

Date : 2024-09-25

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code** : 24111-PTH03

**Customer Identification** : Palmarosa - India - P10114R

**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 :** 2024-09-18

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.4725 \pm 0.0003$  (20 °C)

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

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

**Date :** 2024-09-17

## 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	0.03	Aliphatic alcohol
Isobutyral	tr	Aliphatic aldehyde
2-Methyl-3-buten-2-ol	0.01	Aliphatic alcohol
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.03	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
(3Z)-Hexenol	tr	Aliphatic alcohol
Hexanol	tr	Aliphatic alcohol
Isoamyl acetate	tr	Aliphatic ester
Unknown	tr	Unknown
2-Heptanone	tr	Aliphatic ketone
Hashishene	tr	Monoterpene
$\alpha$ -Pinene	tr	Monoterpene
Camphene	tr	Monoterpene
Sabinene	tr	Monoterpene
$\beta$ -Pinene	tr	Monoterpene
6-Methyl-5-hepten-2-one	0.06	Aliphatic ketone
<i>trans</i> -Dehydroxylinalool oxide	tr	Monoterpenic ether
Myrcene	0.17	Monoterpene
6-Methyl-5-hepten-2-ol	0.01	Aliphatic alcohol
$\alpha$ -Phellandrene	0.02	Monoterpene
Pseudolimonene	tr	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.02	Monoterpenic ether
$\alpha$ -Terpinene	0.01	Monoterpene
<i>para</i> -Cymene	0.01	Monoterpene
Limonene	0.10	Monoterpene
1,8-Cineole	0.01	Monoterpenic ether
(Z)- $\beta$ -Ocimene	0.35	Monoterpene
(E)- $\beta$ -Ocimene	1.43	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.01	Aliphatic aldehyde
$\gamma$ -Terpinene	0.01	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
<i>para</i> -Cymenene	0.01	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Terpinolene	0.02	Monoterpene
Rosefuran	0.01	Monoterpenic ether
Linalool	2.54	Monoterpenic alcohol

Nonanal	0.01	Aliphatic aldehyde
(Z)-6-Methyl-3,5-heptadien-2-one	0.02	Aliphatic ketone
(E)-6-Methyl-3,5-heptadien-2-one	0.01	Aliphatic ketone
Unknown	0.01	Unknown
Camphor	0.01	Monoterpenic ketone
Citronellal	0.02	Monoterpenic aldehyde
Borneol	tr	Monoterpenic alcohol
$\alpha$ -Phellandren-8-ol	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.01	Monoterpenic alcohol
Menthol	0.01	Monoterpenic alcohol
$\alpha$ -Terpineol	0.03	Monoterpenic alcohol
Decanal	tr	Aliphatic aldehyde
Unknown	0.05	Unknown
Citronellol	0.03	Monoterpenic alcohol
Nerol	0.17	Monoterpenic alcohol
Neral	0.19	Monoterpenic aldehyde
Isoamyl hexanoate	0.02	Aliphatic ester
Geraniol	78.26	Monoterpenic alcohol
Geranial	0.37	Monoterpenic aldehyde
Unknown	0.01	Oxygenated monoterpene
Geranyl formate	0.09	Monoterpenic ester
2,3-Epoxygeraniol?	0.02	Oxygenated monoterpene
Neryl acetate	0.01	Monoterpenic ester
Geranic acid	0.01	Aliphatic acid
Geranyl acetate	10.09	Monoterpenic ester
$\beta$ -Elemene	0.09	Sesquiterpene
$\alpha$ -Gurjunene	0.01	Sesquiterpene
$\beta$ -Caryophyllene	1.55	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	[0.01]	Sesquiterpene
$\alpha$ -Guaiene	[0.01]	Sesquiterpene
$\alpha$ -Humulene	0.10	Sesquiterpene
Germacrene D	0.06	Sesquiterpene
Unknown	0.05	Sesquiterpene
Valencene	0.04	Sesquiterpene
$\alpha$ -Selinene	0.01	Sesquiterpene
$\alpha$ -Murolene	0.01	Sesquiterpene
$\gamma$ -Cadinene	0.03	Sesquiterpene
$\delta$ -Cadinene	0.03	Sesquiterpene
$\alpha$ -Elemol	0.01	Sesquiterpenic alcohol
Unknown	0.02	Unknown
Geranyl butyrate	0.19	Monoterpenic ester
(E)-Nerolidol	0.11	Sesquiterpenic alcohol
Caryophyllene oxide	0.16	Sesquiterpenic ether
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Humulene epoxide II	0.02	Sesquiterpenic ether

Caryophylladienol II	0.02	Sesquiterpenic alcohol
Neointermedeol	0.01	Sesquiterpenic alcohol
Precocene II	0.01	Chromane
(3Z)-Caryophylla-3,8(13)-dien-5 $\beta$ -ol	0.01	Sesquiterpenic alcohol
(2E,6E)-Farnesol	0.87	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.01	Sesquiterpenic aldehyde
Geranyl caproate	0.76	Monoterpenic ester
(2E,6E)-Farnesyl acetate	0.11	Sesquiterpenic ester
Phytone	0.02	Terpenic ketone
Geranyl caprylate	0.17	Monoterpenic ester
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Unknown	0.03	Unknown
Unknown	0.06	Unknown
Unknown	0.02	Unknown
<b>Consolidated total</b>	<b>99.00</b>	

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

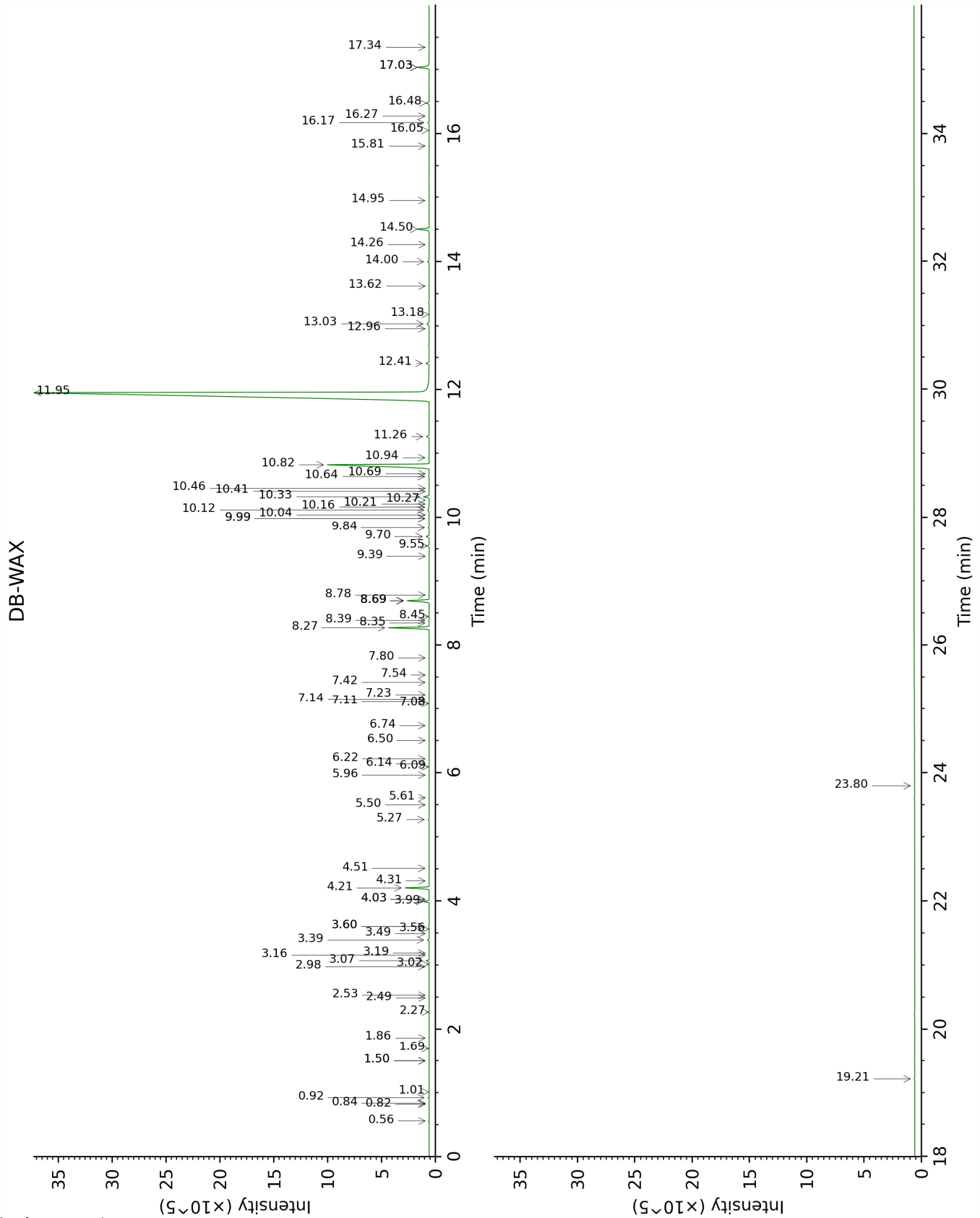
Note: no correction factor was applied

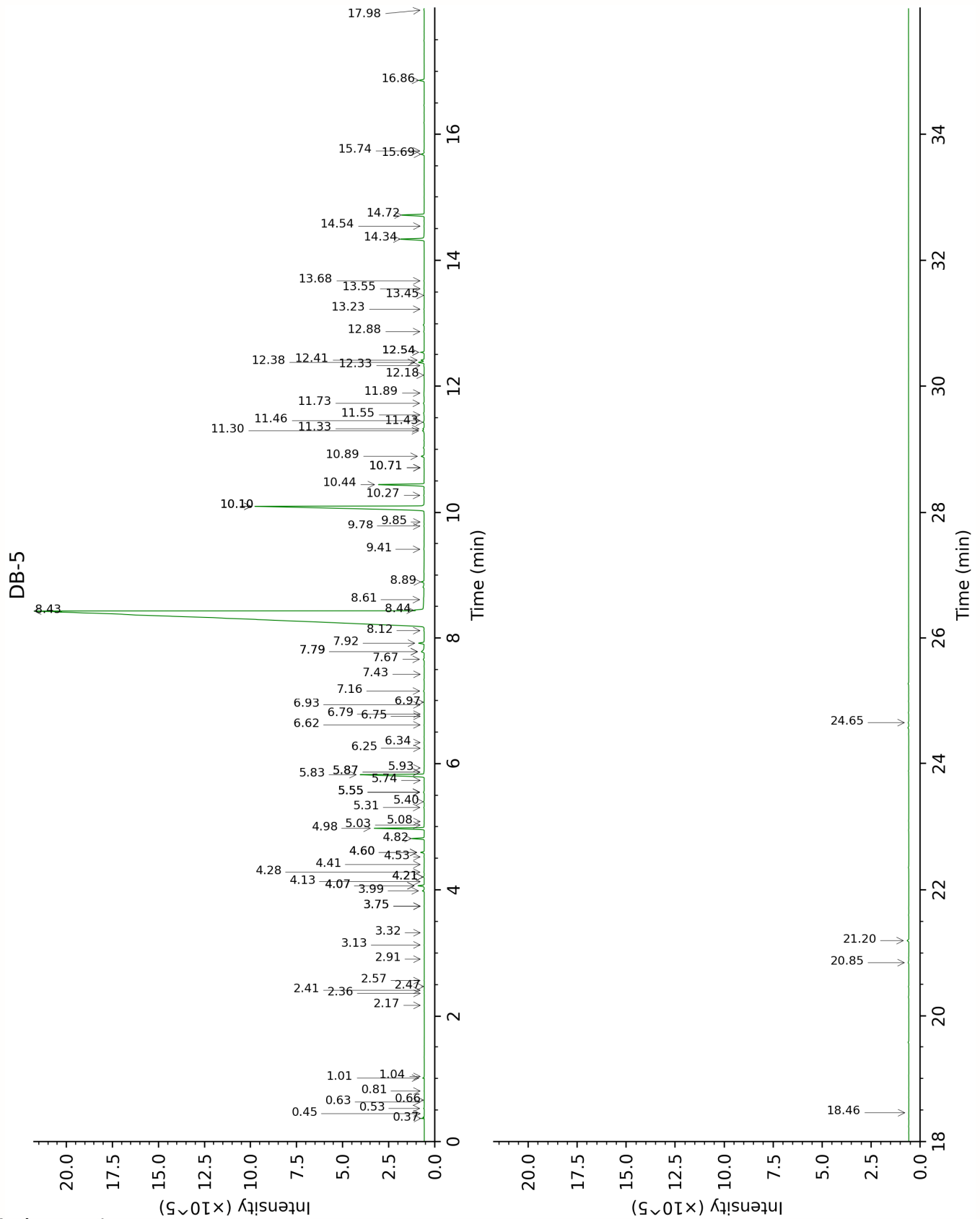
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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







FULL ANALYSIS DATA

Ethanol	Column DB-WAX			Column DB-5		
	0.92	904.3	0.04	0.37	499.0	0.03
Isobutylal	0.56	782.4	tr	0.45	537.3	tr
2-Methyl-3-buten-2-ol	1.69	1013.1	0.01	0.53	605.3	0.01
Isovaleral	0.84	884.8	tr	0.63	640.8	tr
2-Methylbutylal	0.82	878.8	tr	0.66	650.9	tr
2-Ethylfuran	1.01	918.1	tr	0.80	701.2	tr
Isoamyl alcohol	3.60*	1174.8	[0.05]	1.01	731.5	0.03
2-Methylbutanol	3.60*	1174.8	[0.05]	1.04	735.1	tr
(3Z)-Hexenol	5.96	1344.9	0.01	2.17	857.6	tr
Hexanol	5.61	1319.5	0.01	2.36	873.3	tr
Isoamyl acetate	2.53	1093.0	0.01	2.41	877.4	tr
Unknown ZIOF II [m/z 59, 85 (88), 41 (57), 43 (43)...]	6.14	1357.4	0.01	2.47	882.3	tr
2-Heptanone	3.19	1143.5	0.01	2.57	890.1	tr
Hashishene	1.50*	993.1	[tr]	2.91	915.3	tr
α-Pinene	1.50*	993.1	[tr]	3.13	930.2	tr
Camphene	1.86	1029.4	tr	3.32	942.9	tr
Sabinene	2.49	1088.9	tr	3.74*	970.8	[0.01]
β-Pinene	2.27	1068.1	tr	3.74*	970.8	[0.01]
6-Methyl-5-hepten-2-one	5.27	1292.8	0.06	3.99	986.8	0.06
<i>trans</i> - Dehydroxylinalool oxide	3.56	1171.8	tr	4.07*	992.2	[0.18]
Myrcene	3.07	1134.6	0.17	4.07*	992.2	[0.18]
6-Methyl-5-hepten-2-ol	7.11	1428.1	0.01	4.13	996.5	0.01
α-Phellandrene	2.98	1127.6	0.02	4.21*	1001.3	[0.02]
Pseudolimonene	3.02	1130.4	tr	4.21*	1001.3	[0.02]
<i>cis</i> - Dehydroxylinalool oxide	4.03*	1205.9	[0.02]	4.28	1006.3	0.02
α-Terpinene	3.16	1141.1	tr	4.40	1013.9	0.01
<i>para</i> -Cymene	4.31	1226.1	0.01	4.52	1021.4	0.01
Limonene	3.39	1158.9	0.10	4.60*	1025.8	[0.11]
1,8-Cineole	3.49	1166.4	0.01	4.60*	1025.8	[0.11]
(Z)-β-Ocimene	3.99	1203.5	0.35	4.82	1039.6	0.35
(E)-β-Ocimene	4.20	1218.4	1.44	4.98	1049.8	1.43
2,6-Dimethyl-5-heptenal (melonal)	5.50	1311.6	0.01	5.03	1053.0	0.01

$\gamma$ -Terpinene	4.03*	1205.9	[0.02]	5.08	1056.5	0.01
<i>cis</i> -Linalool oxide (fur.)	6.74	1400.3	0.02	5.31	1070.4	0.02
Octanol	8.39	1523.7	0.02	5.40	1076.1	0.02
<i>para</i> -Cymenene	6.50	1383.6	0.01	5.55*	1085.6	[0.03]
<i>trans</i> -Linalool oxide (fur.)	7.08	1425.8	0.01	5.55*	1085.6	[0.03]
Terpinolene	4.51	1239.8	0.02	5.55*	1085.6	[0.03]
Rosefuran	6.22	1363.0	0.01	5.74	1097.3	0.01
Linalool	8.27	1514.9	2.54	5.83	1103.0	2.54
Nonanal	6.09	1354.1	0.01	5.87*	1105.6	[0.02]
( <i>Z</i> )-6-Methyl-3,5-heptadien-2-one	8.45	1528.5	0.02	5.87*	1105.6	[0.02]
( <i>E</i> )-6-Methyl-3,5-heptadien-2-one	8.35	1520.6	0.02	5.93	1109.8	0.01
Unknown COGU I [m/z 95, 123 (73), 67 (64), 82 (54), 41 (47), 55 (27)...]				6.25	1129.7	0.01
Camphor	7.42	1451.0	0.01	6.34	1135.6	0.01
Citronellal	7.23	1436.6	0.01	6.62	1153.4	0.02
Borneol	9.99*	1649.8	[0.04]	6.75	1162.1	tr
$\alpha$ -Phellandren-8-ol	10.41	1684.0	0.02	6.79	1164.3	0.01
Terpinen-4-ol	8.78	1554.4	0.01	6.93	1173.7	0.01
Menthol	9.39	1601.4	0.01	6.98	1176.3	0.01
$\alpha$ -Terpineol	9.99*	1649.8	[0.04]	7.16	1188.4	0.03
Decanal	7.54	1459.5	0.01	7.43	1205.4	tr
Unknown ARAB I [m/z 69, 41 (55), 111 (25), 93 (14), 109 (14)...]				7.67	1221.3	0.05
Citronellol	10.94	1728.0	0.03	7.79*	1229.4	[0.20]
Nerol	11.26	1755.7	0.17	7.79*	1229.4	[0.20]
Neral	9.70	1626.3	0.20	7.92	1238.4	0.19
Isoamyl hexanoate	7.14	1430.5	0.02	8.12	1251.7	0.02
Geraniol	11.95	1814.6	78.26	8.43*†	1272.5	[78.40]
Geranial	10.33	1677.2	0.37	8.44*†	1273.3	[0.40]
Unknown CYFL VII [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	13.18	1924.4	tr	8.61	1284.5	0.01
Geranyl formate	10.12	1660.4	0.13	8.89	1303.3	0.09
2,3-				9.41	1339.8	0.02

Epoxygeraniol?						
Neryl acetate	10.46	1687.9	0.01	9.78	1365.8	0.01
Geranic acid				9.85	1371.1	0.01
Geranyl acetate	10.82	1718.6	10.09	10.10*	1388.6	[10.18]
β-Elemene	8.69*	1547.5	[1.61]	10.10*	1388.6	[10.18]
α-Gurjunene	7.80	1479.3	0.01	10.27	1400.8	0.01
β-Caryophyllene	8.69*	1547.5	[1.61]	10.44	1413.4	1.55
<i>trans</i> -α-Bergamotene	8.69*	1547.5	[1.61]	10.71*	1433.3	[0.01]
α-Guaiene	8.69*	1547.5	[1.61]	10.71*	1433.3	[0.01]
α-Humulene	9.55	1614.6	0.10	10.89	1446.8	0.10
Germacrene D	10.04	1654.3	0.01	11.30	1476.9	0.06
Unknown CASA VII [m/z 189, 133 (75), 91 (71), 105 (69), 93 (44)... 204 (33)]	9.84	1637.6	0.06	11.33	1479.2	0.05
Valencene	10.16	1664.1	0.03	11.43	1486.9	0.04
α-Selinene	10.21	1668.1	0.01	11.46	1488.8	0.01
α-Murolene	10.27	1672.9	0.02	11.55	1495.6	0.01
γ-Cadinene	10.64	1703.1	0.05	11.73	1509.7	0.03
δ-Cadinene	10.68	1706.8	0.01	11.89	1522.4	0.03
α-Elemol	14.26	2025.6	0.01	12.18	1544.6	0.01
Unknown CYMA I [m/z 59, 68 (63), 43 (31), 67 (27), 81 (27), 94 (25), 69 (23), 41 (22), 84 (20)...]				12.33	1556.5	0.02
Geranyl butyrate	12.41	1855.1	0.20	12.38	1560.5	0.19
( <i>E</i> )-Nerolidol	14.00	2000.2	0.10	12.42	1563.3	0.11
Caryophyllene oxide	13.03	1911.0	0.16	12.54*	1573.5	[0.16]
Caryophyllene oxide isomer	12.96	1903.9	0.01	12.54*	1573.5	[0.16]
Humulene epoxide II	13.62	1964.9	0.01	12.88	1599.6	0.02
Caryophylladienol II	16.27	2224.9	0.02	13.23	1628.6	0.02
Neointermedeol	15.81	2177.1	0.02	13.45	1646.5	0.01
Precocene II	17.34	2337.9	0.01	13.55	1655.2	0.01
(3 <i>Z</i> )-Caryophylla-3,8(13)-dien-5β-ol	17.03*	2304.5	[0.88]	13.68	1665.5	0.01
(2 <i>E</i> ,6 <i>E</i> )-Farnesol	17.03*	2304.5	[0.88]	14.34	1720.8	0.87
(2 <i>E</i> ,6 <i>E</i> )-Farnesal	16.05	2202.0	0.01	14.54	1738.6	0.01

Geranyl caproate	14.50	2048.7	0.78	14.72	1753.7	0.76
(2E,6E)-Farnesyl acetate	16.17	2214.5	0.10	15.69	1839.7	0.11
Phytone	14.95	2091.5	0.02	15.74	1844.4	0.02
Geranyl caprylate	16.48	2246.0	0.18	16.86	1948.0	0.17
Unknown DRMO VII [m/z 69, 41 (49), 81 (47), 93 (21), 95 (30), 43 (26)...]				17.98	2056.5	0.01
Unknown DRMO VI [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...]	19.21	2546.4	0.04	18.46	2104.6	0.01
Unknown CYMA III [m/z 69, 81 (70), 93 (37), 95 (31), 41 (24)...]				20.85	2360.5	0.03
Unknown MOFI VII [m/z 69, 81 (54), 95 (26), 41 (20), 82 (16), 123 (16)...]				21.20	2399.7	0.06
Unknown CYWI IV [m/z 69, 81 (64), 95 (29), 137 (19), 41 (19)...]	23.80	3128.2	0.02	24.65	2825.5	0.02
Total reported		98.88%			99.16%	

\*: 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