

Date : April 06, 2020

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 20C23-PTH01

Customer identification : Petitgrain - Paraguay - P60105910R

Type : Essential oil

Source : *Citrus x aurantium*

Customer : Plant Therapy

ANALYSIS

Method: PC-MAT-007 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID (in French); identifications validated by GC-MS.

Analyst : Fanny Charlier, B. Sc.

Analysis date : March 24, 2020

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4595 ± 0.0003 (20 °C)

ISO 3064:2015 - ESSENTIAL OIL OF PETITGRAIN, PARAGUAYAN TYPE

Compound	Min. %	Max. %	Observed %	Complies?
β-Pinene	0.5	2.0	1.1	Yes
Geranyl acetate	2.0	5.0	4.1	Yes
Neryl acetate	1.0	3.0	2.4	Yes
Geraniol	2.0	4.5	3.3	Yes
Nerol	0.5	2.0	1.3	Yes
α-Terpineol	3.0	7.0	6.2	Yes
β-Caryophyllene	0.3	1.5	0.8	Yes
Linalyl acetate	40.0	60.0	43.9	Yes
Linalool	15.0	30.0	24.6	Yes
(E)-β-Ocimene	0.5	3.5	2.4	Yes
(Z)-β-Ocimene	0.7	1.5	0.8	Yes
Limonene	0.7	3.5	1.1	Yes
Sabinene	0.1	0.5	0.3	Yes
Myrcene	1.3	3.0	2.3	Yes
Refractive index	1.4540	1.4630	1.4595	Yes

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method. The oil complies with the ISO standard for petitgrain oil, Paraguayan type.

ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Classe
Acetone	tr	Aliphatic ketone
Ethanol	0.22	Aliphatic alcohol
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Toluene	tr	Simple phenolic
(3Z)-Hexenol	0.01	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
α -Thujene	0.03	Monoterpene
α -Pinene	0.14	Monoterpene
α -Fenchene	tr	Monoterpene
Camphene	0.01	Monoterpene
Sabinene	0.26	Monoterpene
β -Pinene	1.10	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	2.27	Monoterpene
Pseudolimonene	tr	Monoterpene
α -Phellandrene	0.04	Monoterpene
Δ^3 -Carene	0.49	Monoterpene
α -Terpinene	0.04	Monoterpene
ortho-Cymene	tr	Monoterpene
para-Cymene	0.02	Monoterpene
Limonene	1.09	Monoterpene
β -Phellandrene	0.05	Monoterpene
1,8-Cineole	0.06	Monoterpenic ether
(Z)- β -Ocimene	0.84	Monoterpene
(E)- β -Ocimene	2.39	Monoterpene
γ -Terpinene	0.06	Monoterpene
<i>cis</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (fur.)	0.06	Monoterpenic alcohol
Terpinolene	0.49	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
para-Cymenene	tr	Monoterpene
Linalool	24.64	Monoterpenic alcohol
Hotrienol	0.06	Monoterpenic alcohol
<i>cis</i> -para-Menth-2-en-1-ol	0.03	Monoterpenic alcohol
allo-Ocimene	0.01	Monoterpene
<i>trans</i> -para-Menth-2-en-1-ol	0.01	Monoterpenic alcohol
neo-allo-Ocimene	0.01	Monoterpene
Isopulegol	0.01	Monoterpenic alcohol
Citronellal	0.02	Monoterpenic aldehyde
Terpinen-4-ol	0.12	Monoterpenic alcohol
para-Cymen-8-ol	0.01	Monoterpenic alcohol
α -Terpineol	6.16	Monoterpenic alcohol
Safranal	tr	Monoterpenic aldehyde
Hodiendiol	0.01	Monoterpenic alcohol
Nerol	1.33	Monoterpenic alcohol

Citronellol	0.03	Monoterpenic alcohol
Neral	0.07	Monoterpenic aldehyde
Geraniol	3.25	Monoterpenic alcohol
Linalyl acetate	43.93	Monoterpenic ester
(<i>trans</i> ?) - Linalool oxide acetate (fur.)?	0.02	Monoterpenic ester
Geranial	0.10	Monoterpenic aldehyde
Methyl anthranilate	0.01	Phenolic ester
α -Terpinyl acetate	0.11	Monoterpenic ester
Eugenol	0.04	Phenylpropanoid
Neryl acetate	2.45	Monoterpenic ester
α -Copaene	0.01	Sesquiterpene
Geranyl acetate	4.13	Monoterpenic ester
β -Elemene	0.02	Sesquiterpene
β -Caryophyllene	0.77	Sesquiterpene
Aromadendrene	0.03	Sesquiterpene
α -Humulene	0.10	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.04	Sesquiterpene
Germacrene D	0.01	Sesquiterpene
Bicyclogermacrene	0.24	Sesquiterpene
(3 <i>Z</i> ,6 <i>E</i>)- α -Farnesene	0.03	Sesquiterpene
γ -Cadinene	0.06	Sesquiterpene
δ -Cadinene	0.05	Sesquiterpene
(<i>E</i>)-Nerolidol	0.07	Sesquiterpenic alcohol
Spathulenol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
τ -Cadinol	0.02	Sesquiterpenic alcohol
Unknown	0.03	Sesquiterpenic alcohol
α -Cadinol	0.04	Sesquiterpenic alcohol
Mint sulfide?	0.03	Sesquiterpenic sulfide
Phytol	0.03	Diterpenic alcohol
Consolidated total	97.92%	

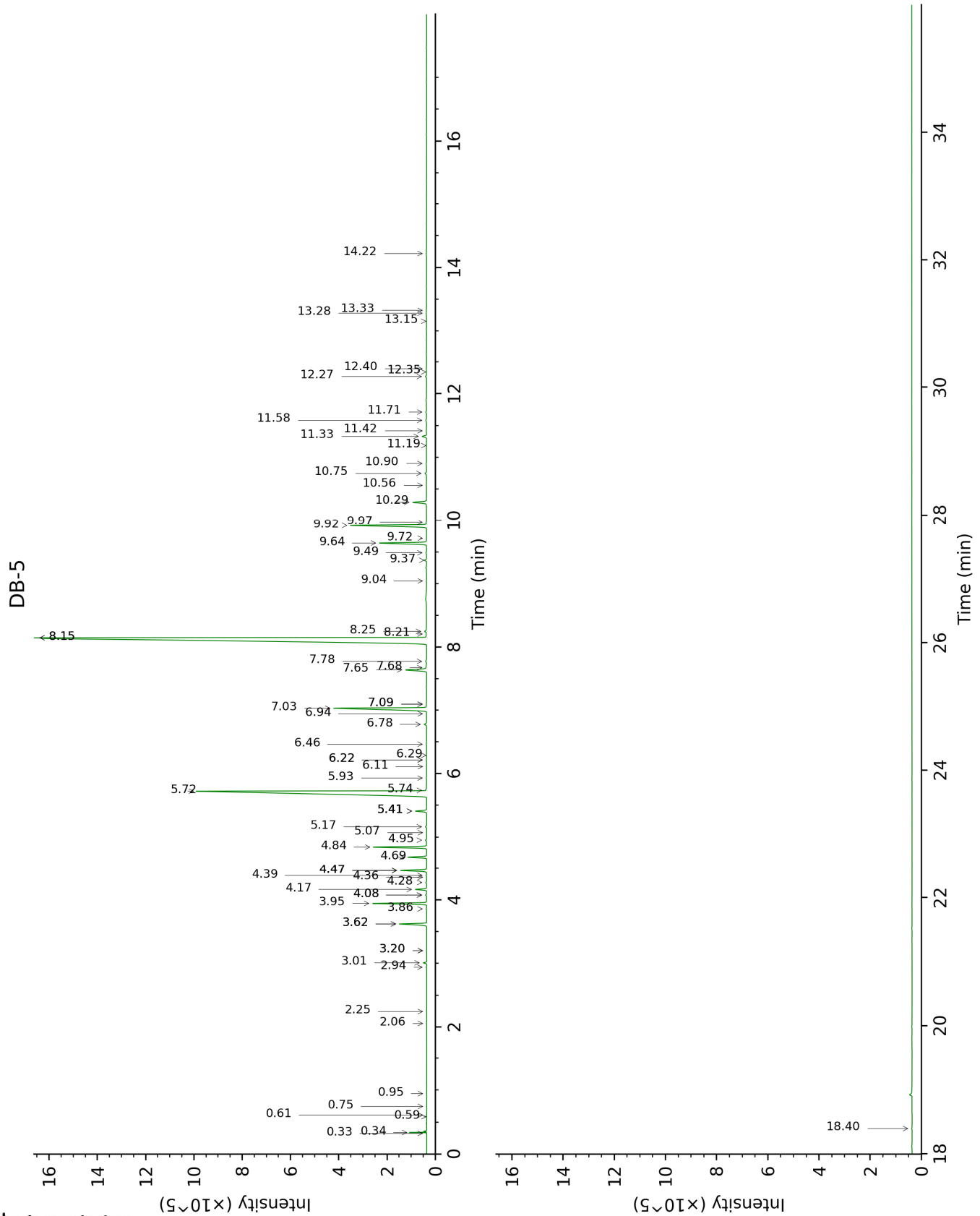
tr: The compound has been detected below 0.005% of total signal.

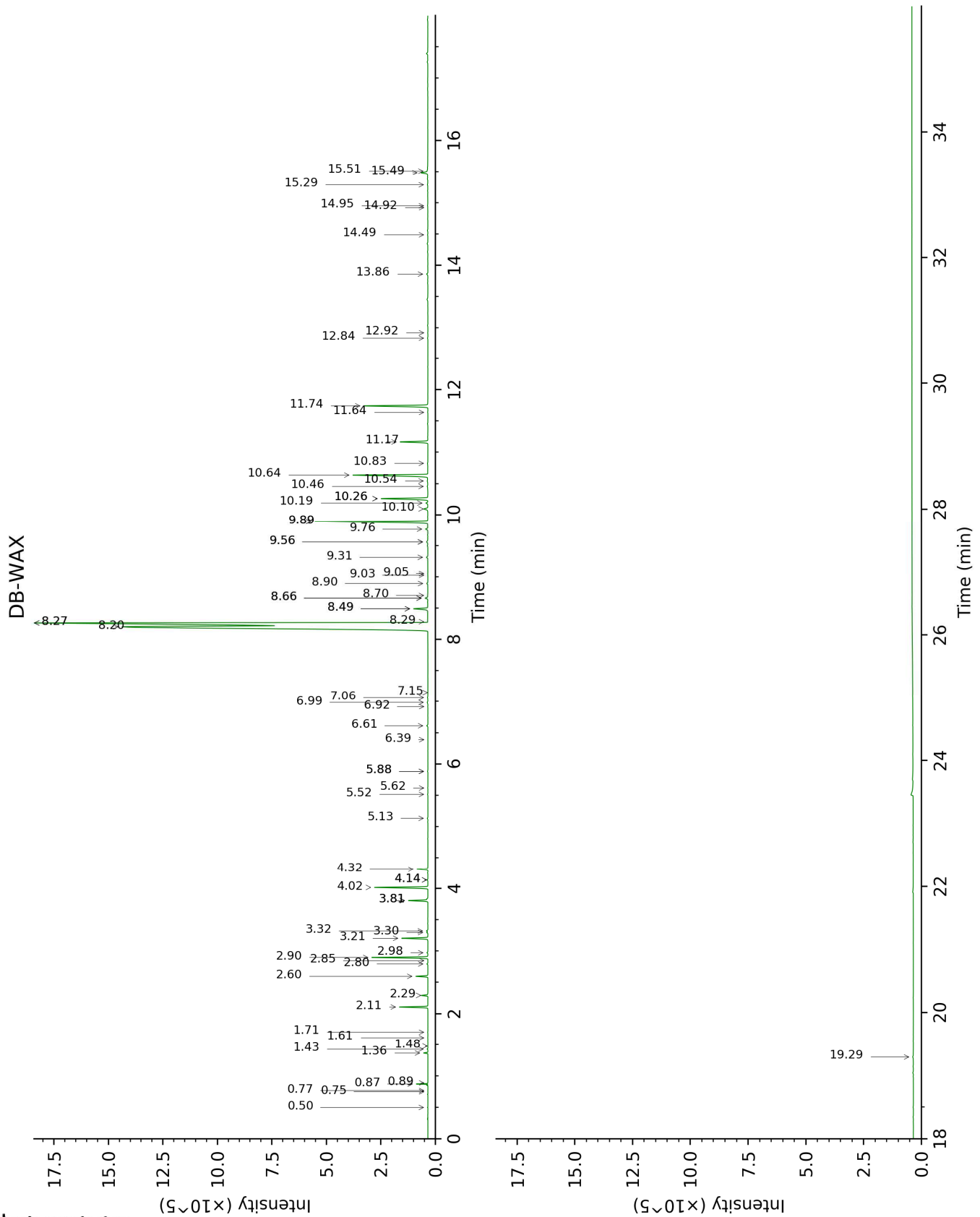
Note: no correction factor was applied

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	%
Acetone	0.33	522	tr	0.50	788	0.01
Ethanol	0.34	522	0.22	0.87	911	0.24
Isovaleral	0.59	640	tr	0.77	892	tr
2-Methylbutyral	0.61	650	tr	0.75	885	tr
2-Ethylfuran	0.75	707	tr	0.89	914	tr
Toluene	0.95	738	tr	1.48	1004	tr
(3Z)-Hexenol	2.06	858	0.01	5.88*	1352	0.02
Hexanol	2.24	873	0.01	5.52	1326	0.02
α-Thujene	2.94	925	0.03	1.43	999	0.02
α-Pinene	3.01	930	0.14	1.36	992	0.13
α-Fenchene	3.20*	942	0.01	1.61	1018	tr
Camphene	3.20*	942	[0.01]	1.71	1027	0.01
Sabinene	3.62*	970	1.35	2.29	1085	0.26
β-Pinene	3.62*	970	[1.35]	2.11	1067	1.10
6-Methyl-5-hepten-2-one	3.86	986	0.02	5.13	1298	0.03
Myrcene	3.95	992	2.27	2.90	1134	2.26
Pseudolimonene	4.08*	1000	0.04	2.85	1130	tr
α-Phellandrene	4.08*	1000	[0.04]	2.80	1126	0.04
Δ3-Carene	4.17	1006	0.49	2.60	1110	0.47
α-Terpinene	4.28	1013	0.04	2.98	1140	0.04
ortho-Cymene	4.36	1018	tr	4.14*	1227	0.03
para-Cymene	4.39	1020	0.02	4.14*	1227	[0.03]
Limonene	4.47*	1025	1.20	3.21	1158	1.09
β-Phellandrene	4.47*	1025	[1.20]	3.30	1165	0.05
1,8-Cineole	4.47*	1025	[1.20]	3.32	1167	0.06
(Z)-β-Ocimene	4.69	1039	0.84	3.81*	1203	0.83
(E)-β-Ocimene	4.84	1049	2.39	4.02	1218	2.38
γ-Terpinene	4.95	1056	0.06	3.81*	1203	[0.83]
cis-Sabinene hydrate	5.07	1063	0.01	6.99	1432	0.05
cis-Linalool oxide (fur.)	5.16	1069	0.06	6.61	1404	0.06
Terpinolene	5.41*	1085	0.53	4.32	1240	0.49
trans-Linalool oxide (fur.)	5.41*	1085	[0.53]	6.92	1427	0.01
para-Cymenene	5.41*	1085	[0.53]	6.39	1388	tr
Linalool	5.72†	1105	24.70	8.20†	1523	68.60
Hotrienol	5.74†	1106	[24.70]	8.90	1576	0.06
cis-para-Menth-2-en-1-ol	5.93	1118	0.03	8.27*†	1528	[68.60]
allo-Ocimene	6.11	1130	0.01	5.62	1333	0.01
trans-para-Menth-2-en-1-ol	6.22*	1137	0.02	9.05	1589	0.01
neo-allo-Ocimene	6.22*	1137	[0.02]	5.88*	1352	[0.02]
Isopulegol	6.29	1142	0.01	8.29	1529	0.02
Citronellal	6.46	1153	0.02	7.06	1438	0.02
Terpinen-4-ol	6.78	1174	0.12	8.66*	1558	0.14

para-Cymen-8-ol	6.94	1184	0.01	11.64	1802	0.01
α-Terpineol	7.03	1190	6.16	9.89*	1656	6.16
Safranal	7.09*	1194	0.02	9.03	1586	tr
Hodiendiol	7.09*	1194	[0.02]	12.92	1916	0.01
Nerol	7.65†	1232	1.34	11.17	1762	1.33
Citronellol	7.68†	1234	[1.34]	10.83	1733	0.03
Neral	7.78	1241	0.07	9.56*	1629	0.09
Geraniol	8.15*	1267	47.91	11.74	1811	3.25
Linalyl acetate	8.15*	1267	[47.91]	8.27*†	1528	[68.60]
(<i>trans</i> ?) - Linalool oxide acetate (<i>fur.</i>)?	8.21	1271	0.02	8.70	1562	0.01
Geranial	8.25	1274	0.10	10.19	1680	0.10
Methyl anthranilate	9.04	1331	0.01	15.49	2162	0.42
α-Terpinyl acetate	9.37	1355	0.11	9.76	1646	0.11
Eugenol	9.49	1356	0.04	14.92	2105	0.01
Neryl acetate	9.64	1366	2.45	10.26*	1686	2.43
α-Copaene	9.72	1372	0.01	7.15	1444	0.01
Geranyl acetate	9.92	1386	4.13	10.64	1717	4.15
β-Elemene	9.97	1390	0.02	8.49*	1545	0.72
β-Caryophyllene	10.29	1413	0.77	8.49*	1545	[0.72]
Aromadendrene	10.56	1433	0.03	8.66*	1558	[0.14]
α-Humulene	10.75	1447	0.10	9.31	1609	0.07
(<i>E</i>)-β-Farnesene	10.90	1458	0.04	9.56*	1629	[0.09]
Germacrene D	11.19	1479	0.01	9.89*	1656	[6.16]
Bicyclogermacrene	11.33	1490	0.24	10.10	1672	0.24
(3 <i>Z</i> ,6 <i>E</i>)-α- Farnesene	11.42	1497	0.03	10.26*	1686	[2.43]
γ-Cadinene	11.58	1509	0.06	10.46	1702	0.04
δ-Cadinene	11.72	1520	0.05	10.54	1709	0.05
(<i>E</i>)-Nerolidol	12.27	1563	0.07	13.86	2003	0.08
Spathulenol	12.34	1569	0.01	14.49	2063	0.01
Caryophyllene oxide	12.40	1573	0.02	12.84	1908	0.02
τ-Cadinol	13.16	1634	0.02	14.95	2108	0.02
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109)40)... 204 (35), 222 (2)]	13.28	1645	0.03	15.29	2142	0.02
α-Cadinol	13.33	1648	0.04	15.51	2164	0.04
Mint sulfide?	14.22	1723	0.03			
Phytol	18.40	2114	0.03	19.29	2574	0.04
Total identified		98.63%			98.03%	
Total reported		98.66%			98.05%	

*: 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

