

Date : March 16, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21B23-FEP12

Customer identification : Grapefruit - Mexico - 51303-03

Type : Essential oil

Source : *Citrus x paradisi*

Customer : Fern & Petal

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

Analysis date : March 16, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Bright orange liquid

Refractive index: 1.4769 ± 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
α -Thujene	tr	Monoterpene
α -Pinene	0.53	Monoterpene
Sabinene	0.35	Monoterpene
β -Pinene	0.04	Monoterpene
Myrcene	1.88	Monoterpene
α -Phellandrene	0.03	Monoterpene
Octanal	0.26	Aliphatic aldehyde
para-Cymene	0.02	Monoterpene
Limonene	91.93	Monoterpene
β -Phellandrene	0.27	Monoterpene
(<i>E</i>)- β -Ocimene	0.05	Monoterpene
<i>cis</i> -Sabinene hydrate	0.01	Monoterpenic alcohol
Octanol	0.07	Aliphatic alcohol
Terpinolene	0.01	Monoterpene
Linalool	0.09	Monoterpenic alcohol
Nonanal	0.07	Aliphatic aldehyde
(<i>E</i>)-4,8-Dimethylnona-1,3,7-triene	0.02	Terpene derivative
<i>trans</i> -para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
<i>cis</i> -Limonene oxide	0.02	Monoterpenic ether
<i>cis</i> -para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
<i>trans</i> -Limonene oxide	0.02	Monoterpenic ether
(<i>E</i>)-Myroxide	0.01	Monoterpenic ether
Citronellal	0.07	Monoterpenic aldehyde
Terpinen-4-ol	0.01	Monoterpenic alcohol
α -Terpineol	0.27	Monoterpenic alcohol
Decanal	0.29	Aliphatic aldehyde
Octyl acetate	0.04	Aliphatic ester
<i>trans</i> -Carveol	0.01	Monoterpenic alcohol
<i>cis</i> -Carveol	0.01	Monoterpenic alcohol
Neral	0.04	Monoterpenic aldehyde
Geraniol	0.01	Monoterpenic alcohol
Geranial	0.07	Monoterpenic aldehyde
Undecanal	0.02	Aliphatic aldehyde
α -Terpinyl acetate	0.03	Monoterpenic ester
Limonene hydroperoxide IV	0.01	Monoterpenic peroxide
Neryl acetate	0.01	Monoterpenic ester
<i>trans</i> -para-Mentha-6,8-diene-2-hydroperoxide	0.01	Monoterpenic peroxide
α -Copaene	0.10	Sesquiterpene
β -Cubebene	0.10	Sesquiterpene
Geranyl acetate	0.04	Monoterpenic ester
β -Elemene	0.03	Sesquiterpene
Dodecanal	0.04	Aliphatic aldehyde
β -Caryophyllene	0.26	Sesquiterpene
α -Humulene	0.04	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.04	Sesquiterpene

Germacrene D	0.09	Sesquiterpene
Bicyclogermacrene	0.03	Sesquiterpene
α -Muurolene	0.02	Sesquiterpene
Cubebol	0.01	Sesquiterpenic alcohol
δ -Cadinene	0.11	Sesquiterpene
α -Elemol	0.03	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.01	Sesquiterpenic alcohol
Germacrene D-4-ol	0.02	Sesquiterpenic alcohol
Spathulenol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
β -Sinensal	0.06	Sesquiterpenic aldehyde
Myristic acid	0.02	Aliphatic acid
Nootkatone	0.09	Sesquiterpenic ketone
Hexadecanal	0.01	Aliphatic aldehyde
Palmitic acid	0.10	Aliphatic acid
Bergapten	0.03	Furanocoumarin
Osthole	0.08	Coumarin
Linoleic acid	0.10	Aliphatic acid
Oleic acid	0.06	Aliphatic acid
<i>cis</i> -Vaccenic acid?	0.02	Aliphatic acid
Stearic acid	0.02	Aliphatic acid
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	0.02	Coumarin
Isoauraptene	0.12	Coumarin
Meranzin	0.27	Coumarin
Meranzin hydrate	0.01	Coumarin
Unknown	0.01	Coumarin
Auraptene	0.89	Coumarin
Epoxyaurapten	0.24	Coumarin
Tangeretin	0.03	Flavonoid
3,5,6,7,8,3',4'-Heptamethoxyflavone?	0.07	Flavonoid
Consolidated total	99.88%	

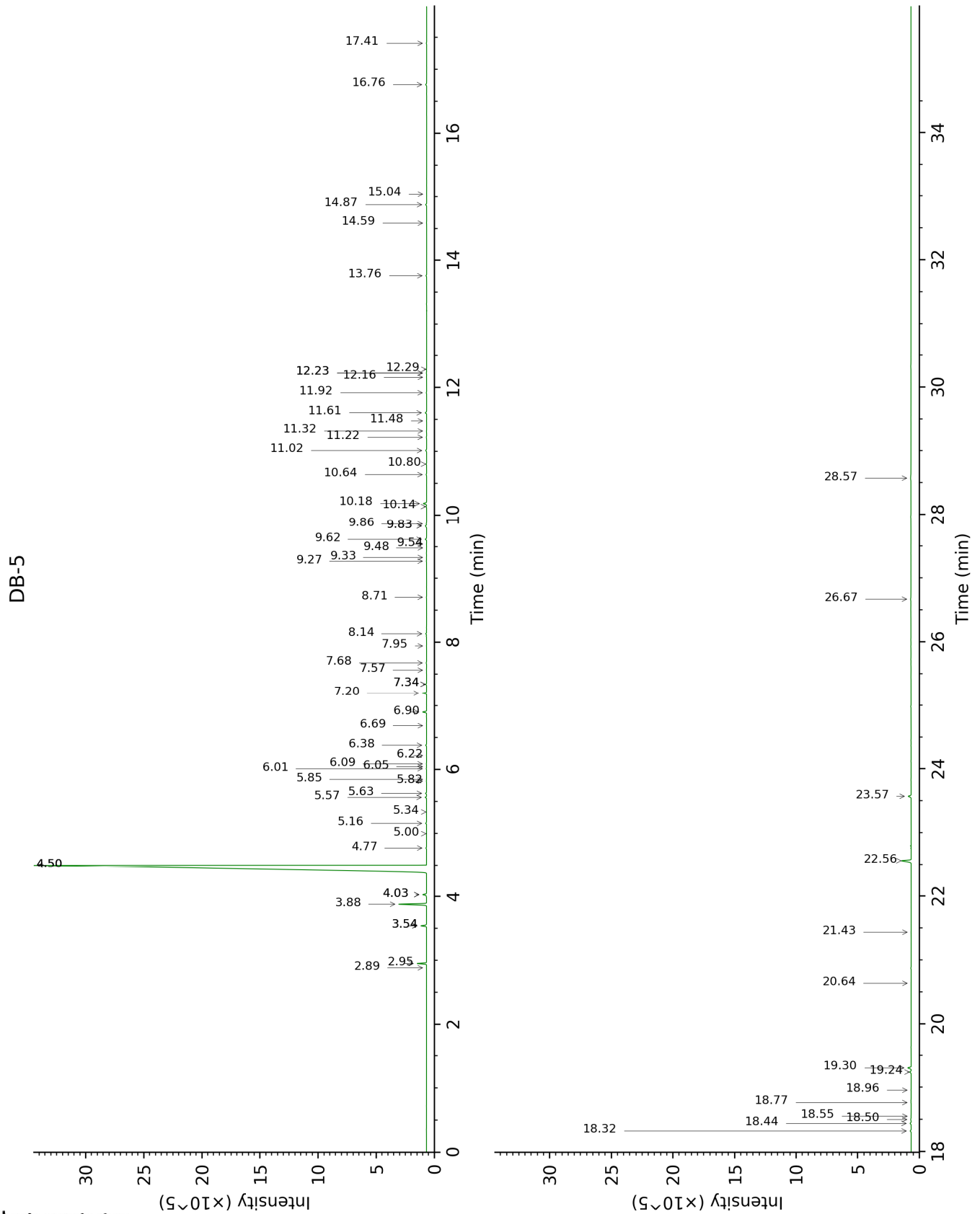
tr: The compound has been detected below 0.005% of total signal.

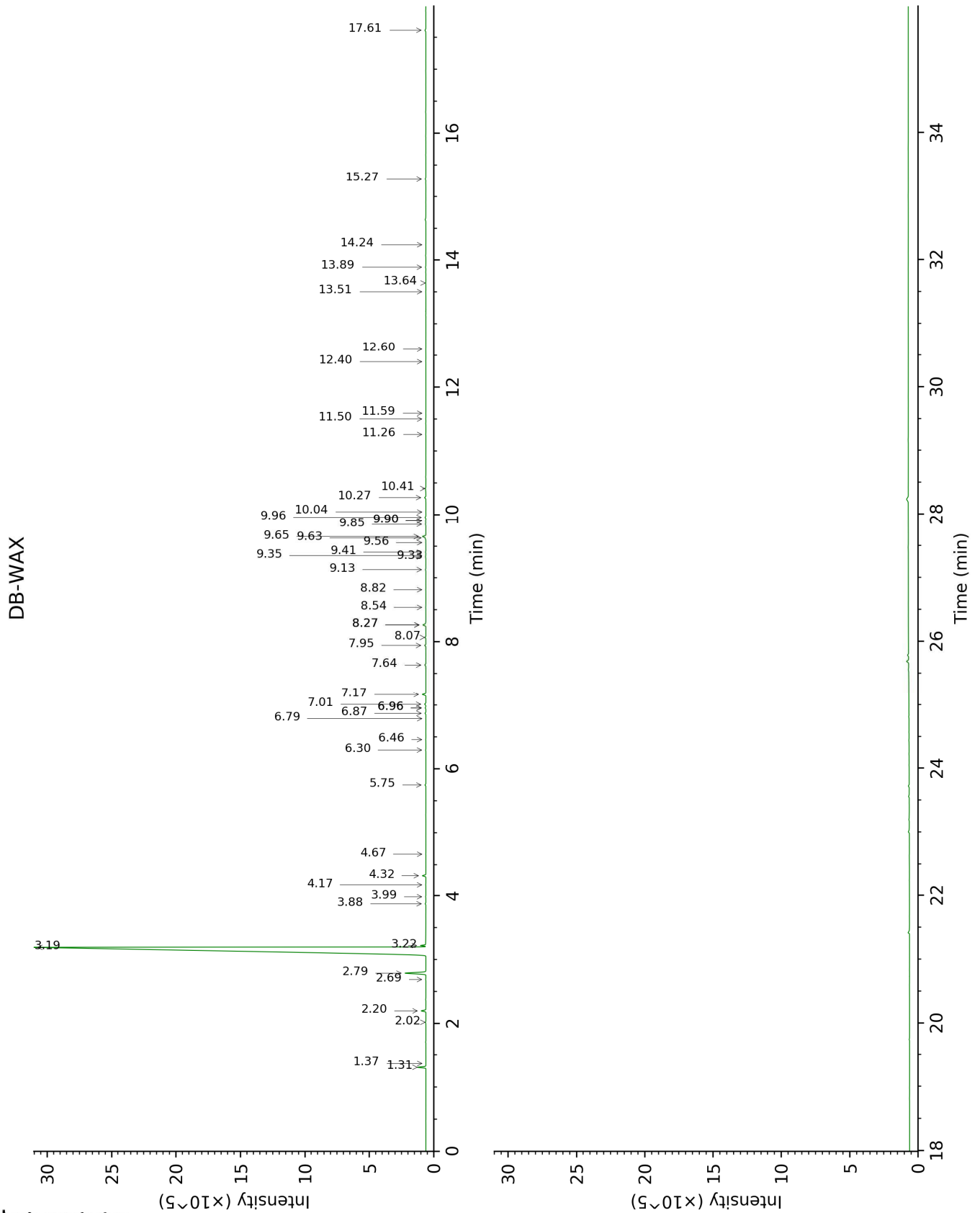
Note: no correction factor was applied

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	%
α -Thujene	2.89	927	tr	1.37	1002	tr
α -Pinene	2.95	931	0.53	1.31	992	0.54
Sabinene	3.54*	971	0.37	2.20	1085	0.35
β -Pinene	3.54*	971	[0.37]	2.02	1067	0.04
Myrcene	3.88	994	1.88	2.79	1135	1.88
α -Phellandrene	4.03*	1004	0.29	2.69	1127	0.03
Octanal	4.03*	1004	[0.29]	4.32	1251	0.26
para-Cymene	4.50*	1034	91.60	3.99	1227	0.02
Limonene	4.50*	1034	[91.60]	3.20	1167	91.93
β -Phellandrene	4.50*	1034	[91.60]	3.22	1169	0.27
(E)- β -Ocimene	4.77	1051	0.05	3.88	1219	0.05
cis-Sabinene hydrate	5.00	1065	0.01	6.79	1431	0.01
Octanol	5.16	1075	0.07	8.07	1528	0.07
Terpinolene	5.34	1087	0.01	4.17	1241	0.02
Linalool	5.56	1101	0.09	7.95	1518	0.10
Nonanal	5.63	1105	0.07	5.75	1355	0.07
(E)-4,8-Dimethylnona-1,3,7-triene	5.82	1118	0.02	4.66	1276	0.01
trans-para-Mentha-2,8-dien-1-ol	5.85	1119	0.01	8.82	1587	0.02
cis-Limonene oxide	6.01	1130	0.02	6.30	1394	0.03
cis-para-Mentha-2,8-dien-1-ol	6.05	1132	0.01	9.35	1630	0.01
trans-Limonene oxide	6.09	1135	0.02	6.46	1406	0.02
(E)-Myroxide	6.22	1143	0.01	6.96*	1444	0.06
Citronellal	6.38	1154	0.07	6.87	1437	0.07
Terpinen-4-ol	6.69	1173	0.01			
α -Terpineol	6.90	1187	0.27	9.65	1654	0.30
Decanal	7.20	1206	0.29	7.17	1460	0.28
Octyl acetate	7.34*	1216	0.06	6.96*	1444	[0.06]
trans-Carveol	7.34*	1216	[0.06]	11.26	1789	0.01
cis-Carveol	7.57	1231	0.01	11.59	1818	0.01
Neral	7.68	1239	0.04	9.33	1628	0.04
Geraniol	7.95	1256	0.01	11.50	1810	0.02
Geranial	8.14	1269	0.07	9.96	1679	0.06
Undecanal	8.71	1308	0.02	8.54	1565	0.02
α -Terpinyl acetate	9.27	1348	0.03	9.56	1646	0.01
Limonene hydroperoxide IV	9.33	1352	0.01			
Neryl acetate	9.48	1363	0.01	10.04	1686	0.01
trans-para-Mentha-6,8-diene-2-hydroperoxide	9.54	1367	0.01			
α -Copaene	9.62	1372	0.10	7.02	1448	0.10
β -Cubebene	9.83*	1387	0.13	7.64	1495	0.10
Geranyl acetate	9.83*	1387	[0.13]	10.41	1717	0.04
β -Elemene	9.86	1390	0.03	8.27*	1544	0.29
Dodecanal	10.14	1409	0.04	9.85	1670	0.04
β -Caryophyllene	10.18	1413	0.26	8.27*	1544	[0.29]

α-Humulene	10.64	1447	0.04	9.13	1612	0.04
(E)-β-Farnesene	10.80	1459	0.04	9.41	1634	0.03
Germacrene D	11.02	1475	0.09	9.63	1652	0.07
Bicyclogermacrene	11.22	1490	0.03	9.90*	1675	0.04
α-Murolene	11.32	1498	0.02	9.90*	1675	[0.04]
Cubebol	11.48	1510	0.01	12.40	1891	0.01
δ-Cadinene	11.60	1520	0.11	10.27	1705	0.11
α-Elemol	11.92	1545	0.03	13.89	2030	0.04
(E)-Nerolidol	12.16	1564	0.01	13.64	2006	0.02
Germacrene D-4-ol	12.23*	1569	0.03	13.51	1993	0.02
Spathulenol	12.23*	1569	[0.03]	14.24	2064	0.01
Caryophyllene oxide	12.29	1574	0.02	12.60	1908	0.01
β-Sinensal	13.76	1694	0.06	15.27	2166	0.06
Myristic acid	14.58	1765	0.02			
Nootkatone	14.87	1790	0.09	17.61	2414	0.09
Hexadecanal	15.04	1805	0.01			
Palmitic acid	16.76	1965	0.10			
Bergapten	17.41	2027	0.03			
Osthole	18.32	2119	0.08			
Linoleic acid	18.44	2131	0.10			
Oleic acid	18.50	2137	0.06			
cis-Vaccenic acid?	18.55	2143	0.02			
Stearic acid	18.76	2165	0.02			
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	18.96	2185	0.02			
Isoauraptene	19.24	2214	0.12			
Meranzin	19.30	2222	0.27			
Meranzin hydrate	20.64	2368	0.01			
Unknown [m/z 219, 247 (85), 217 (61), 161 (48), 189 (33), 232 (23)... 290 (18)]	21.44	2460	0.01			
Auraptene	22.56	2595	0.89			
Epoxyaurapten	23.57	2722	0.24			
Tangeretin	26.67	3136	0.03			
3,5,6,7,8,3',4'-Heptamethoxyflavone?	28.57	3323	0.07			
Total identified		99.22%			97.78%	
Total reported		99.23%			97.78%	

*: Two or more compounds are coeluting on this column

[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
R.T.: Retention time (minutes)
R.I.: Retention index