

Date : September 10, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

**Internal code** : 21I08-PTH13

**Customer identification** : Palmarosa - India - P10109215R

**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** : Sarah-Eve Tremblay, M. Sc. A., Chimiste

**Analysis date** : September 09, 2021

Checked and approved by :

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Alexis St-Gelais, M. Sc., Chimiste 2013-174

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Light yellow liquid

**Refractive index:**  $1.4736 \pm 0.0003$  (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	tr	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Hexanol	tr	Aliphatic alcohol
Isoamyl acetate	tr	Aliphatic ester
Unknown	tr	Unknown
2-Heptanone	0.01	Aliphatic ketone
Hashishene	tr	Monoterpene
$\alpha$ -Thujene	0.01	Monoterpene
$\alpha$ -Pinene	0.01	Monoterpene
Camphene	tr	Monoterpene
6-Methyl-5-hepten-2-one	0.05	Aliphatic ketone
Myrcene	0.21	Monoterpene
$\alpha$ -Phellandrene	0.02	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.01	Monoterpenic ether
$\Delta^3$ -Carene	0.02	Monoterpene
para-Cymene	0.01	Monoterpene
Limonene	0.11	Monoterpene
1,8-Cineole	tr	Monoterpenic ether
$\beta$ -Phellandrene	tr	Monoterpene
( <i>Z</i> )- $\beta$ -Ocimene	0.39	Monoterpene
( <i>E</i> )- $\beta$ -Ocimene	1.61	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.02	Aliphatic aldehyde
$\gamma$ -Terpinene	0.01	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
<i>trans</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Terpinolene	0.03	Monoterpene
Rosefuran	0.01	Monoterpenic ether
Linalool	2.69	Monoterpenic alcohol
Nonanal	0.04	Aliphatic aldehyde
Unknown	0.01	Unknown
Camphor	0.01	Monoterpenic ketone
Nerol oxide	0.01	Aliphatic ether
Citronellal	0.01	Monoterpenic aldehyde
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
Nerol	0.16	Monoterpenic alcohol
2,3-Epoxygeranial?	0.06	Monoterpenic aldehyde

Citronellol	0.03	Monoterpenic alcohol
Neral	0.17	Monoterpenic aldehyde
Geraniol	78.49	Monoterpenic alcohol
Geranial	0.46	Monoterpenic aldehyde
Perilla alcohol	0.08	Monoterpenic alcohol
Geranyl formate	0.10	Monoterpenic ester
2,3-Epoxygeraniol?	0.03	Oxygenated monoterpene
Neryl acetate	0.04	Monoterpenic ester
Geranyl acetate	9.00	Monoterpenic ester
β-Elemene	0.02	Sesquiterpene
β-Caryophyllene	1.98	Sesquiterpene
<i>trans</i> -α-Bergamotene	0.01*	Sesquiterpene
α-Guaiene	[0.01]*	Sesquiterpene
α-Humulene	0.14	Sesquiterpene
Selina-4,11-diene	0.01	Sesquiterpene
Germacrene D	0.01	Sesquiterpene
Unknown	0.08	Sesquiterpene
β-Selinene	0.02	Sesquiterpene
Valencene	0.05	Sesquiterpene
α-Murolene	0.04	Sesquiterpene
γ-Cadinene	0.04	Sesquiterpene
7-epi-α-Selinene	0.01	Sesquiterpene
δ-Cadinene	0.02	Sesquiterpene
α-Elemol	0.01	Sesquiterpenic alcohol
Unknown	0.02	Unknown
Geranyl butyrate	0.16	Monoterpenic ester
( <i>E</i> )-Nerolidol	0.14	Sesquiterpenic alcohol
Caryophyllene oxide	0.17	Sesquiterpenic ether
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Humulene epoxide II	0.01	Sesquiterpenic ether
Caryophylladienol II	0.02	Sesquiterpenic alcohol
(3 <i>Z</i> )-Caryophylla-3,8(13)-dien-5β-ol	0.01	Sesquiterpenic alcohol
(2 <i>E</i> ,6 <i>Z</i> )-Farnesal	0.01	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>E</i> )-Farnesol	0.87	Sesquiterpenic alcohol
(2 <i>E</i> ,6 <i>E</i> )-Farnesal	0.01	Sesquiterpenic aldehyde
Geranyl caproate	0.65	Monoterpenic ester
(2 <i>E</i> ,6 <i>E</i> )-Farnesyl acetate	0.10	Sesquiterpenic ester
Phytone	0.02	Terpenic ketone
Geranyl caprylate	0.15	Monoterpenic ester
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Unknown	0.04	Unknown
<b>Consolidated total</b>	<b>98.95%</b>	

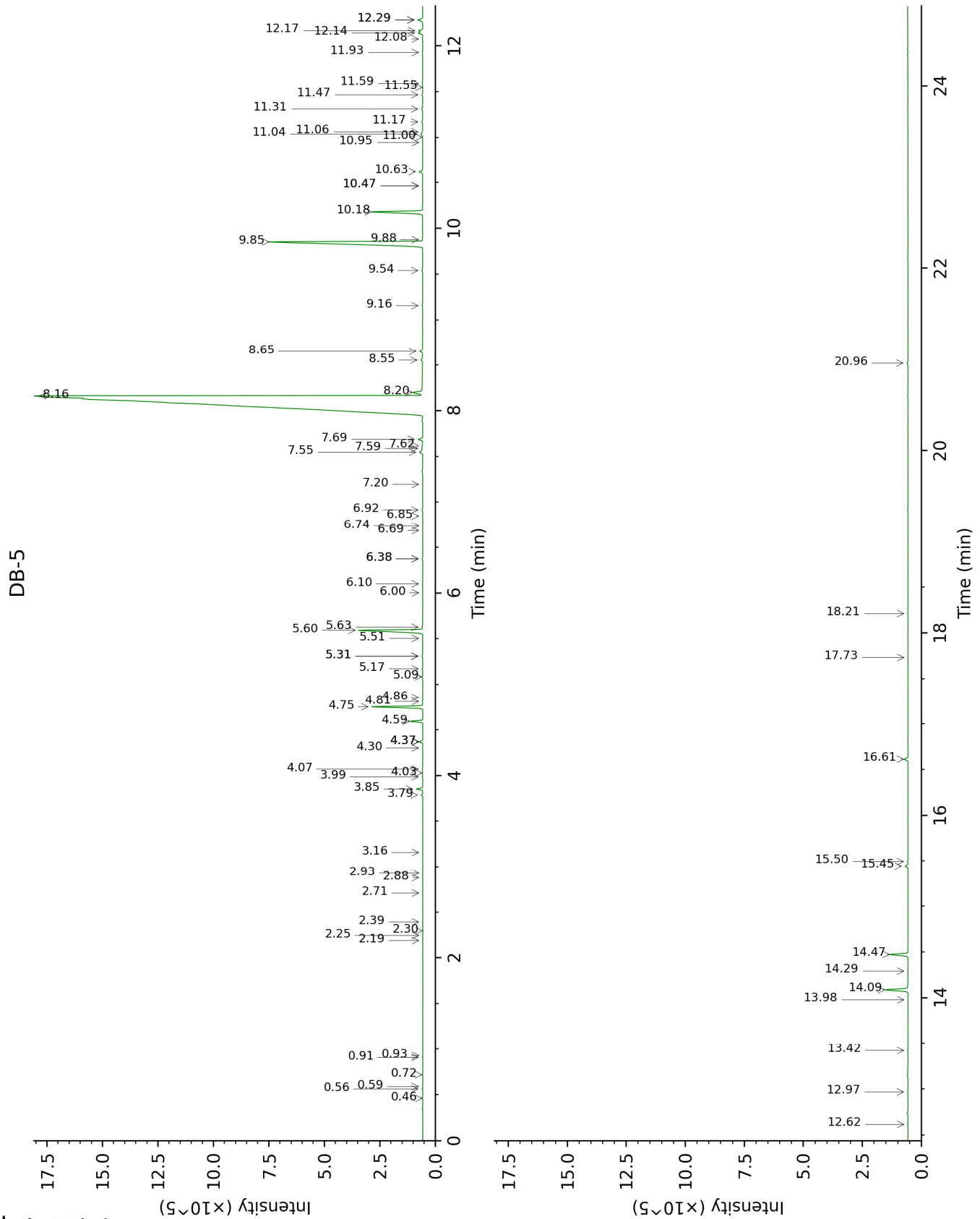
\*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered  
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total  
tr: The compound has been detected below 0.005% of total signal.

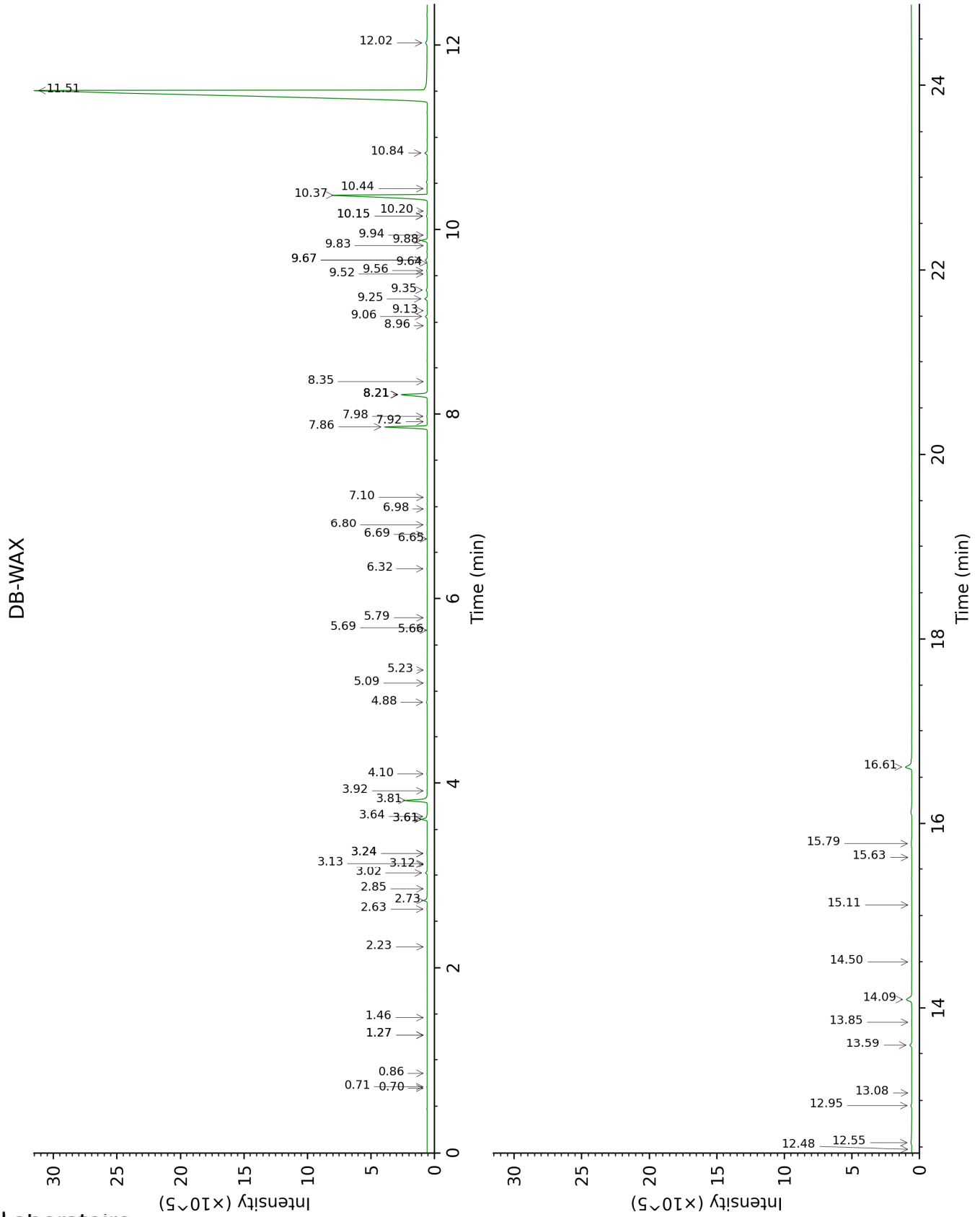
Note: no correction factor was applied

**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	600	tr	1.46	1014	tr
Isovaleral	0.56	641	0.01	0.71	888	0.01
2-Methylbutyral	0.59	652	0.01	0.70	882	tr
2-Ethylfuran	0.72	700	tr	0.86	920	tr
Isoamyl alcohol	0.91	731	0.01	3.24*	1177	0.02
2-Methylbutanol	0.93	734	tr	3.24*	1177	[0.02]
Hexanol	2.19	873	tr	5.23	1322	0.01
Isoamyl acetate	2.25	878	tr	2.23	1093	tr
Unknown [m/z 59, 85 (88), 41 (57), 43 (43)...]	2.30	883	tr	5.69	1355	0.01
2-Heptanone	2.39	891	0.01	2.85	1145	tr
Hashishene	2.71	915	tr	1.27*	991	0.01
$\alpha$ -Thujene	2.88	926	0.01			
$\alpha$ -Pinene	2.93	930	0.01	1.27*	991	[0.01]
Camphene	3.16	946	tr			
6-Methyl-5-hepten-2-one	3.79	988	0.05	4.88	1303	0.05
Myrcene	3.85	992	0.21	2.73	1135	0.24
$\alpha$ -Phellandrene	3.99	1001	0.02	2.63	1127	0.01
<i>cis</i> -Dehydroxylinalool oxide	4.03	1004	0.01	3.61*	1207	0.40
$\Delta$ 3-Carene	4.07	1007	0.02			
para-Cymene	4.30	1021	0.01	3.92	1230	0.01
Limonene	4.37*	1026	0.12	3.02	1159	0.11
1,8-Cineole	4.37*	1026	[0.12]	3.13	1168	tr
$\beta$ -Phellandrene	4.37*	1026	[0.12]	3.12	1167	tr
( <i>Z</i> )- $\beta$ -Ocimene	4.59	1040	0.39	3.61*	1207	[0.40]
( <i>E</i> )- $\beta$ -Ocimene	4.75	1050	1.61	3.82	1222	1.63
2,6-Dimethyl-5-heptenal (melonal)	4.81	1054	0.02	5.09	1311	0.01
$\gamma$ -Terpinene	4.86	1057	0.01	3.64	1209	0.03
<i>cis</i> -Linalool oxide (fur.)	5.09	1071	0.02	6.32	1401	0.02
Octanol	5.17	1077	0.02	7.92	1522	0.01
<i>trans</i> -Linalool oxide (fur.)	5.31*†	1085	0.04	6.69	1429	0.02
Terpinolene	5.31*†	1085	[0.04]	4.10	1244	0.03
Rosefuran	5.51	1098	0.01	5.80	1363	0.01
Linalool	5.60	1103	2.69	7.86	1518	2.74
Nonanal	5.63	1105	0.04	5.66	1353	0.01
Unknown [m/z 95, 123 (73), 67 (64), 82 (54), 41 (47), 55 (27)...]	6.00	1130	0.01			

Camphor	6.10	1136	0.01	6.98	1451	0.01
Nerol oxide	6.38*	1153	0.03	6.65	1426	0.01
Citronellal	6.38*	1153	[0.03]	6.80	1437	0.01
Terpinen-4-ol	6.69	1173	0.01	8.35	1556	0.01
Menthol	6.74	1177	0.01	8.96	1604	tr
Isogeranial	6.85	1184	0.01	7.98	1527	0.04
$\alpha$ -Terpineol	6.92	1188	0.03	9.56	1653	0.04
Decanal	7.20	1206	0.01	7.10	1460	0.01
Nerol	7.55	1230	0.16	10.84	1760	0.17
2,3-Epoxygeranial?	7.59	1233	0.06			
Citronellol	7.62	1235	0.03	10.44	1727	0.04
Neral	7.69	1239	0.17	9.25	1628	0.18
Geraniol	8.16	1271	78.49	11.51	1819	79.08
Geranial	8.20	1274	0.46	9.88	1680	0.41
Perilla alcohol	8.56	1297	0.08	12.95	1949	0.07
Geranyl formate	8.65	1304	0.10	9.67*	1662	0.14
2,3-Epoxygeraniol?	9.16	1340	0.03			
Neryl acetate	9.54	1367	0.04	9.94	1684	0.01
Geranyl acetate	9.85	1389	9.00	10.37	1720	8.90
$\beta$ -Elemene	9.88	1391	0.02	8.21*	1545	2.09
$\beta$ -Caryophyllene	10.18	1413	1.98	8.21*	1545	[2.09]
<i>trans</i> - $\alpha$ -Bergamotene	10.47*	1434	0.01	8.21*	1545	[2.09]
$\alpha$ -Guaiene	10.47*	1434	[0.01]	8.21*	1545	[2.09]
$\alpha$ -Humulene	10.63	1446	0.14	9.06	1612	0.13
Selina-4,11-diene	10.95	1470	0.01	9.13	1618	0.01
Germacrene D	11.00	1474	0.01	9.52	1650	0.02
Unknown [m/z 189, 133 (75), 91 (71), 105 (69), 93 (44)... 204 (33)]	11.04	1476	0.08	9.35	1636	0.09
$\beta$ -Selinene	11.06	1478	0.02	9.64	1660	0.02
Valencene	11.17	1486	0.05	9.67*	1662	[0.14]
$\alpha$ -Muurolene	11.31	1497	0.04	9.83	1675	0.01
$\gamma$ -Cadinene	11.47	1509	0.04	10.15*	1701	0.06
7-epi- $\alpha$ -Selinene	11.55	1515	0.01	10.20	1706	0.02
$\delta$ -Cadinene	11.59	1518	0.02	10.15*	1701	[0.06]
$\alpha$ -Elemol	11.93	1545	0.01	13.85	2034	tr
Unknown [m/z 59, 68 (63), 43 (31), 67 (27), 81 (27), 94 (25), 69 (23), 41 (22), 84 (20)...]	12.08	1557	0.02			
Geranyl butyrate	12.14	1562	0.16	12.02	1864	0.15
( <i>E</i> )-Nerolidol	12.17	1564	0.14	13.59	2009	0.14
Caryophyllene oxide	12.29*	1573	0.21	12.55	1912	0.17
Caryophyllene oxide isomer	12.29*	1573	[0.21]	12.48	1905	0.01

Humulene epoxide II	12.62	1599	0.01	13.08	1961	tr
Caryophylladienol II	12.97	1628	0.02	15.78	2227	0.10
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	13.42	1665	0.01			
(2E,6Z)-Farnesal	13.98	1712	0.01	15.11	2159	tr
(2E,6E)-Farnesol	14.09	1722	0.87	16.61	2314	0.75
(2E,6E)-Farnesal	14.29	1739	0.01	15.64	2211	0.01
Geranyl caproate	14.47	1755	0.65	14.09	2058	0.66
(2E,6E)-Farnesyl acetate	15.45	1841	0.10			
Phytone	15.50	1846	0.02	14.50	2097	0.01
Geranyl caprylate	16.62	1950	0.15			
Unknown [m/z 69, 41 (49), 81 (47), 93 (21), 95 (30), 43 (26)...]	17.73	2059	0.01			
Unknown [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...]	18.21	2106	0.01			
Unknown [m/z 69, 81 (54), 95 (26), 41 (20), 82 (16), 123 (16)...]	20.96	2402	0.04			
<b>Total identified</b>		<b>98.80%</b>			<b>98.89%</b>	
<b>Total reported</b>		<b>98.97%</b>			<b>98.99%</b>	

\*: 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