

Date : August 19, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21H05-PTH03


Customer identification : Grapefruit, Pink ORGANIC - GK0105214R

Type : Essential oil

Source : *Citrus x paradisi*

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 : Pamela Lavoie, M.Sc., Chimiste

Analysis date : August 13, 2021

Checked and approved by :

Alexis St-Gelais, M. Sc., 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

PHYSICOCHEMICAL DATA

Physical aspect: Bright yellow liquid

Refractive index: 1.4761 ± 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	0.01	Monoterpene
α -Pinene	0.51	Monoterpene
Camphene	tr	Monoterpene
meta-Cymene	0.01	Monoterpene
β -Pinene	0.06	Monoterpene
Sabinene	0.36	Monoterpene
Myrcene	1.84	Monoterpene
α -Phellandrene	0.02	Monoterpene
Pseudolimonene	tr	Monoterpene
Octanal	0.35	Aliphatic aldehyde
β -Phellandrene	0.27*	Monoterpene
1,8-Cineole	[0.27]*	Monoterpenic ether
Limonene	92.00	Monoterpene
(Z)- β -Ocimene	0.01	Monoterpene
(E)- β -Ocimene	0.14	Monoterpene
Octanol	0.03	Aliphatic alcohol
Terpinolene	0.01	Monoterpene
Linalool	0.12	Monoterpenic alcohol
Nonanal	0.05	Aliphatic aldehyde
(E)-4,8-Dimethylnona-1,3,7-triene	0.02	Terpene derivative
cis-Limonene oxide	0.01	Monoterpenic ether
trans-Limonene oxide	0.02	Monoterpenic ether
(E)-Myroxide	0.01	Monoterpenic ether
Citronellal	0.06	Monoterpenic aldehyde
α -Terpineol	0.04	Monoterpenic alcohol
Decanal	0.28	Aliphatic aldehyde
Octyl acetate	0.02	Aliphatic ester
trans-Carveol	0.01	Monoterpenic alcohol
Citronellol	0.01	Monoterpenic alcohol
Neral	0.05	Monoterpenic aldehyde
Geranial	0.07	Monoterpenic aldehyde
Undecanal	0.01	Aliphatic aldehyde
α -Terpinyl acetate	0.01	Monoterpenic ester
Neryl acetate	0.01	Monoterpenic ester
α -Copaene	0.10	Sesquiterpene
β -Cubebene	0.09	Sesquiterpene
Geranyl acetate	0.07	Monoterpenic ester
β -Elemene	0.02	Sesquiterpene
Dodecanal	0.03	Aliphatic aldehyde
β -Caryophyllene	0.24	Sesquiterpene
α -Humulene	0.04	Sesquiterpene
(E)- β -Farnesene	0.01	Sesquiterpene
Germacrene D	0.08	Sesquiterpene
Bicyclogermacrene	0.03	Sesquiterpene
α -Muurolene	0.03	Sesquiterpene

Cubebol	0.02	Sesquiterpenic alcohol
δ-Cadinene	0.11	Sesquiterpene
α-Elemol	0.02	Sesquiterpenic alcohol
(E)-Nerolidol	0.03	Sesquiterpenic alcohol
Germacrene D-4-ol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
β-Sinensal	0.01	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	0.15	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
Myristic acid	0.02	Aliphatic acid
Nootkatone	0.16	Sesquiterpenic ketone
Palmitic acid	0.08	Aliphatic acid
Osthole	0.04	Coumarin
Linoleic acid	0.11	Aliphatic acid
Oleic acid	0.06	Aliphatic acid
cis-Vaccenic acid?	0.03	Aliphatic acid
Stearic acid	0.02	Aliphatic acid
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	0.02	Coumarin
Isoauraptene	0.07	Coumarin
Meranzin	0.17	Coumarin
Auraptenol	0.01	Coumarin
Auraptene	0.67	Coumarin
Epoxyaurapten	0.09	Coumarin
Tangeretin	0.03	Flavonoid
3,3',4',5,6,7,8-Heptamethoxyflavone	0.03	Flavonoid
Consolidated total	99.16%	

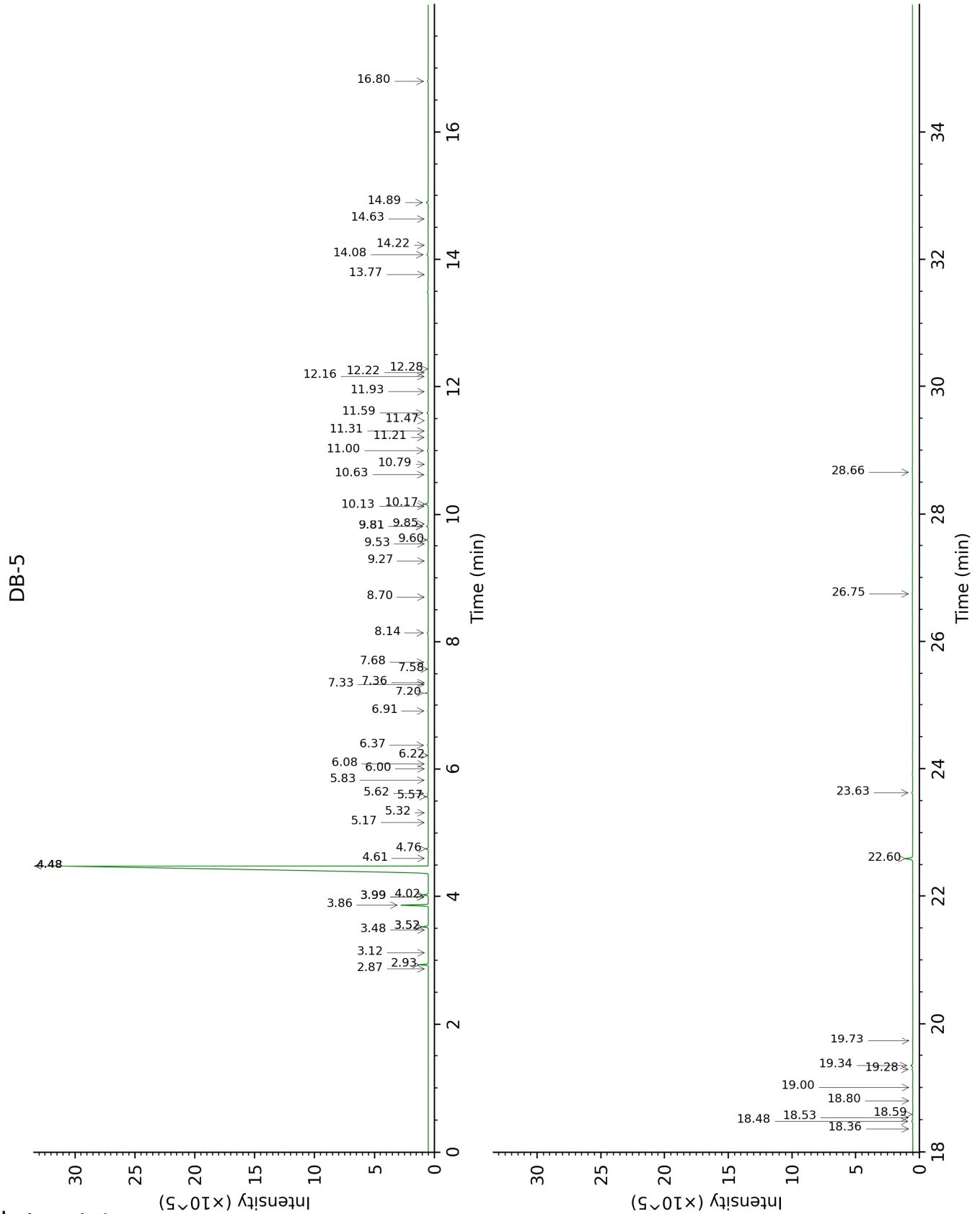
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered [xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

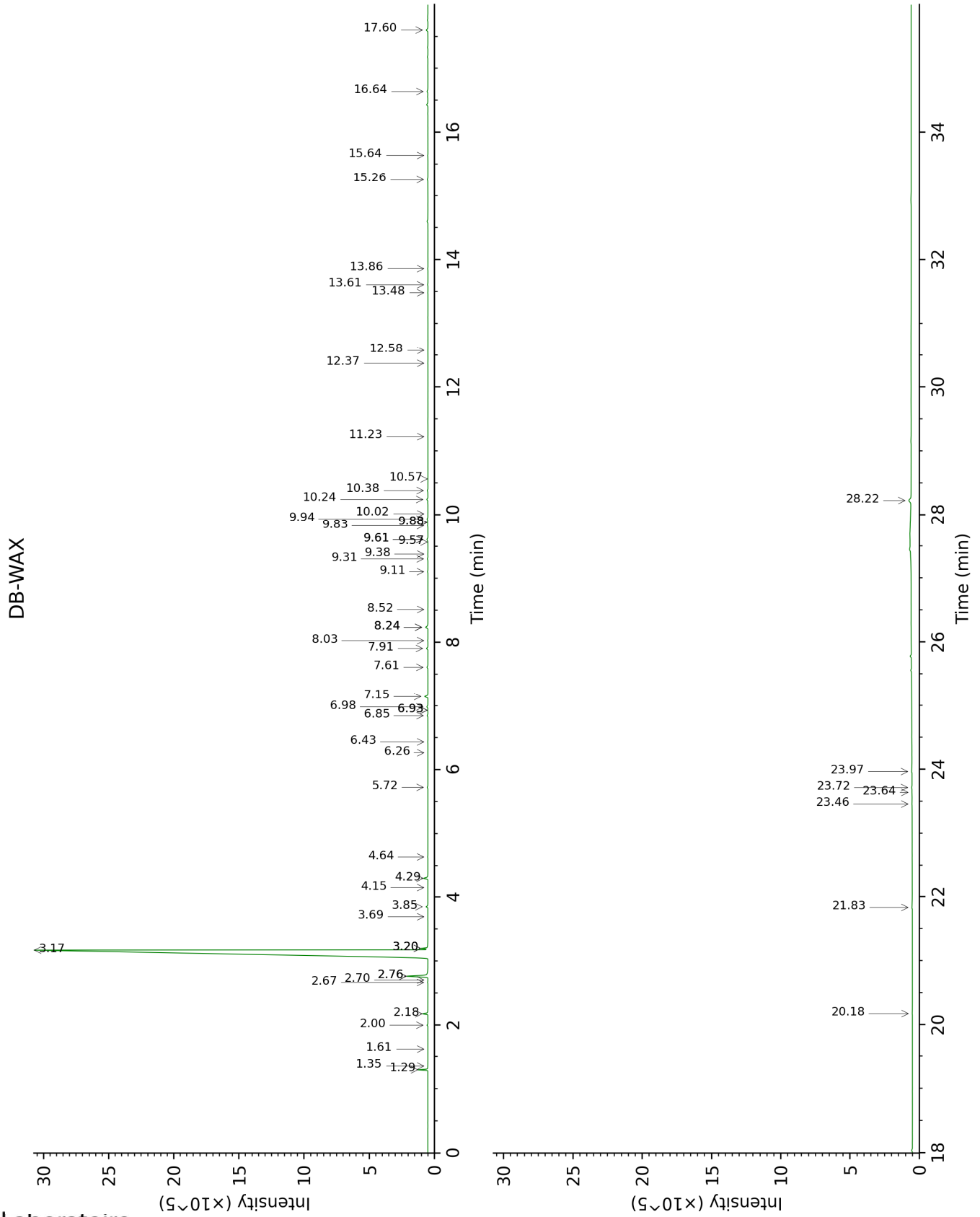
Note: no correction factor was applied

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	%
α -Thujene	2.87	926	0.01	1.35	1000	0.01
α -Pinene	2.93	930	0.51	1.29	991	0.50
Camphene	3.12	943	tr	1.61	1026	tr
meta-Cymene	3.48	967	0.01	2.76*	1134	1.83
β -Pinene	3.52*	970	0.42	2.00	1066	0.06
Sabinene	3.52*	970	[0.42]	2.18	1084	0.36
Myrcene	3.86	993	1.84	2.76*	1134	[1.83]
α -Phellandrene	3.99*	1002	0.03	2.67	1126	0.02
Pseudolimonene	3.99*	1002	[0.03]	2.70	1129	tr
Octanal	4.02	1004	0.35	4.29	1254	0.35
β -Phellandrene	4.48*	1033	92.26	3.20*	1169	0.41
1,8-Cineole	4.48*	1033	[92.26]	3.20*	1169	[0.41]
Limonene	4.48*	1033	[92.26]	3.17	1167	92.00
(Z)- β -Ocimene	4.61	1041	0.01	3.69	1208	0.01
(E)- β -Ocimene	4.76	1050	0.14	3.85	1220	0.14
Octanol	5.17	1076	0.03	8.03	1525	0.02
Terpinolene	5.32	1086	0.01	4.15	1243	0.01
Linalool	5.57	1102	0.12	7.91	1516	0.12
Nonanal	5.62	1105	0.05	5.72	1354	0.05
(E)-4,8-Dimethylnona-1,3,7-triene	5.83	1118	0.02	4.64	1280	0.02
cis-Limonene oxide	6.00	1130	0.01	6.26	1393	0.01
trans-Limonene oxide	6.08	1135	0.02	6.44	1405	0.02
(E)-Myroxide	6.22	1143	0.01	6.93*	1442	0.03
Citronellal	6.37	1154	0.06	6.85	1436	0.06
α -Terpineol	6.91	1188	0.04	9.61*	1651	0.11
Decanal	7.20	1206	0.28	7.15	1458	0.28
Octyl acetate	7.33	1216	0.02	6.93*	1442	[0.03]
trans-Carveol	7.36	1218	0.01	11.23	1786	0.01
Citronellol	7.58	1232	0.01	10.57	1730	0.01
Neral	7.68	1239	0.05	9.31	1626	0.05
Geranial	8.14	1270	0.07	9.94	1677	0.09
Undecanal	8.70	1308	0.01	8.52	1563	0.01
α -Terpinyl acetate	9.27	1348	0.01	9.57	1647	0.01
Neryl acetate	9.53	1367	0.01	10.02	1684	0.01
α -Copaene	9.60	1371	0.10	6.98	1446	0.10
β -Cubebene	9.81*	1386	0.14	7.61	1493	0.09
Geranyl acetate	9.81*	1386	[0.14]	10.38	1714	0.07
β -Elemene	9.84	1389	0.02	8.24*	1542	0.26
Dodecanal	10.13	1409	0.03	9.83	1668	0.04
β -Caryophyllene	10.17	1412	0.24	8.24*	1542	[0.26]
α -Humulene	10.63	1446	0.04	9.10	1610	0.04
(E)- β -Farnesene	10.79	1458	0.01	9.38	1632	0.02
Germacrene D	11.00	1474	0.08	9.61*	1651	[0.11]
Bicyclgermacrene	11.21	1490	0.03	9.88*	1673	0.05
α -Muurolene	11.31	1497	0.03	9.88*	1673	[0.05]
Cubebol	11.47	1509	0.02	12.37	1887	0.02
δ -Cadinene	11.59	1519	0.11	10.24	1703	0.11

α-Elemol	11.92	1545	0.02	13.86	2026	0.02
(E)-Nerolidol	12.16	1564	0.03	13.61	2002	0.03
Germacrene D-4-ol	12.22	1569	0.02	13.48	1990	0.02
Caryophyllene oxide	12.28	1573	0.02	12.58	1906	0.01
β-Sinensal	13.77	1694	0.01	15.26	2163	0.06
(2E,6E)-Farnesol	14.08	1721	0.15	16.64	2306	0.10
(2E,6E)-Farnesal	14.22	1734	0.02	15.64	2201	0.02
Myristic acid	14.63	1769	0.02	20.18	2709	0.04
Nootkatone	14.89	1792	0.16	17.60	2410	0.18
Palmitic acid	16.80	1968	0.08	21.83	2918	0.11
Osthole	18.36	2122	0.04			
Linoleic acid	18.48	2134	0.11	23.97	3207	0.11
Oleic acid	18.53	2140	0.06	23.72	3172	0.06
cis-Vaccenic acid?	18.58	2145	0.03	23.64	3161	0.02
Stearic acid	18.80	2167	0.02	23.46	3136	0.03
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	19.00	2189	0.02			
Isoauraptene	19.28	2218	0.07			
Meranzin	19.34	2225	0.17			
Auraptenol	19.73	2266	0.01			
Auraptene	22.60	2597	0.67	28.22	3770	0.35
Epoxyaurapten	23.63	2726	0.09			
Tangeretin	26.75	3141	0.03			
3,3',4',5,6,7,8-Heptamethoxyflavone	28.66	3325	0.03			
Total identified		99.13%			98.58%	
Total reported		99.13%			98.58%	

*: 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