

Date : 2023-12-21

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code** : 23L14-PTH04

**Customer Identification** : Palmarosa - India - P10112R

**Type** : Essential Oil

**Source** : *Cymbopogon martini*

**Customer** : Plant Therapy

Checked and approved by:

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Alexis St-Gelais, Ph. D., Chimiste 2013-174

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## GAS CHROMATOGRAPHIC ANALYSIS

**Method :** PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID

**\*ISO**

**Results :** See analysis summary (next page)

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

**Date :** 2023-12-20

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.4727 \pm 0.0003$  (20 °C)

**Method :** PC-MAT-016 - Measure of the refractive index of a liquid.

**Analyst :** Cindy Caron B. Sc.

**Date :** 2023-12-19

## 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	0.04	Aliphatic alcohol
Isobutyral	tr	Aliphatic aldehyde
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	0.04	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Hexanal	tr	Aliphatic aldehyde
(3Z)-Hexenol	0.01	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
Isoamyl acetate	0.01	Aliphatic ester
Unknown	0.01	Unknown
2-Heptanone	0.01	Aliphatic ketone
Hashishene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	0.11	Aliphatic ketone
<i>trans</i> -Dehydroxylinalool oxide	0.03	Monoterpenic ether
Myrcene	0.19	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.02	Monoterpenic ether
<i>para</i> -Cymene	0.01	Monoterpene
Limonene	0.11	Monoterpene
(Z)- $\beta$ -Ocimene	0.42	Monoterpene
(E)- $\beta$ -Ocimene	1.53	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.03	Aliphatic aldehyde
$\gamma$ -Terpinene	0.01	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.03	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
<i>trans</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Terpinolene	0.01	Monoterpene
Rosefuran	0.01	Monoterpenic ether
Linalool	2.55	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
Unknown	0.01	Unknown
Camphor	0.01	Monoterpenic ketone
neo-allo-Ocimene	0.01	Monoterpene
Citronellal	0.03	Monoterpenic aldehyde
Nerol oxide	0.01	Aliphatic ether
Terpinen-4-ol	0.01	Monoterpenic alcohol
Menthol	0.01	Monoterpenic alcohol
Isogeranial	0.01	Monoterpenic aldehyde
$\alpha$ -Terpineol	0.03	Monoterpenic alcohol

Decanal	0.01	Aliphatic aldehyde
Unknown	0.05	Unknown
Nerol	0.18	Monoterpenic alcohol
Citronellol	0.04	Monoterpenic alcohol
2,3-Epoxygeranial?	0.03	Monoterpenic aldehyde
Neral	0.24	Monoterpenic aldehyde
Isoamyl hexanoate	0.03	Aliphatic ester
Geraniol	79.65	Monoterpenic alcohol
Geranial	0.47	Monoterpenic aldehyde
Unknown	0.02	Oxygenated monoterpene
Perilla alcohol	0.07	Monoterpenic alcohol
Geranyl formate	0.10	Monoterpenic ester
2,3-Epoxygeraniol?	0.04	Oxygenated monoterpene
Neryl acetate	0.02	Monoterpenic ester
Geranyl acetate	8.05	Monoterpenic ester
$\beta$ -Elemene	0.08	Sesquiterpene
$\alpha$ -Gurjunene	0.03	Sesquiterpene
$\beta$ -Caryophyllene	1.25	Sesquiterpene
$\alpha$ -Humulene	0.09	Sesquiterpene
Germacrene D	0.01	Sesquiterpene
Unknown	0.06	Sesquiterpene
$\beta$ -Selinene	0.03	Sesquiterpene
Valencene	0.04	Sesquiterpene
$\alpha$ -Muurolene	0.01	Sesquiterpene
$\gamma$ -Cadinene	0.03	Sesquiterpene
$\alpha$ -Elemol	0.01	Sesquiterpenic alcohol
Unknown	0.01	Unknown
Geranyl butyrate	0.19	Monoterpenic ester
(E)-Nerolidol	0.10	Sesquiterpenic alcohol
Caryophyllene oxide	0.22	Sesquiterpenic ether
Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
Humulene epoxide II	0.01	Sesquiterpenic ether
Caryophylladienol II	0.02	Sesquiterpenic alcohol
(3Z)-Caryophylla-3,8(13)-dien-5 $\beta$ -ol	0.01	Sesquiterpenic alcohol
(2E,6Z)-Farnesal	0.01	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	1.08	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
Geranyl caproate	0.94	Monoterpenic ester
(2E,6E)-Farnesyl acetate	0.11	Sesquiterpenic ester
Phytone	0.03	Terpenic ketone
Geranyl caprylate	0.19	Monoterpenic ester
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Unknown	0.02	Unknown
Unknown	0.03	Unknown

<b>Consolidated total</b>	<b>99.10</b>
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tr: The compound has been detected below 0.005% of the total signal

Note: no correction factor was applied

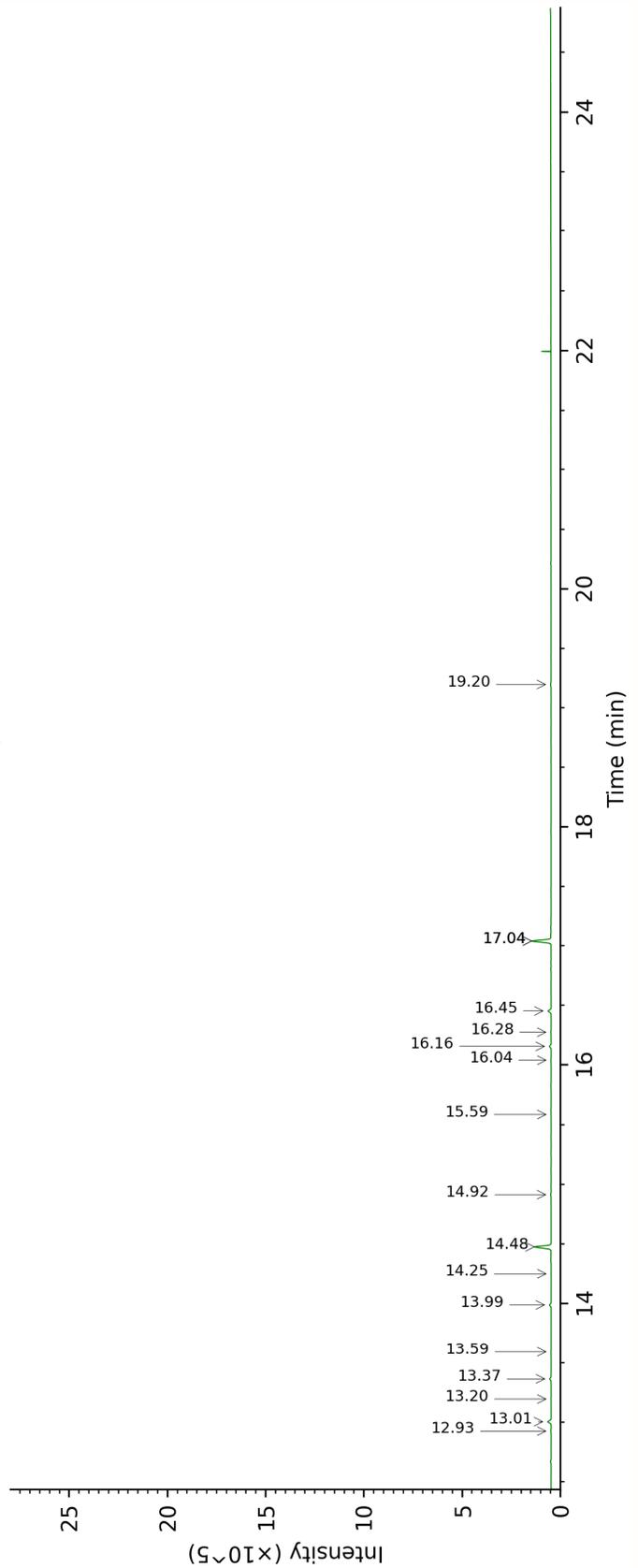
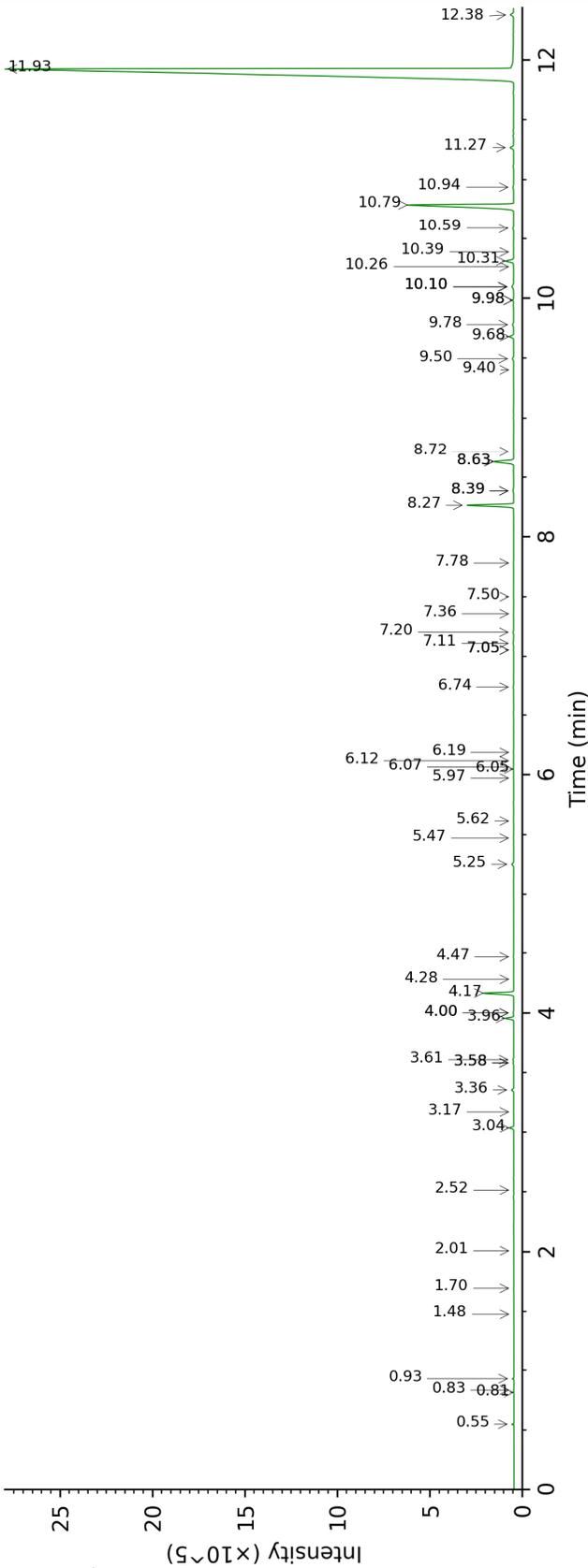
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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.

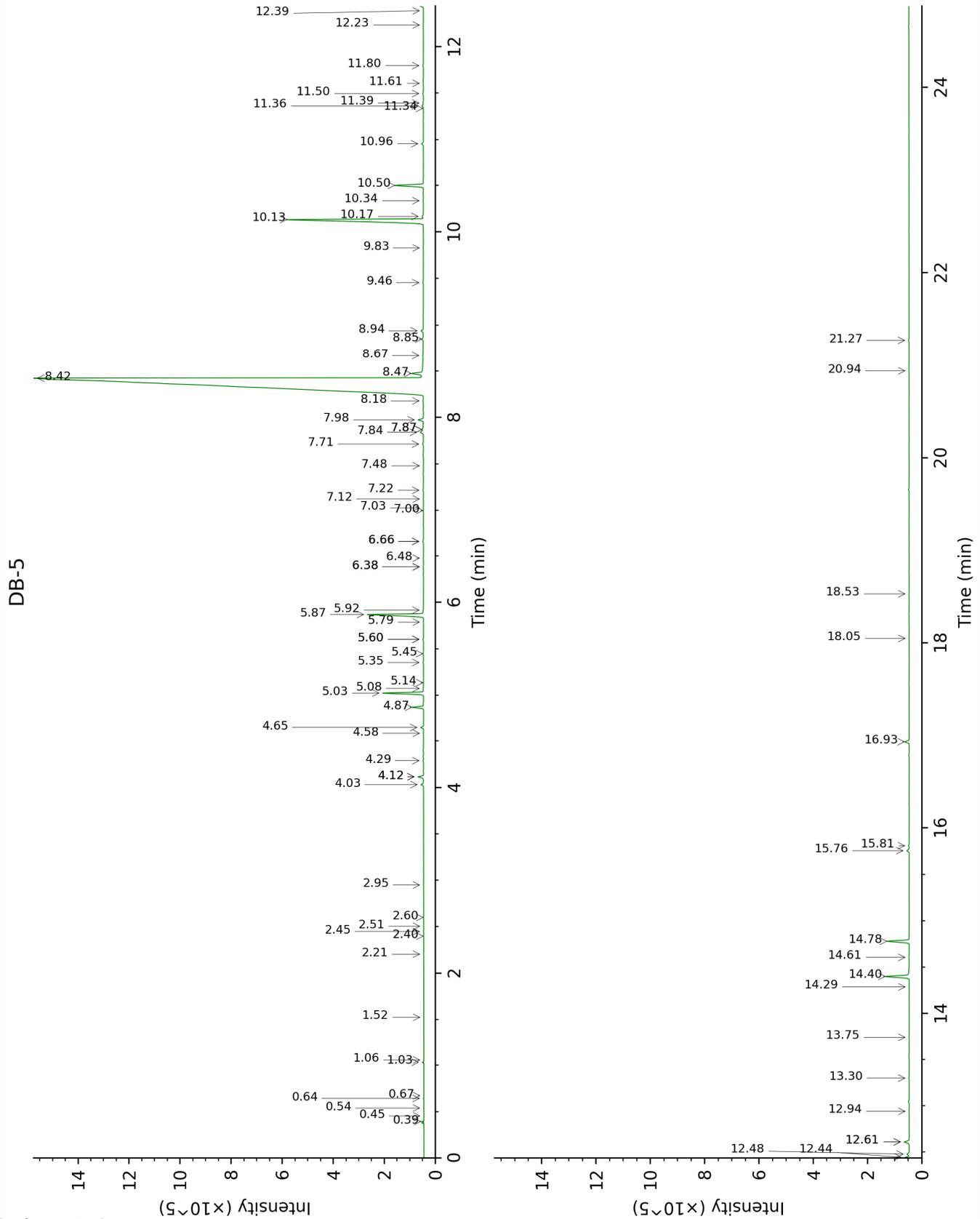
**Unknowns:** Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

**Bracketed value ([xx]):** A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

This page was intentionally left blank. The following pages present the complete data of the analysis.

DB-WAX





FULL ANALYSIS DATA

Ethanol	Column DB-WAX			Column DB-5		
	0.93	908.6	0.04	0.39	500.3	0.04
Isobutyral	0.55	777.8	0.04	0.45	537.6	tr
2-Methyl-3-buten-2-ol	1.70	1014.8	0.01	0.54	606.6	0.01
Isovaleral	0.84	886.3	0.01	0.64	641.3	0.01
2-Methylbutyral	0.82	879.6	tr	0.67	651.4	tr
Isoamyl alcohol	3.61	1176.5	0.04	1.03	732.6	0.04
2-Methylbutanol	3.58*	1174.5	[0.03]	1.06	736.1	tr
Hexanal	2.01	1044.4	tr	1.52	800.3	tr
(3Z)-Hexenol	5.97	1347.8	0.01	2.21	858.0	0.01
Hexanol	5.62	1322.2	0.01	2.40	874.0	0.01
Isoamyl acetate	2.52	1092.4	0.01	2.45	878.1	0.01
Unknown ZIOF II [m/z 59, 85 (88), 41 (57), 43 (43)...]	6.12	1358.2	0.01	2.51	882.7	0.01
2-Heptanone	3.17	1143.3	tr	2.60	890.5	0.01
Hashishene	1.48	991.1	0.01	2.95	916.3	0.01
6-Methyl-5-hepten-2-one	5.25	1294.8	0.11	4.03	987.4	0.11
<i>trans</i> -Dehydroxylinalool oxide	3.58*	1174.5	[0.03]	4.12*	993.0	[0.22]
Myrcene	3.04	1133.2	0.19	4.12*	993.0	[0.22]
<i>cis</i> -Dehydroxylinalool oxide	4.00*	1205.8	[0.02]	4.29	1004.4	0.02
<i>para</i> -Cymene	4.28	1225.8	tr	4.58	1022.8	0.01
Limonene	3.36	1157.3	0.10	4.65	1026.8	0.11
(Z)- $\beta$ -Ocimene	3.96	1202.6	0.41	4.86	1040.4	0.42
(E)- $\beta$ -Ocimene	4.17	1217.5	1.52	5.02	1050.4	1.53
2,6-Dimethyl-5-heptenal (melonal)	5.47	1312.0	0.01	5.08	1053.5	0.03
$\gamma$ -Terpinene	4.00*	1205.8	[0.02]	5.14	1057.4	0.01
<i>cis</i> -Linalool oxide (fur.)	6.74	1402.4	0.03	5.35	1071.0	0.03
Octanol	8.39*	1525.5	[0.04]	5.45	1076.9	0.02
<i>trans</i> -Linalool oxide (fur.)	7.05*	1425.9	[0.01]	5.60*	1086.5	[0.03]
Terpinolene	4.47	1239.2	0.01	5.60*	1086.5	[0.03]
Rosefuran	6.19	1363.2	0.01	5.79	1098.2	0.01
Linalool	8.27	1516.2	2.50	5.87	1103.3	2.55
Nonanal	6.07	1354.4	0.01	5.92	1106.3	0.02

Unknown COGU I [m/z 95, 123 (73), 67 (64), 82 (54), 41 (47), 55 (27)...]				6.38*	1136.0	[0.02]
Camphor	7.36	1448.3	0.01	6.38*	1136.0	[0.02]
neo-allo-Ocimene	6.05	1353.3	0.01	6.48	1142.0	0.01
Citronellal	7.20	1436.9	0.03	6.66*	1153.4	[0.04]
Nerol oxide	7.05*	1425.9	[0.01]	6.66*	1153.4	[0.04]
Terpinen-4-ol	8.72	1551.2	0.01	7.00	1175.2	0.01
Menthol	9.40	1604.2	0.01	7.03	1177.0	0.01
Isogeranial	8.39*	1525.5	[0.04]	7.12	1183.0	0.01
α-Terpineol	9.98*	1651.1	[0.04]	7.22	1189.0	0.03
Decanal	7.50	1458.8	0.01	7.48	1205.9	0.01
Unknown ARAB I [m/z 69, 41 (55), 111 (25), 93 (14), 109 (14)...]				7.71	1221.5	0.05
Nerol	11.27	1757.3	0.21	7.84	1230.0	0.18
Citronellol	10.94	1729.3	0.04	7.87*	1232.0	[0.08]
2,3- Epoxygeranial?				7.87*	1232.0	[0.08]
Neral	9.68	1626.7	0.25	7.98	1239.0	0.24
Isoamyl hexanoate	7.11	1430.0	0.03	8.18	1252.6	0.03
Geraniol	11.93	1813.6	79.65	8.42*†	1269.0	[79.75]
Geranial	10.31	1677.5	0.47	8.48*†	1272.4	[0.54]
Unknown CYFL VII [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	13.20	1926.9	0.01	8.67	1285.3	0.02
Perilla alcohol	13.37	1942.5	0.09	8.85	1297.5	0.07
Geranyl formate	10.10*	1660.2	[0.15]	8.94	1303.5	0.10
2,3- Epoxygeraniol?				9.46	1339.8	0.04
Neryl acetate	10.39	1683.6	0.01	9.83	1366.0	0.02
Geranyl acetate	10.79	1716.8	7.98	10.13	1387.5	8.05
β-Elemene	8.63*	1544.4	[1.29]	10.17	1389.9	0.08
α-Gurjunene	7.78	1479.7	0.01	10.34	1401.7	0.03
β-Caryophyllene	8.63*	1544.4	[1.29]	10.50	1413.8	1.25
α-Humulene	9.50	1611.7	0.08	10.96	1447.7	0.09
Germacrene D	9.98*	1651.1	[0.04]	11.34	1476.0	0.01
Unknown CASA VII [m/z 189, 133 (75), 91 (71), 105 (69), 93 (44)... 204	9.78	1634.7	0.08	11.36	1477.9	0.06

(33)]						
β-Selinene	10.10*	1660.2	[0.15]	11.39	1480.2	0.03
Valencene	10.10*	1660.2	[0.15]	11.50	1487.9	0.04
α-Murolene	10.26	1673.6	0.01	11.61	1496.0	0.01
γ-Cadinene	10.59	1699.9	0.06	11.80	1510.5	0.03
α-Elemol	14.25	2025.4	0.01	12.24	1544.8	0.01
Unknown CYMA I [m/z 59, 68 (63), 43 (31), 67 (27), 81 (27), 94 (25), 69 (23), 41 (22), 84 (20)...]				12.39	1556.9	0.01
Geranyl butyrate	12.38	1853.7	0.19	12.44	1561.1	0.19
(E)-Nerolidol	13.99	2000.4	0.10	12.48	1564.0	0.10
Caryophyllene oxide	13.01	1909.4	0.22	12.61*	1574.4	[0.22]
Caryophyllene oxide isomer	12.93	1902.1	0.02	12.61*	1574.4	[0.22]
Humulene epoxide II	13.59	1963.5	0.01	12.94	1600.2	0.01
Caryophylladienol II	16.28	2225.7	0.02	13.30	1629.5	0.02
(3Z)-Caryophylla- 3,8(13)-dien-5β-ol	17.04*	2305.3	[1.15]	13.75	1666.4	0.01
(2E,6Z)-Farnesal	15.59	2155.6	0.01	14.29	1711.5	0.01
(2E,6E)-Farnesol	17.04*	2305.3	[1.15]	14.40	1721.3	1.08
(2E,6E)-Farnesal	16.04	2201.4	0.01	14.61	1739.1	0.02
Geranyl caproate	14.48	2047.0	1.00	14.78	1754.2	0.94
(2E,6E)-Farnesyl acetate	16.16	2213.4	0.10	15.76	1840.3	0.11
Phytone	14.92	2088.8	0.03	15.81	1845.2	0.03
Geranyl caprylate	16.45	2244.1	0.20	16.93	1948.8	0.19
Unknown DRMO VII [m/z 69, 41 (49), 81 (47), 93 (21), 95 (30), 43 (26)...]				18.05	2057.5	0.01
Unknown DRMO VI [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...]	19.20	2544.7	0.05	18.53	2105.1	0.01
Unknown CYMA III [m/z 69, 81 (70), 93 (37), 95 (31), 41 (24)...]				20.94	2363.0	0.02

Unknown MOFI VII [m/z 69, 81 (54), 95 (26), 41 (20), 82 (16), 123 (16)...]			21.27	2400.4	0.03
Total reported	98.85%		99.26%		

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is 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