Date : May 04, 2021

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 21D20-ORA05
Customer identification : Grapefruit - Paraguay - 3 years - B715002
Type : Essential oil
Source : *Citrus x paradisi* cv. White
Customer : Organic Aromas Inc.

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 : Benoit Roger, Ph. D.
Analysis date : May 03, 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

Laboratoire PhytoChemia
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PHYSICOCHEMICAL DATA

Physical aspect: Bright yellow liquid
Refractive index: 1.4779 ± 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
α-Thujene	0.01	Monoterpene
α-Pinene	0.51	Monoterpene
Camphene	tr	Monoterpene
Sabinene	0.61	Monoterpene
β-Pinene	0.05	Monoterpene
Myrcene	1.80	Monoterpene
α-Phellandrene	0.02	Monoterpene
Octanal	0.28	Aliphatic aldehyde
para-Cymene	0.02	Monoterpene
1,8-Cineole	0.27	Monoterpenic ether
Limonene	90.32	Monoterpene
(*Z*)-β-Ocimene	0.01	Monoterpene
(*E*)-β-Ocimene	0.14	Monoterpene
γ-Terpinene	0.04	Monoterpene
cis-Sabinene hydrate	tr	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Terpinolene	0.01	Monoterpene
Linalool	0.06	Monoterpenic alcohol
Nonanal	0.07	Aliphatic aldehyde
trans-para-Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol
cis-Limonene oxide	0.04	Monoterpenic ether
cis-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
trans-Limonene oxide	0.04	Monoterpenic ether
Citronellal	0.05	Monoterpenic aldehyde
Terpinen-4-ol	0.01	Monoterpenic alcohol
α-Terpineol	0.03	Monoterpenic alcohol
Decanal	0.34	Aliphatic aldehyde
Octyl acetate	0.05	Aliphatic ester
trans-Carveol	0.01	Monoterpenic alcohol
cis-Carveol	0.01	Monoterpenic alcohol
Neral	0.05	Monoterpenic aldehyde
Geraniol	0.01	Monoterpenic alcohol
Geranial	0.06	Monoterpenic aldehyde
Undecanal	0.02	Aliphatic aldehyde
α-Terpinyl acetate	0.01	Monoterpenic ester
Limonene hydroperoxide IV	0.01	Monoterpenic peroxide
α-Copaene	0.14	Sesquiterpene
Geranyl acetate	0.05	Monoterpenic ester
β-Cubebene	0.13	Sesquiterpene
β-Elemene	0.03	Sesquiterpene
β-Caryophyllene	0.44	Sesquiterpene
α-Humulene	0.06	Sesquiterpene
(*E*)-β-Farnesene	0.02	Sesquiterpene
Germacrene D	0.12	Sesquiterpene
Bicyclogermacrene	0.03	Sesquiterpene

α-Muurolene	0.03	Sesquiterpene
Cubebol	0.02	Sesquiterpenic alcohol
δ-Cadinene	0.15	Sesquiterpene
α-Elemol	0.03	Sesquiterpenic alcohol
(*E*)-Nerolidol	0.02	Sesquiterpenic alcohol
Caryophyllene oxide	0.04	Sesquiterpenic ether
β-Sinensal	0.02	Sesquiterpenic aldehyde
Nootkatone	0.04	Sesquiterpenic ketone
Palmitic acid	0.15	Aliphatic acid
Osthole	0.05	Coumarin
Linoleic acid	0.11	Aliphatic acid
Oleic acid	0.07	Aliphatic acid
Stearic acid	0.06	Aliphatic acid
Isoauraptene	0.05	Coumarin
Meranzin	0.13	Coumarin
Auraptenol	0.01	Coumarin
Auraptene	1.23	Coumarin
Epoxyaurapten	0.39	Coumarin
Tangeretin	0.05	Flavonoid
Consolidated total	**98.65%**	

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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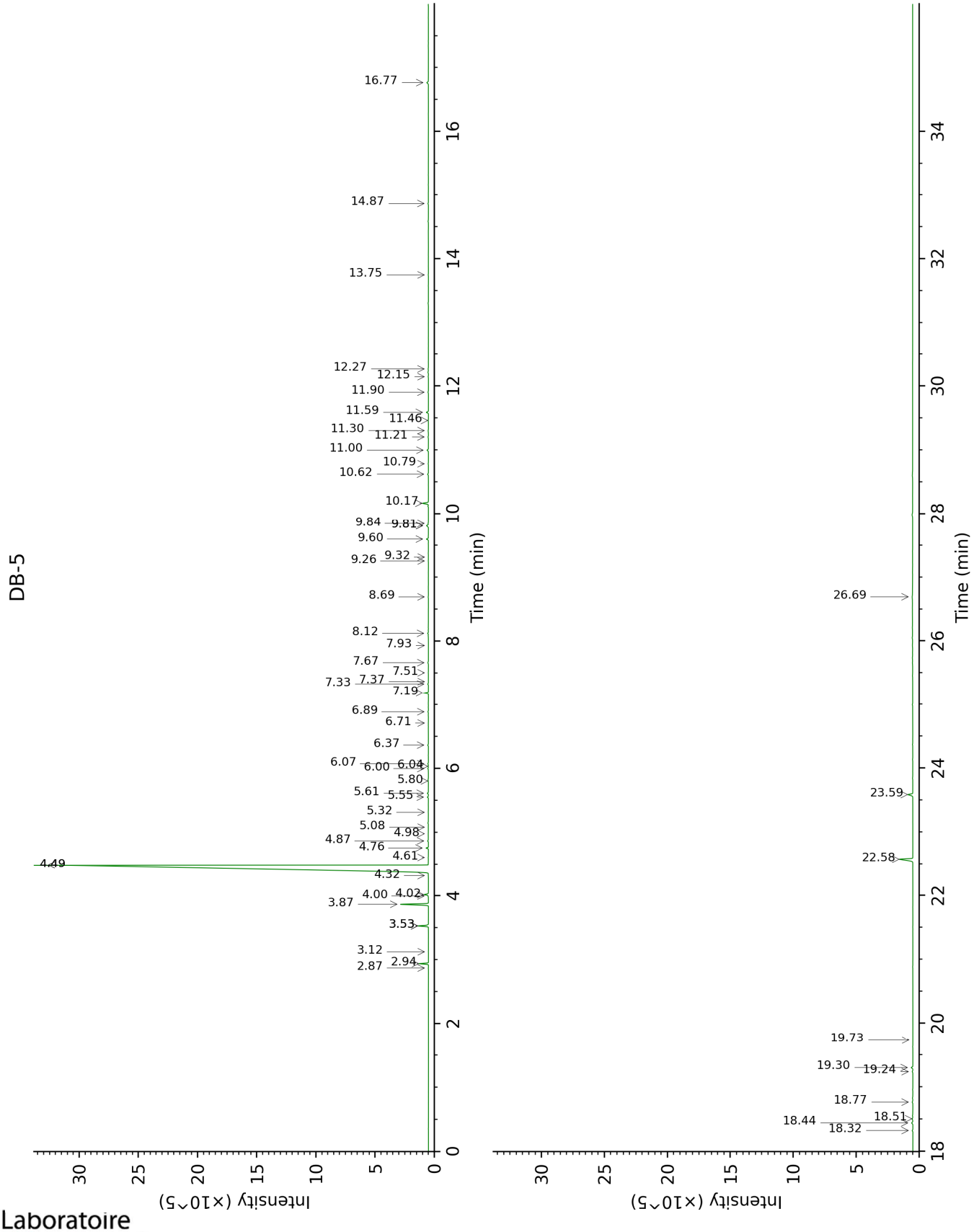
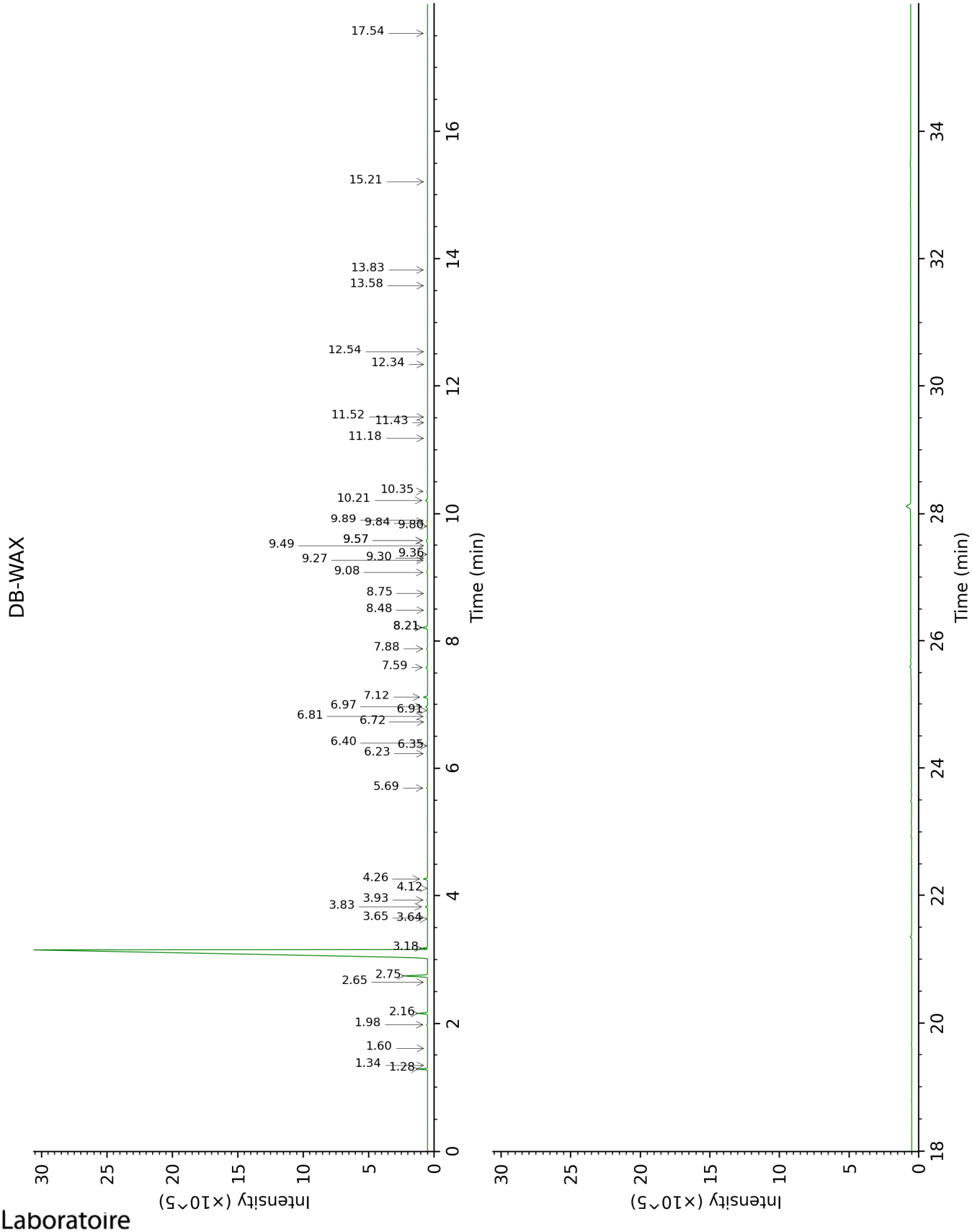

DB-5
Intensity (×10^5)
Time (min)
16.77
14.87
13.75
12.27
12.15
11.90
11.59
11.46
11.30
11.21
11.00
10.79
10.62
10.17
9.84
9.81
9.60
9.26
9.32
8.69
8.12
7.93
7.67
7.51
7.33
7.37
7.19
6.89
6.71
6.37
6.07
6.00
6.04
5.80
5.61
5.55
5.32
5.08
4.98
4.87
4.76
4.61
4.49
4.32
4.00
4.02
3.87
3.53
3.12
2.94
2.87
26.69
23.59
22.58
19.73
19.30
19.24
18.77
18.51
18.44
18.32


DB-WAX
17.54
15.21
13.83
13.58
12.54
12.34
11.52
11.43
11.18
10.35
10.21
9.89
9.84
9.80
9.57
9.49
9.36
9.30
9.27
9.08
8.75
8.48
8.21
7.88
7.59
7.12
6.97
6.91
6.81
6.72
6.40
6.35
6.23
5.69
4.26
4.12
3.93
3.83
3.65
3.64
3.18
2.75
2.65
2.16
1.98
1.60
1.34
1.28
Time (min)
Intensity (×10^5)

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
α-Thujene	2.87	927	0.01	1.34	1001	0.01
α-Pinene	2.94	932	0.51	1.28	992	0.52
Camphene	3.12	944	tr	1.60	1027	tr
Sabinene	3.53*	972	0.64	2.16	1084	0.61
β-Pinene	3.53*	972	[0.64]	1.98	1066	0.05
Myrcene	3.87	994	1.80	2.75	1134	1.83
α-Phellandrene	4.00	1003	0.02	2.65	1126	0.03
Octanal	4.02	1005	0.28	4.26	1251	0.27
para-Cymene	4.32	1024	0.02	3.93	1227	0.04
1,8-Cineole	4.49*	1034	90.59	3.18	1168	0.27
Limonene	4.49*	1034	[90.59]			
(*Z*)-β-Ocimene	4.61	1042	0.01	3.64	1205	0.01
(*E*)-β-Ocimene	4.76	1052	0.14	3.83	1219	0.14
γ-Terpinene	4.87	1058	0.04	3.65	1206	0.05
cis-Sabinene hydrate	4.98	1066	tr	6.72	1429	0.01
cis-Linalool oxide (fur.)	5.08	1072	0.01	6.35	1402	0.01
Terpinolene	5.32	1087	0.01	4.12	1240	0.01
Linalool	5.55	1102	0.06	7.88	1517	0.07
Nonanal	5.61	1106	0.07	5.69	1354	0.06
trans-para-Mentha-2,8-dien-1-ol	5.80	1118	0.02	8.75	1584	0.02
cis-Limonene oxide	6.00	1130	0.04	6.23	1393	0.04
cis-para-Mentha-2,8-dien-1-ol	6.04	1133	0.01	9.30	1628	0.01
trans-Limonene oxide	6.07	1135	0.04	6.40	1405	0.04
Citronellal	6.37	1154	0.05	6.81	1436	0.04
Terpinen-4-ol	6.71	1176	0.01			
α-Terpineol	6.89	1188	0.03	9.57*	1651	0.16
Decanal	7.19	1207	0.34	7.12	1458	0.31
Octyl acetate	7.33	1217	0.05	6.91	1443	0.03
trans-Carveol	7.37	1219	0.01	11.18	1786	0.02
cis-Carveol	7.51	1228	0.01	11.52	1815	0.02
Neral	7.66	1239	0.05	9.27	1626	0.04
Geraniol	7.93	1257	0.01	11.43	1808	0.01
Geranial	8.12	1270	0.06	9.89	1677	0.05
Undecanal	8.69	1308	0.02	8.48	1564	0.02
α-Terpinyl acetate	9.26	1348	0.01	9.49	1644	0.01
Limonene hydroperoxide IV	9.32	1352	0.01			
α-Copaene	9.60	1372	0.14	6.97	1447	0.14
Geranyl acetate	9.81*	1387	0.17	10.35	1715	0.05
β-Cubebene	9.81*	1387	[0.17]	7.59	1494	0.13
β-Elemene	9.84	1390	0.03	8.21*	1543	0.47

β-Caryophyllene	10.17	1413	0.44	8.21*	1543	[0.47]
α-Humulene	10.62	1447	0.06	9.08	1610	0.06
(*E*)-β-Farnesene	10.79	1459	0.02	9.36	1633	0.03
Germacrene D	11.00	1475	0.12	9.57*	1651	[0.16]
Bicyclogermacrene	11.21	1491	0.03	9.84	1673	0.04
α-Muurolene	11.30	1498	0.03	9.80	1669	0.03
Cubebol	11.46	1510	0.02	12.34	1889	0.01
δ-Cadinene	11.59	1520	0.15	10.21	1703	0.15
α-Elemol	11.90	1545	0.03	13.83	2028	0.04
(*E*)-Nerolidol	12.15	1564	0.02	13.58	2004	0.02
Caryophyllene oxide	12.27	1574	0.04	12.54	1906	0.02
β-Sinensal	13.75	1695	0.02	15.21	2164	0.01
Nootkatone	14.87	1791	0.04	17.54	2410	0.03
Palmitic acid	16.77	1966	0.15			
Osthole	18.32	2120	0.05			
Linoleic acid	18.44	2133	0.11			
Oleic acid	18.51	2139	0.07			
Stearic acid	18.76	2166	0.06			
Isoauraptene	19.24	2216	0.05			
Meranzin	19.30	2222	0.13			
Auraptenol	19.73	2269	0.01			
Auraptene	22.58	2597	1.23			
Epoxyaurapten	23.59	2724	0.39			
Tangeretin	26.69	3138	0.05			
Total identified		**98.62%**			**6.05%**	
Total reported		**98.62%**			**6.05%**	

*: 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