

Date : July 06, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21F21-PTH09


Customer identification : Palmarosa Organic - India - PK0104920R

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 : Seydou Ka, Ph. D.

Analysis date : July 05, 2021

Checked and approved by :

Sylvain Mercier, M. Sc., chimiste 2014-005

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia. This report is digitally signed, it is only considered valid if the digital signature is intact. The results only describe the samples that were submitted to the assays.

PHYSICOCHEMICAL DATA

Physical aspect: Light yellow liquid

Refractive index: 1.4738 ± 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	tr	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutyl acetate	tr	Aliphatic ester
2-Heptanone	tr	Aliphatic ketone
Hashishene	tr	Monoterpene
6-Methyl-5-hepten-2-one	0.05	Aliphatic ketone
<i>trans</i> -Dehydroxylinalool oxide	0.01	Monoterpenic ether
Myrcene	0.19	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.02	Monoterpenic ether
para-Cymene	tr	Monoterpene
Limonene	0.11	Monoterpene
(<i>Z</i>)- β -Ocimene	0.39	Monoterpene
(<i>E</i>)- β -Ocimene	1.49	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
<i>trans</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Terpinolene	0.02	Monoterpene
Linalool	2.59	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
Camphor	tr	Monoterpenic ketone
Terpinen-4-ol	0.01	Monoterpenic alcohol
α -Terpineol	0.03	Monoterpenic alcohol
Decanal	tr	Aliphatic aldehyde
Nerol	0.17	Monoterpenic alcohol
Citronellol	0.04	Monoterpenic alcohol
Neral	0.17	Monoterpenic aldehyde
Geraniol	80.79	Monoterpenic alcohol
Geranial	0.37	Monoterpenic aldehyde
Geranyl formate	0.10	Monoterpenic ester
2,3-Epoxygeraniol?	0.03	Oxygenated monoterpene
Geranic acid	0.05	Aliphatic acid
Neryl acetate	0.02	Monoterpenic ester
Unknown	0.09	Unknown
Geranyl acetate	6.85	Monoterpenic ester
β -Elemene	0.02	Sesquiterpene
β -Caryophyllene	1.60	Sesquiterpene
α -Guaiene	0.02*	Sesquiterpene
<i>trans</i> - α -Bergamotene	[0.02]*	Sesquiterpene
α -Humulene	0.11	Sesquiterpene
Selina-4,11-diene	0.02	Sesquiterpene
Unknown	0.06	Sesquiterpene
β -Selinene	0.02	Sesquiterpene
Valencene	0.04	Sesquiterpene

α-Muurolene	0.01	Sesquiterpene
7-epi-α-Selinene	0.03	Sesquiterpene
δ-Cadinene	0.01	Sesquiterpene
α-Elemol	0.01	Sesquiterpenic alcohol
Unknown	0.02	Unknown
Geranyl butyrate	0.18	Monoterpenic ester
(E)-Nerolidol	0.11	Sesquiterpenic alcohol
Caryophyllene oxide	0.20	Sesquiterpenic ether
Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
Humulene epoxide II	0.01	Sesquiterpenic ether
Caryophylladienol II	0.01	Sesquiterpenic alcohol
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	0.01	Sesquiterpenic alcohol
(2E,6Z)-Farnesal	tr	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	0.87	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.01	Sesquiterpenic aldehyde
Geranyl caproate	0.71	Monoterpenic ester
(2E,6E)-Farnesyl acetate	0.08	Sesquiterpenic ester
Phytone	0.03	Terpenic ketone
Geranyl caprylate	0.17	Monoterpenic ester
Unknown	tr	Unknown
Unknown	0.03	Unknown
Unknown	0.02	Unknown
Consolidated total	98.13%	

*: 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

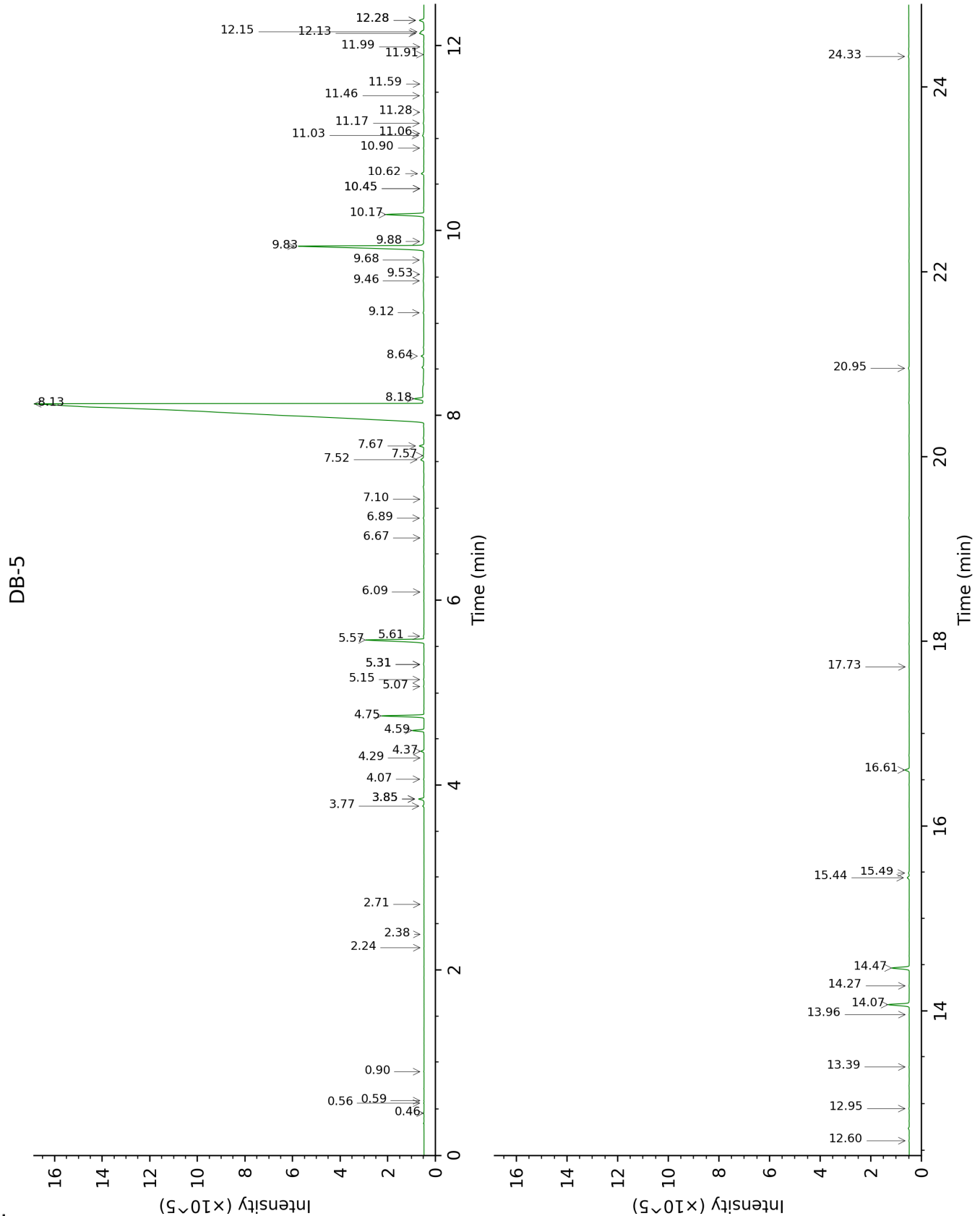
tr: The compound has been detected below 0.005% of total signal.

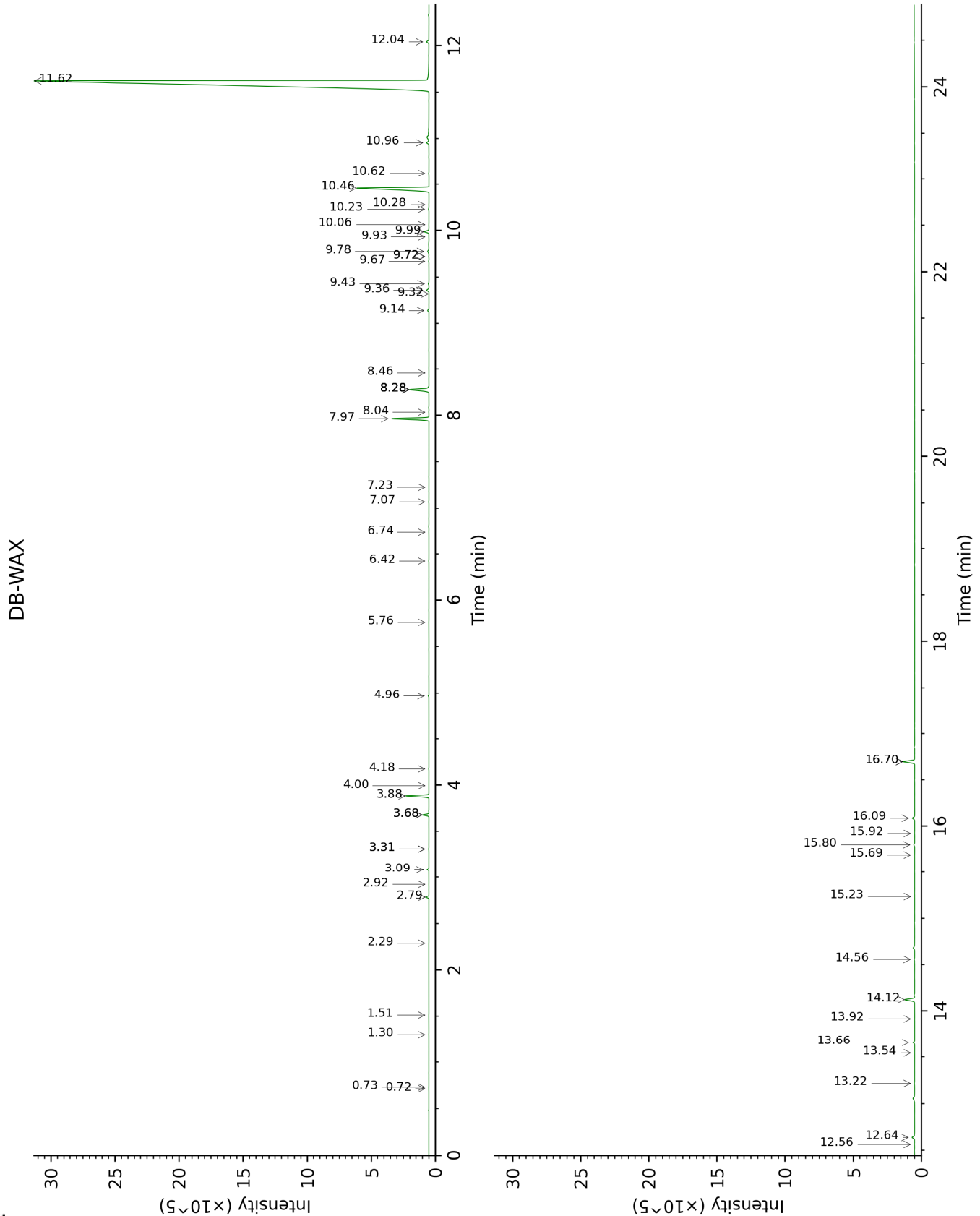
Note: no correction factor was applied

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	596	tr	1.51	1014	tr
Isovaleral	0.56	643	0.01	0.73	888	0.01
2-Methylbutyral	0.59	653	tr	0.72	882	tr
Isoamyl alcohol	0.90	731	0.01	3.31*	1176	0.02
2-Methylbutyl acetate	2.24	878	tr	2.29	1094	tr
2-Heptanone	2.38	891	tr	2.92	1145	tr
Hashishene	2.71	915	tr	1.30	990	tr
6-Methyl-5-hepten-2-one	3.78	988	0.05	4.96	1298	0.05
<i>trans</i> -Dehydroxylinalool oxide	3.85*	993	0.20	3.31*	1176	[0.02]
Myrcene	3.85*	993	[0.20]	2.79	1134	0.19
<i>cis</i> -Dehydroxylinalool oxide	4.06	1007	0.02	3.68*	1206	0.39
para-Cymene	4.29	1022	tr	4.00	1229	tr
Limonene	4.37	1026	0.11	3.09	1158	0.11
(<i>Z</i>)- β -Ocimene	4.59	1041	0.39	3.68*	1206	[0.39]
(<i>E</i>)- β -Ocimene	4.75	1051	1.49	3.88	1221	1.47
<i>cis</i> -Linalool oxide (fur.)	5.07	1071	0.02	6.42	1403	0.02
Octanol	5.15	1076	0.02	8.04	1524	0.02
<i>trans</i> -Linalool oxide (fur.)	5.31*	1086	0.02	6.74	1426	0.01
Terpinolene	5.31*	1086	[0.02]	4.18	1243	0.02
Linalool	5.57	1103	2.59	7.97	1519	2.56
Nonanal	5.61	1106	0.02	5.76	1355	0.01
Camphor	6.09	1137	tr	7.07	1451	0.02
Terpinen-4-ol	6.67	1175	0.01	8.46	1557	0.01
α -Terpineol	6.89	1189	0.03	9.67†	1653	0.05
Decanal	7.10	1202	tr	7.23	1463	tr
Nerol	7.52	1231	0.17	10.96	1760	0.48
Citronellol	7.57	1234	0.04	10.62	1732	0.03
Neral	7.67	1242	0.17	9.36	1628	0.19
Geraniol	8.13†	1272	81.92	11.62	1818	80.79
Geranial	8.18†	1276	[81.92]	9.99	1679	0.37
Geranyl formate	8.64	1308	0.10	9.78	1662	0.15
2,3-Epoxygeraniol?	9.12	1338	0.03			
Geranic acid	9.46	1362	0.05			
Neryl acetate	9.53	1367	0.02	10.06	1685	0.02
Unknown [m/z 43, 41 (25), 67 (24), 109 (23), 93 (20), 69 (19)...]	9.68	1378	0.09	13.54	1991	tr

Geranyl acetate	9.83	1389	6.85	10.46	1718	6.70
β-Elemene	9.88	1392	0.02	8.28*	1543	1.65
β-Caryophyllene	10.17	1413	1.60	8.28*	1543	[1.65]
α-Guaiene	10.45*	1434	0.02	8.28*	1543	[1.65]
<i>trans</i> -α-Bergamotene	10.45*	1434	[0.02]	8.28*	1543	[1.65]
α-Humulene	10.62	1447	0.11	9.14	1610	0.10
Selina-4,11-diene	10.90	1468	0.02	9.32	1625	0.01
Unknown [m/z 189, 133 (75), 91 (71), 105 (69), 93 (44)... 204 (33)]	11.03	1478	0.06	9.43	1634	0.06
β-Selinene	11.06	1480	0.02	9.72*†	1658	[0.05]
Valencene	11.17	1488	0.04	9.72*†	1658	[0.05]
α-Muurolene	11.28	1497	0.01	9.93	1675	0.02
7-epi-α-Selinene	11.46	1510	0.03	10.23	1699	0.05
δ-Cadinene	11.59	1520	0.01	10.28	1703	0.01
α-Elemol	11.91	1545	0.01	13.92	2027	0.01
Unknown [m/z 59, 68 (63), 43 (31), 67 (27), 81 (27), 94 (25), 69 (23), 41 (22), 84 (20)...]	11.99	1552	0.02			
Geranyl butyrate	12.14	1563	0.18	12.04	1855	0.21
(<i>E</i>)-Nerolidol	12.15	1565	0.11	13.66	2002	0.12
Caryophyllene oxide	12.28*	1574	0.22	12.64	1908	0.20
Caryophyllene oxide isomer	12.28*	1574	[0.22]	12.56	1901	0.02
Humulene epoxide II	12.60	1600	0.01	13.22	1961	0.03
Caryophylladienol II	12.95	1629	0.01	15.92	2226	0.02
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5β-ol	13.39	1666	0.01	16.70*	2306	0.89
(2 <i>E</i> ,6 <i>Z</i>)-Farnesal	13.96	1714	tr	15.24	2156	0.01
(2 <i>E</i> ,6 <i>E</i>)-Farnesol	14.07	1723	0.87	16.70*	2306	[0.89]
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	14.27	1740	0.01	15.69	2202	0.01
Geranyl caproate	14.47	1757	0.71	14.12	2047	0.78
(2 <i>E</i> ,6 <i>E</i>)-Farnesyl acetate	15.44	1844	0.08	15.80	2213	0.07
Phytone	15.49	1848	0.03	14.56	2088	0.04
Geranyl caprylate	16.61	1953	0.17	16.09	2243	0.17
Unknown [m/z 69, 41 (49), 81 (47), 93 (21), 95 (30), 43 (26)...]	17.73	2062	tr			
Unknown [m/z 69, 81 (54), 95 (26), 41 (20), 82 (16), 123 (16)...]	20.95	2406	0.03			

Unknown [m/z 69, 81 (64), 95 (29), 137 (19), 41 (19)...]	24.33	2823	0.02	
Total identified		98.66%		98.08%
Total reported		98.89%		98.15%

*: 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