CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23F19-PTH01
Customer identification : Pink Grapefruit - USA - G50111R
Type : Essential oil
Source : *Citrus x paradisi* cv. Pink
Customer : Plant Therapy

ANALYSIS

Method: PC-MAT-014 ✲ISO - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.
Analyst : Amélie Simard, Analyste
Analysis date : June 21, 2023

Checked and approved by :

_____

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

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

MÉTHODE CERTIFIÉE
✲ISO 17025:2017
CERTIFIED METHOD

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PHYSICOCHEMICAL DATA

Physical aspect: Bright orange liquid
Refractive index: 1.4766 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

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ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

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

Identification	%	Class
Heptanal	0.01	Aliphatic aldehyde
α-Thujene	0.02	Monoterpene
α-Pinene	0.58	Monoterpene
Camphene	0.01	Monoterpene
3,7,7-Trimethylcyclohepta-1,3,5-triene	0.01	Monoterpene
Sabinene	0.37	Monoterpene
β-Pinene	0.14	Monoterpene
Myrcene	1.95	Monoterpene
Octanal	0.36	Aliphatic aldehyde
α-Phellandrene	0.03	Monoterpene
para-Cymene	0.02	Monoterpene
Limonene	92.98	Monoterpene
(*Z*)-β-Ocimene	0.01	Monoterpene
(*E*)-β-Ocimene	0.10	Monoterpene
γ-Terpinene	0.06	Monoterpene
Octanol	0.03	Aliphatic alcohol
Terpinolene	0.01	Monoterpene
Linalool	0.05	Monoterpenic alcohol
Nonanal	0.04	Aliphatic aldehyde
trans-para-Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol
cis-Limonene oxide	0.03	Monoterpenic ether
trans-Limonene oxide	0.03	Monoterpenic ether
Citronellal	0.03	Monoterpenic aldehyde
α-Terpineol	0.02	Monoterpenic alcohol
Decanal	0.14	Aliphatic aldehyde
Octyl acetate	0.02	Aliphatic ester
trans-Carveol	0.01	Monoterpenic alcohol
cis-Carveol	0.01	Monoterpenic alcohol
Neral	0.04	Monoterpenic aldehyde
Geranial	0.06	Monoterpenic aldehyde
Undecanal	0.01	Aliphatic aldehyde
α-Terpinyl acetate	0.01	Monoterpenic ester
α-Copaene	0.05	Sesquiterpene
Geranyl acetate	0.02	Monoterpenic ester
β-Cubebene	0.05	Sesquiterpene
β-Elemene	0.02	Sesquiterpene
Dodecanal	0.02	Aliphatic aldehyde
β-Caryophyllene	0.11	Sesquiterpene
α-Humulene	0.03	Sesquiterpene
(*E*)-β-Farnesene	0.03	Sesquiterpene
Germacrene D	0.04	Sesquiterpene
Bicyclogermacrene	0.02	Sesquiterpene
α-Muurolene	0.01	Sesquiterpene
Cubebol	0.01	Sesquiterpenic alcohol
δ-Cadinene	0.05	Sesquiterpene

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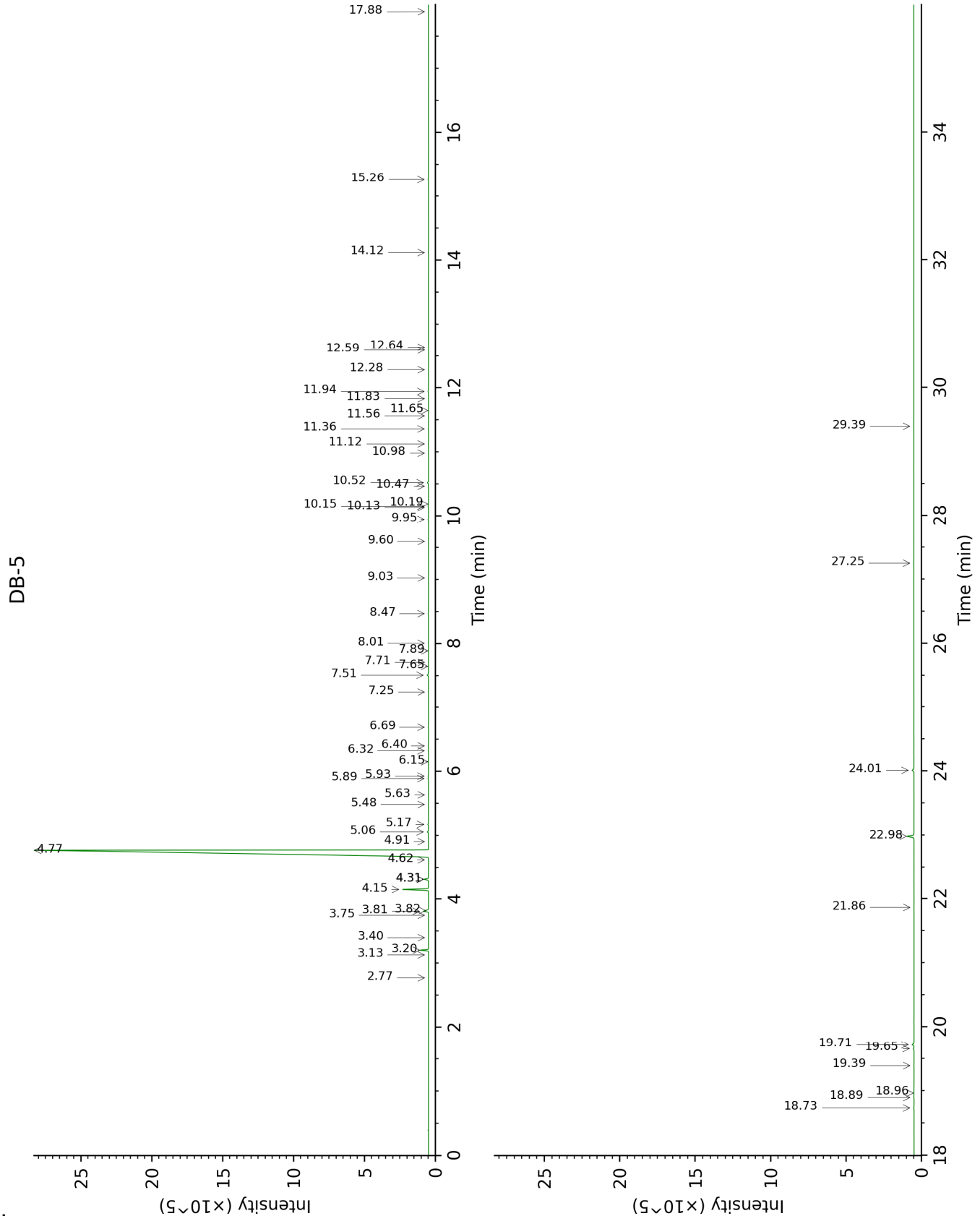|		
α-Elemol	0.02	Sesquiterpenic alcohol
Spathulenol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	Sesquiterpenic ether
β-Sinensal	0.02	Sesquiterpenic aldehyde
Nootkatone	0.06	Sesquiterpenic ketone
Bergapten	0.01	Furanocoumarin
Osthole	0.05	Coumarin
Linoleic acid	0.05	Aliphatic acid
cis-Vaccenic acid?	0.06	Aliphatic acid
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	0.03	Coumarin
Isoauraptene	0.08	Coumarin
Meranzin	0.21	Coumarin
Auraptenol	0.01	Coumarin
Auraptene	0.76	Coumarin
Epoxyaurapten	0.23	Coumarin
Tangeretin	0.05	Flavonoid
3,3',4',5,6,7,8-Heptamethoxyflavone	0.03	Flavonoid
β-Phellandrene	0.26	Monoterpene
Consolidated total	**99.65%**	

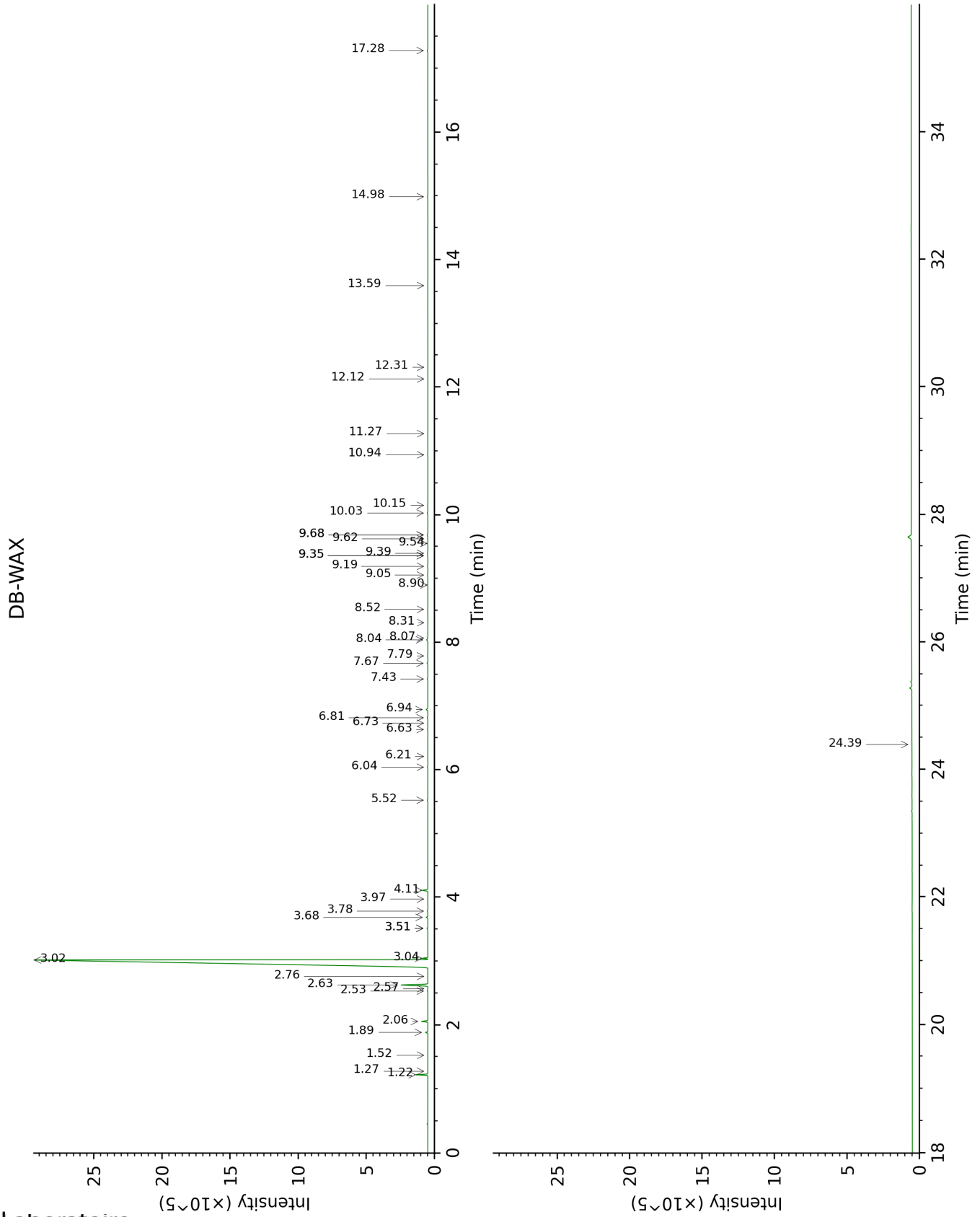tr: The compound has been detected below 0.005% of total signal.

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.

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Pink Grapefruit - USA - G50111R

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This page was intentionally left blank. The following pages present the complete data of the analysis.

Essential oil, *Citrus x paradisi* cv. Pink
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Pink Grapefruit - USA - G50111R

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DB-5

Time (min)

Intensity (×10^5)

Time (min)

Intensity (×10^5)

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Essential oil, *Citrus x paradisi* cv. Pink
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DB-WAX

Time (min)

Intensity (×10^5)

Time (min)

Intensity (×10^5)

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Pink Grapefruit - USA - G50111R

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Heptanal	2.77	902	0.01	2.76	1146	0.01
α-Thujene	3.13	926	0.02	1.27	1002	0.01
α-Pinene	3.20	931	0.58	1.22	993	0.56
Camphene	3.40	944	0.01	1.52	1029	tr
3,7,7-Trimethylcyclohepta-1,3,5-triene	3.75	967	0.01	2.57	1131	0.01
Sabinene	3.81†	971	0.52	2.06	1085	0.37
β-Pinene	3.82†	972	[0.52]	1.89	1067	0.14
Myrcene	4.15	993	1.95	2.63	1136	1.97
Octanal	4.31*	1004	0.38	4.10	1254	0.36
α-Phellandrene	4.31*	1004	[0.38]	2.53	1128	0.03
para-Cymene	4.62	1023	0.02	3.78	1229	0.03
Limonene	4.77	1033	92.98	3.02	1167	93.70
(*Z*)-β-Ocimene	4.90	1041	0.01	3.51*	1208	0.07
(*E*)-β-Ocimene	5.06	1051	0.10	3.68	1221	0.11
γ-Terpinene	5.17	1058	0.06	3.51*	1208	[0.07]
Octanol	5.48	1077	0.03	7.79	1525	0.03
Terpinolene	5.63	1087	0.01	3.97	1243	0.02
Linalool	5.89	1102	0.05	7.67	1516	0.06
Nonanal	5.93	1105	0.04	5.52	1355	0.04
trans-para-Mentha-2,8-dien-1-ol	6.15	1119	0.02	8.52	1582	0.02
cis-Limonene oxide	6.32	1130	0.03	6.04	1393	0.03
trans-Limonene oxide	6.40	1135	0.03	6.21	1405	0.02
Citronellal	6.69	1154	0.03	6.63	1437	0.03
α-Terpineol	7.25	1189	0.02	9.35*	1650	0.03
Decanal	7.51	1206	0.14	6.94	1460	0.13
Octyl acetate	7.65	1215	0.02	6.73	1444	0.02
trans-Carveol	7.71	1219	0.01	10.94	1784	0.02
cis-Carveol	7.89	1231	0.01	11.27	1812	0.01
Neral	8.01	1239	0.04	9.05	1625	0.03
Geranial	8.47	1270	0.06	9.68*	1676	0.06
Undecanal	9.03	1307	0.01	8.31	1565	0.01
α-Terpinyl acetate	9.60	1347	0.01	9.35*	1650	[0.03]
α-Copaene	9.95	1372	0.05	6.81	1450	0.05
Geranyl acetate	10.13	1385	0.02	10.15	1716	0.03
β-Cubebene	10.15	1387	0.05	7.43	1497	0.04
β-Elemene	10.19	1389	0.02	8.07	1546	0.02
Dodecanal	10.47	1409	0.02	9.54	1665	0.02
β-Caryophyllene	10.52	1413	0.11	8.04	1544	0.11
α-Humulene	10.98	1447	0.03	8.90	1612	0.02
(*E*)-β-Farnesene	11.12	1458	0.03	9.19	1636	0.03
Germacrene D	11.36	1475	0.04	9.39	1653	0.03
Bicyclogermacrene	11.56	1490	0.02	9.62	1671	0.01
α-Muurolene	11.65	1497	0.01	9.68*	1676	[0.06]
Cubebol	11.83	1511	0.01	12.12	1889	0.01
δ-Cadinene	11.94	1519	0.05	10.03	1705	0.05

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Compound	R.T.	R.I.	%	R.T.	R.I.	%
α-Elemol	12.28	1546	0.02	13.59	2028	0.02
Spathulenol	12.59	1570	0.02			
Caryophyllene oxide	12.64	1574	0.01	12.31	1906	0.01
β-Sinensal	14.12	1695	0.02	14.98	2166	0.03
Nootkatone	15.26	1793	0.06	17.28	2414	0.05
Bergapten	17.88	2038	0.01	24.38	3352	0.01
Osthole	18.73	2123	0.05			
Linoleic acid	18.89	2139	0.05			
cis-Vaccenic acid?	18.96	2146	0.06			
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	19.39	2190	0.03			
Isoauraptene	19.65	2218	0.08			
Meranzin	19.71	2225	0.21			
Auraptenol	21.86	2465	0.01			
Auraptene	22.98	2598	0.76			
Epoxyaurapten	24.01	2727	0.23			
Tangeretin	27.25	3141	0.05			
3,3',4',5,6,7,8-Heptamethoxyflavone	29.39	3322	0.03			
β-Phellandrene				3.04	1170	0.26
Total identified		**99.38%**			**98.77%**	
Total reported		**99.38%**			**98.77%**	

*: 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

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