

Date : April 06, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23C30-PTH01

Customer identification : DaiDai Flower - China - DE0101R

Type : Essential oil

Source : Citrus aurantium var. daidai

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 2014-005

Analysis date : April 03, 2023

Checked and approved by :

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

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*P*HYSICO*C*HEMICAL *D*ATA

Physical aspect: Light yellow liquid

Refractive index: 1.4681 ± 0.0003 (20 °C; method PC-MAT-016)

*C*ONCLUSION

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
Tricyclene	0.01	Monoterpene
α-Thujene	0.03	Monoterpene
α-Pinene	0.56	Monoterpene
Camphene	0.04	Monoterpene
Benzaldehyde	0.02	Simple phenolic
β-Pinene	7.27	Monoterpene
Sabinene	0.76	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	1.67	Monoterpene
trans-Dehydroxylinalool oxide	0.02	Monoterpenic ether
α-Phellandrene	0.02	Monoterpene
Δ3-Carene	0.01	Monoterpene
cis-Dehydroxylinalool oxide	0.01	Monoterpenic ether
α-Terpinene	0.07	Monoterpene
para-Cymene	0.02	Monoterpene
β-Phellandrene	0.16	Monoterpene
Limonene	21.98	Monoterpene
(Z)-β-Ocimene	0.59	Monoterpene
(E)-β-Ocimene	4.58	Monoterpene
γ-Terpinene	0.12	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.08	Monoterpenic alcohol
Terpinolene	0.33	Monoterpene
trans-Linalool oxide (fur.)	0.03	Monoterpenic alcohol
Linalool	35.55	Monoterpenic alcohol
cis-para-Menth-2-en-1-ol	0.03	Monoterpenic alcohol
allo-Ocimene	0.03	Monoterpene
cis-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
Benzeneacetonitrile	0.10	Simple phenolic
(E)-Myroxide	0.03	Monoterpenic ether
Lilac aldehyde B	0.01	Monoterpenic aldehyde
Borneol	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.20	Monoterpenic alcohol
α-Terpineol	3.45	Monoterpenic alcohol
2,6-Dimethyl-3,7-octadiene-2,6-diol	0.01	Monoterpenic alcohol
Octyl acetate	0.02	Aliphatic ester
Nerol	0.85	Monoterpenic alcohol
Neral	0.05	Monoterpenic aldehyde
Geraniol	2.37	Monoterpenic alcohol
Linalyl acetate	10.31	Monoterpenic ester
Geranal	0.07	Monoterpenic aldehyde
Bornyl acetate	0.02	Monoterpenic ester
Indole	0.23	Indole
cis-para-Mentha-2,8-diene-1-hydroperoxide?	0.01	Monoterpenic peroxide

δ-Elemene	0.03	Sesquiterpene
Methyl anthranilate	0.19	Phenolic ester
Linalyl propionate	0.02	Monoterpenic ester
α-Terpinyl acetate	0.09	Monoterpenic ester
Neryl acetate	1.25	Monoterpenic ester
Geranyl acetate	2.42	Monoterpenic ester
β-Elemene	0.02	Sesquiterpene
(Z)-Jasmone	0.03	Jasmonate
β-Caryophyllene	0.38	Sesquiterpene
α-Humulene	0.05	Sesquiterpene
Geranylacetone	0.01	Monoterpenic ketone
(E)-β-Farnesene	0.09	Sesquiterpene
Germacrene D	0.08	Sesquiterpene
Bicyclogermacrene	0.18	Sesquiterpene
α-Muurolene	0.02	Sesquiterpene
(3E,6E)-α-Farnesene	0.04	Sesquiterpene
δ-Cadinene	0.04	Sesquiterpene
Germacrene B	0.02	Sesquiterpene
(E)-Nerolidol	1.08	Sesquiterpenic alcohol
Spathulenol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	Sesquiterpenic ether
Globulol	0.02	Sesquiterpenic alcohol
Viridiflorol	0.01	Sesquiterpenic alcohol
τ-Muurolol	0.02	Sesquiterpenic alcohol
α-Cadinol	0.02	Sesquiterpenic alcohol
(8Z)-Heptadecene	0.02	Alkene
Heptadecane	0.01	Alkane
(2E,6Z)-Farnesal	0.01	Sesquiterpenic aldehyde
Pentadecanal?	0.01	Aliphatic aldehyde
(2E,6E)-Farnesol	1.13	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
meta-Camphorene	0.01	Diterpene
Unknown	0.05	Unknown
Phytol	0.02	Diterpenic alcohol
Tricosane	0.08	Alkane
Tetracosane	0.01	Alkane
Pentacosane	0.06	Alkane
Heptacosane	0.03	Alkane
Consolidated total	99.35%	

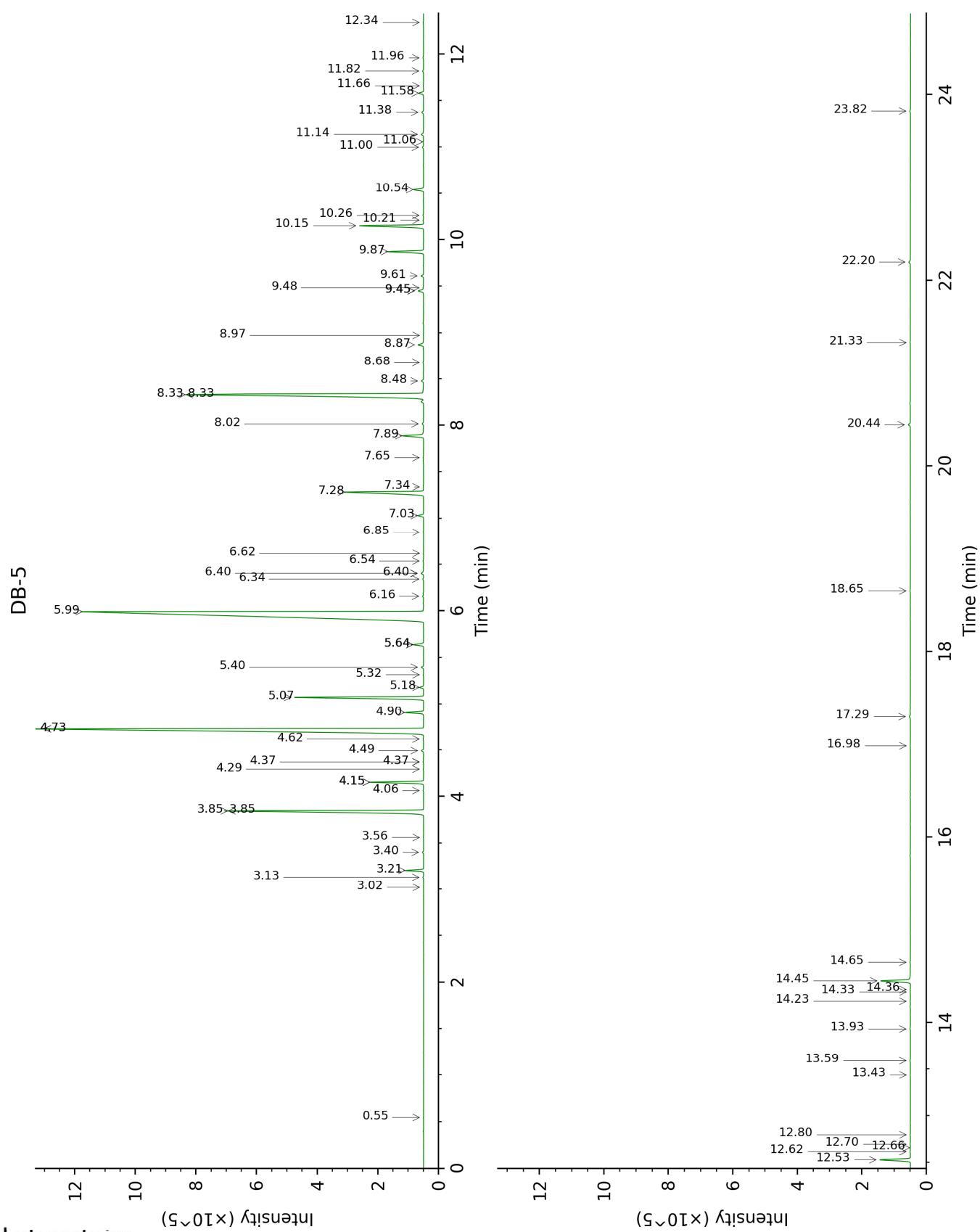
tr: The compound has been detected below 0.005% of total signal.

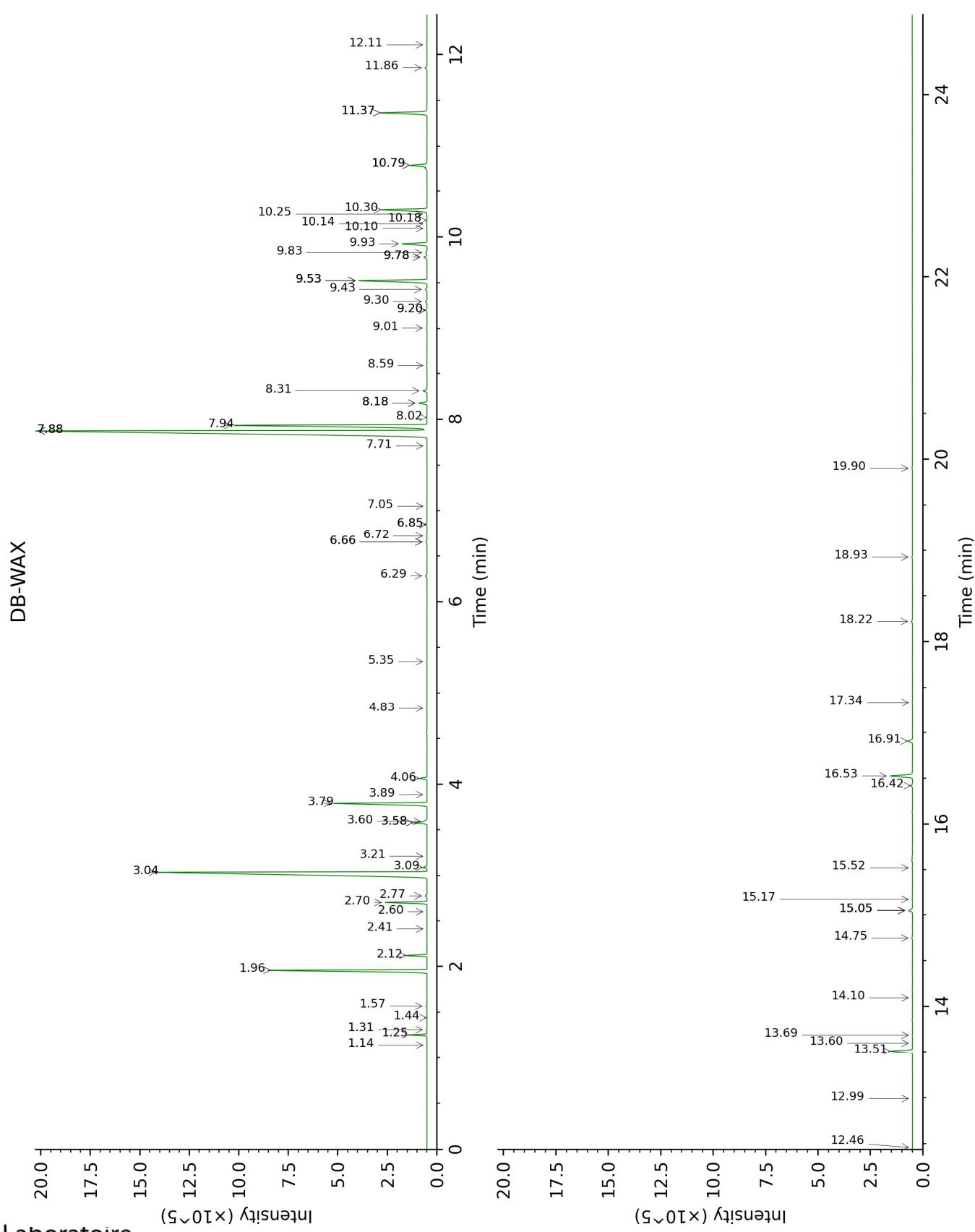
Note: no correction factor was applied

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	0.54	606	tr	1.44	1013	tr
Tricyclene	3.02	919	0.01	1.14	971	tr
α -Thujene	3.13	926	0.03	1.31	999	0.02
α -Pinene	3.21	931	0.56	1.25	991	0.55
Camphene	3.40	944	0.04	1.57	1026	0.04
Benzaldehyde	3.56	954	0.02	7.05	1459	0.01
β -Pinene	3.85*	973	8.05	1.96	1067	7.27
Sabinene	3.85*	973	[8.05]	2.12	1084	0.76
6-Methyl-5-hepten-2-one	4.06	987	0.02	4.83	1303	0.02
Myrcene	4.15*	993	1.68	2.70	1134	1.67
<i>trans</i> -Dehydroxylinalool oxide	4.15*	993	[1.68]	3.21	1176	0.02
α -Phellandrene	4.29	1002	0.02	2.60	1126	0.01
Δ^3 -Carene	4.37*	1007	0.02	2.41	1110	0.01
<i>cis</i> -Dehydroxylinalool oxide	4.37*	1007	[0.02]	3.58*	1206	0.61
α -Terpinene	4.49	1015	0.07	2.77	1140	0.07
para-Cymene	4.62	1023	0.02	3.89	1230	0.02
β -Phellandrene	4.73*	1030	22.16	3.09	1166	0.16
Limonene	4.73*	1030	[22.16]	3.04	1162	21.98
(Z)- β -Ocimene	4.90	1040	0.59	3.58*	1206	[0.61]
(E)- β -Ocimene	5.07	1051	4.58	3.79	1222	4.60
γ -Terpinene	5.18	1058	0.12	3.60	1207	0.10
<i>cis</i> -Sabinene hydrate	5.32	1066	0.01	6.66*	1429	0.05
<i>cis</i> -Linalool oxide (fur.)	5.40	1071	0.08	6.28	1401	0.08
Terpinolene	5.64*	1086	0.36	4.06	1243	0.33
<i>trans</i> -Linalool oxide (fur.)	5.64*	1086	[0.36]	6.66*	1429	[0.05]
Linalool	5.99	1109	35.55	7.88*†	1521	45.88
<i>cis</i> -para-Menth-2-en-1-ol	6.16	1119	0.03	7.88*†	1521	[45.88]
allo-Ocimene	6.34	1131	0.03	5.35	1333	0.03
<i>cis</i> -para-Menth-2,8-dien-1-ol	6.40*	1135	0.11	9.20*	1626	0.06
Benzeneacetonitrile	6.40*	1135	[0.11]	11.86	1852	0.10
(E)-Myroxide	6.54	1143	0.03	6.85*	1444	0.03
Lilac aldehyde B	6.62	1148	0.01	7.71	1509	0.01
Borneol	6.85	1163	0.01	9.52*	1653	3.52
Terpinen-4-ol	7.03	1175	0.20	8.31	1556	0.20
α -Terpineol	7.28	1191	3.45	9.52*	1653	[3.52]
2,6-Dimethyl-3,7-octadiene-2,6-diol	7.34	1194	0.01			

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Octyl acetate	7.65	1215	0.02	6.85*	1444	[0.03]
Nerol	7.89	1230	0.85	10.79*	1759	0.88
Neral	8.02	1239	0.05	9.20*	1626	[0.06]
Geraniol	8.33*	1260	12.81	11.37*	1808	2.39
Linalyl acetate	8.33*	1260	[12.81]	7.94†	1526	[45.88]
Geranial	8.48	1270	0.07	9.83	1678	0.07
Bornyl acetate	8.68	1283	0.02	8.02	1533	0.02
Indole	8.87	1296	0.23	16.91	2349	0.24
<i>cis</i> -para-Mentha-2,8-diene-1-hydroperoxide?	8.97	1303	0.01			
δ-Elemene	9.45*	1336	0.22	6.72	1434	0.03
Methyl anthranilate	9.45*	1336	[0.22]	15.05*	2155	0.21
Linalyl propionate	9.48	1339	0.02	8.59	1577	0.02
α-Terpinyl acetate	9.61	1348	0.09	9.43	1645	0.09
Neryl acetate	9.87	1366	1.25	9.93	1686	1.26
Geranyl acetate	10.15	1386	2.42	10.30	1717	2.41
β-Elemene	10.21	1390	0.02	8.18*	1545	0.39
(Z)-Jasmone	10.26	1393	0.03	12.11	1874	0.03
β-Caryophyllene	10.54	1414	0.38	8.18*	1545	[0.39]
α-Humulene	11.00	1448	0.05	9.01	1610	0.04
Geranylacetone	11.06	1452	0.01	11.37*	1808	[2.39]
(E)-β-Farnesene	11.14	1458	0.09	9.30	1634	0.09
Germacrene D	11.38	1476	0.08	9.52*	1653	[3.52]
Bicyclogermacrene	11.58	1491	0.18	9.78*	1674	0.18
α-Murolene	11.66	1497	0.02	9.78*	1674	[0.18]
(3E,6E)-α-Farnesene	11.82	1509	0.04	10.25	1713	0.03
δ-Cadinene	11.96	1520	0.04	10.14	1704	0.02
Germacrene B	12.34	1550	0.02	10.79*	1759	[0.88]
(E)-Nerolidol	12.53	1565	1.08	13.51	2004	1.08
Spathulenol	12.62	1572	0.02	14.10	2060	0.01
Caryophyllene oxide	12.66	1575	0.01	12.46	1906	0.01
Globulol	12.70	1578	0.02	13.60	2012	0.01
Viridiflorol	12.80	1586	0.01	13.69	2021	0.01
τ-Murolol	13.43	1637	0.02	14.75	2124	0.04
α-Cadinol	13.59	1650	0.02	15.17	2167	0.02
(8Z)-Heptadecene	13.93	1678	0.02	10.18	1707	0.02
Heptadecane	14.23	1703	0.01	10.10	1699	0.02
(2E,6Z)-Farnesal	14.33	1712	0.01	15.05*	2155	[0.21]
Pentadecanal?	14.36	1714	0.01	12.99	1955	0.01
(2E,6E)-Farnesol	14.45	1722	1.13	16.53	2308	1.17
(2E,6E)-Farnesal	14.65	1739	0.02	15.52	2202	0.02
meta-Camphorene	16.98	1950	0.01	15.05*	2155	[0.21]
Unknown [m/z 107, 93 (75), 161 (73), 69 (68), 41 (67), 105 (65)...]	17.29	1979	0.05			
Phytol	18.65	2113	0.02	18.92	2576	0.03
Tricosane	20.44	2302	0.08	16.42	2296	0.07
Tetracosane	21.33	2402	0.01	17.34	2395	0.01
Pentacosane	22.20	2502	0.06	18.22	2495	0.06

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Heptacosane	23.82	2702	0.03	19.90	2693	0.03
Total identified		99.48%			99.26%	
Total reported		99.52%			99.26%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

t: 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