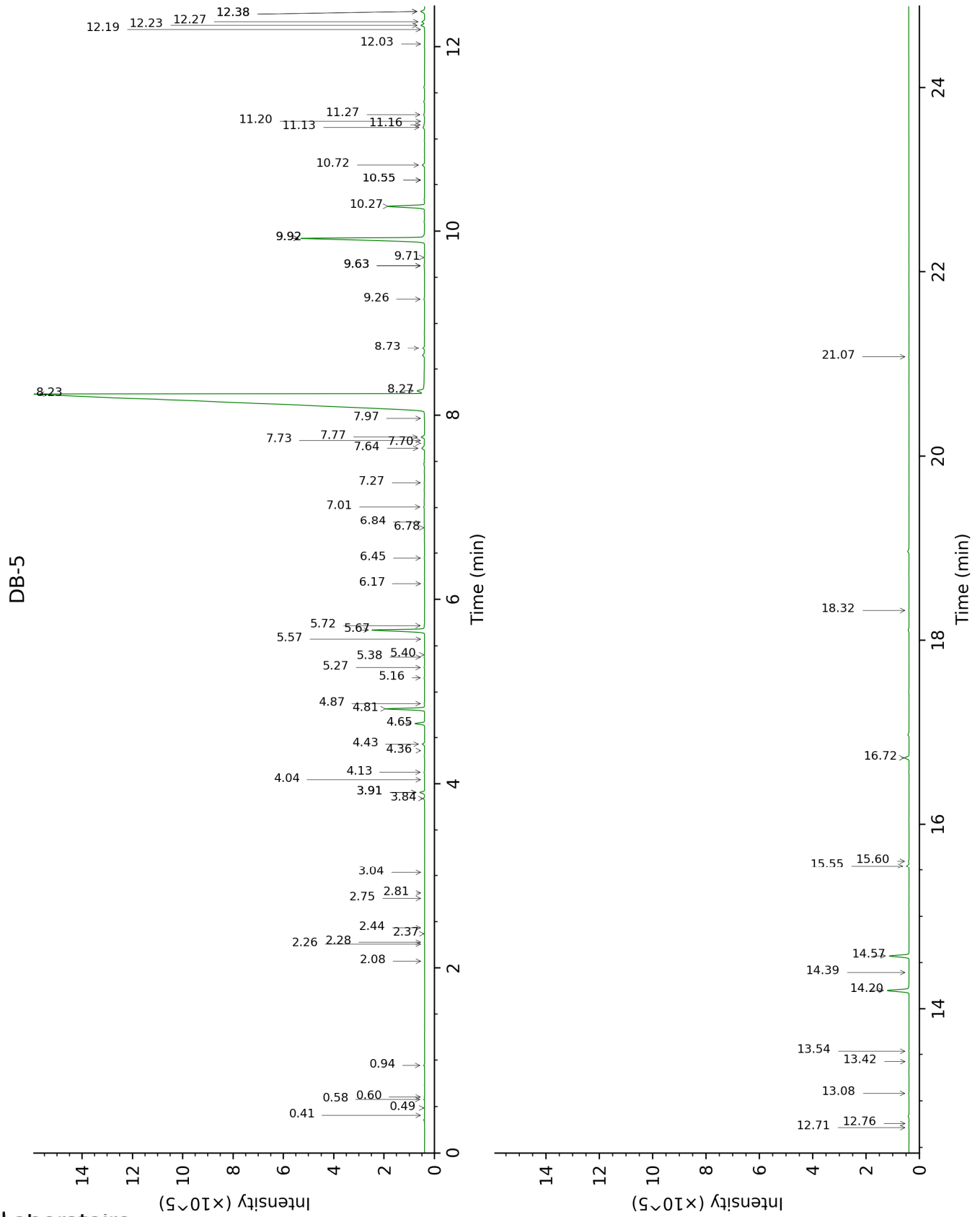
tr: The compound has been detected below 0.005% of total signal.

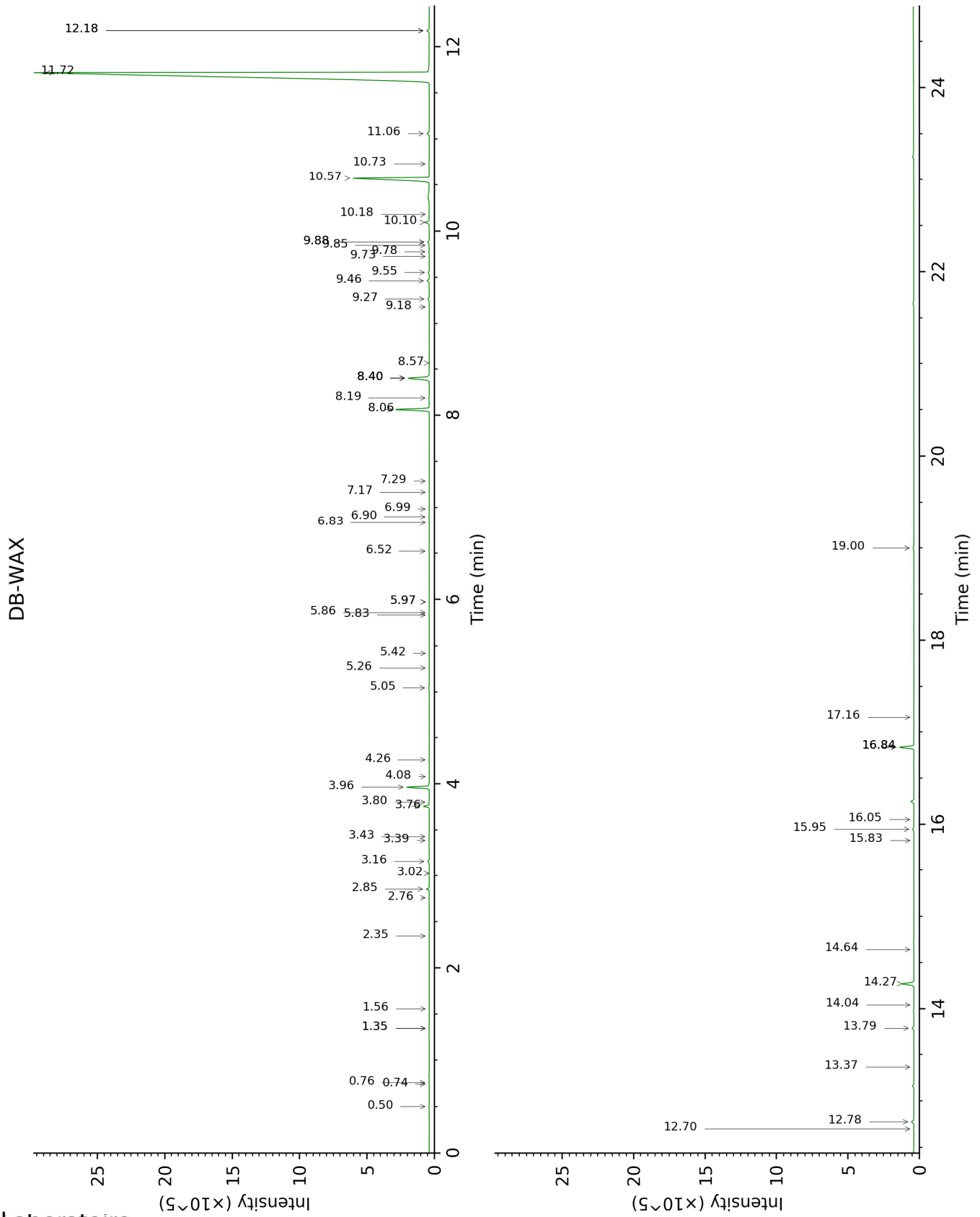
Note: no correction factor was applied

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	%
Isobutylal	0.41	534	tr	0.50	783	0.01
2-Methyl-3-buten-2-ol	0.49	604	tr	1.56	1014	0.01
Isovaleral	0.58	640	0.01	0.76	886	0.01
2-Methylbutylal	0.60	650	0.01	0.74	880	0.01
Isoamyl alcohol	0.94	733	0.02	3.43	1178	0.02
(3Z)-Hexenol	2.08	860	tr	5.83	1350	tr
Hexanol	2.26	875	0.01	5.42	1320	tr
Isoamyl acetate	2.28	877	0.01	2.35	1092	tr
Unknown [m/z 59, 85 (88), 41 (57), 43 (43)...]	2.37	885	0.01	5.98*	1361	0.01
2-Heptanone	2.44	890	0.01	3.02	1146	0.01
Hashishene	2.75	914	tr	1.35*	990	tr
Tricyclene	2.81	918	tr			
α -Pinene	3.04	933	tr	1.35*	990	[tr]
6-Methyl-5-hepten-2-one	3.84	987	0.05	5.05	1296	0.06
Myrcene	3.91*	991	0.22	2.86	1133	0.18
<i>trans</i> -Dehydroxylinalool oxide	3.91*	991	[0.22]	3.39	1174	0.03
α -Phellandrene	4.04	1000	0.01	2.76	1126	tr
<i>cis</i> -Dehydroxylinalool oxide	4.13	1006	0.03	3.80	1206	0.03
para-Cymene	4.36	1020	tr	4.08	1226	tr
Limonene	4.43	1025	0.10	3.16	1157	0.09
(Z)- β -Ocimene	4.65	1039	0.41	3.76	1203	0.40
(E)- β -Ocimene	4.81	1049	1.62	3.96	1218	1.61
2,6-Dimethyl-5-heptenal (melonal)	4.87	1052	0.02	5.26	1309	0.01
<i>cis</i> -Linalool oxide (fur.)	5.16	1070	0.02	6.52	1401	0.03
Octanol	5.27	1077	0.02	8.19	1526	0.03
Terpinolene	5.38	1084	0.02	4.26	1239	0.02
<i>trans</i> -Linalool oxide (fur.)	5.40	1086	0.01	6.90	1429	0.02
Rosefuran	5.57	1096	0.01	5.98*	1361	[0.01]
Linalool	5.67	1102	2.54	8.06	1516	2.52
Nonanal	5.72	1106	0.02	5.86	1352	0.02
Camphor	6.17	1134	0.01	7.17	1449	0.02
Citronellal	6.45	1152	0.02	6.99	1435	0.01
Terpinen-4-ol	6.78	1173	0.01	8.57	1555	0.02
Menthol	6.84	1177	0.01	9.18	1603	0.01
α -Terpineol	7.01	1188	0.02	9.78	1652	0.04
Decanal	7.27	1204	0.01	7.29	1458	0.02

Nerol	7.64	1229	0.17	11.06	1759	0.17
Citronellol	7.70	1233	0.02	10.73	1731	0.02
2,3-Epoxygeranial?	7.73	1235	0.01			
Neral	7.77	1237	0.16	9.46	1626	0.18
Isoamyl hexanoate	7.97	1251	0.01	6.84	1424	0.01
Geraniol	8.23†	1268	80.29	11.72	1816	79.56
Geranial	8.27†	1271	[80.29]	10.10	1678	0.35
Geranyl formate	8.73	1301	0.09	9.88*	1660	0.13
2,3-Epoxygeraniol?	9.26	1338	0.04			
Neryl acetate	9.63*	1364	0.04	10.18	1684	0.01
Unknown [m/z 81, 59 (99), 41 (82), 85 (79), 43 (74), 71 (60)...]	9.63*	1364	[0.04]			
Geranic acid	9.71	1370	0.03	16.84*	2308	1.17
Geranyl acetate	9.92*	1385	7.45	10.57	1717	7.34
β-Elemene	9.92*	1385	[7.45]	8.40*	1543	1.95
β-Caryophyllene	10.27	1410	1.89	8.40*	1543	[1.95]
<i>trans</i> -α-Bergamotene	10.55*	1431	0.01	8.40*	1543	[1.95]
α-Guaiene	10.55*	1431	[0.01]	8.40*	1543	[1.95]
α-Humulene	10.72	1443	0.12	9.27	1610	0.14
Unknown [m/z 189, 133 (75), 91 (71), 105 (69), 93 (44)... 204 (33)]	11.13	1474	0.10	9.55	1634	0.10
Germacrene D	11.16	1476	0.03	9.73	1648	0.02
β-Selinene	11.20	1478	0.01	9.85	1657	0.03
Valencene	11.27	1484	0.06	9.88*	1660	[0.13]
α-Elemol	12.03	1543	0.01	14.04	2027	0.01
Unknown [m/z 59, 68 (63), 43 (31), 67 (27), 81 (27), 94 (25), 69 (23), 41 (22), 84 (20)...]	12.19	1555	0.01			
Geranyl butyrate	12.23	1559	0.19	12.18*	1856	0.19
(<i>E</i>)-Nerolidol	12.27	1562	0.14	13.79	2003	0.14
Caryophyllene oxide	12.38*	1571	0.21	12.78	1910	0.20
Caryophyllene oxide isomer	12.38*	1571	[0.21]	12.70	1902	0.02
Humulene epoxide II	12.71	1597	0.01	13.36	1964	0.01
Geranyl isovalerate	12.76	1600	0.01	12.18*	1856	[0.19]
Caryophylladienol II	13.08	1627	0.02	16.06	2227	0.02
Precocene II	13.42	1655	0.01	17.16	2343	0.01
(3 <i>Z</i>)-Caryophylla-	13.54	1664	0.01	16.84*	2308	[1.17]

3,8(13)-dien-5 β -ol						
(2E,6E)-Farnesol	14.20	1720	1.10	16.84*	2308	[1.17]
(2E,6E)-Farnesol	14.39	1737	0.01	15.83	2203	0.01
Geranyl caproate	14.57	1753	0.94	14.27	2049	0.99
(2E,6E)-Farnesyl acetate	15.55	1840	0.12	15.95	2216	0.11
Phytone	15.60	1845	0.03	14.64	2085	0.02
Geranyl caprylate	16.72	1949	0.23			
Unknown [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...]	18.32	2107	0.02	19.00	2547	0.08
Unknown [m/z 69, 81 (54), 95 (26), 41 (20), 82 (16), 123 (16)...]	21.07	2407	0.02			
Total identified		98.75%			98.06%	
Total reported		98.90%			98.24%	

*: 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