

Date : May 04, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

**Internal code** : 21D20-ORA06


**Customer identification** : Sweet Orange - Brazil - 3 years - 012131A

**Type** : Essential oil

**Source** : *Citrus sinensis*

**Customer** : Organic Aromas Inc.

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** : May 04, 2021

Checked and approved by :

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

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Bright yellow liquid

**Refractive index:**  $1.4737 \pm 0.0003$  (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
Heptanal	tr	Aliphatic aldehyde
$\alpha$ -Thujene	tr	Monoterpene
$\alpha$ -Pinene	0.53	Monoterpene
Camphene	tr	Monoterpene
$\beta$ -Pinene	0.02	Monoterpene
Sabinene	0.28	Monoterpene
Myrcene	1.77	Monoterpene
$\alpha$ -Phellandrene	0.02	Monoterpene
Octanal	0.26	Aliphatic aldehyde
$\Delta^3$ -Carene	0.06	Monoterpene
para-Cymene	tr	Monoterpene
Limonene	94.15	Monoterpene
$\beta$ -Phellandrene	0.24	Monoterpene
(Z)- $\beta$ -Ocimene	tr	Monoterpene
(E)- $\beta$ -Ocimene	0.01	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.02	Monoterpene
Linalool	0.36	Monoterpenic alcohol
Nonanal	0.05	Aliphatic aldehyde
trans-para-Mentha-2,8-dien-1-ol	0.04	Monoterpenic alcohol
(E)-4,8-Dimethyl-1,3,7-nonatriene	tr	Monoterpene
cis-Limonene oxide	0.09	Monoterpenic ether
cis-para-Mentha-2,8-dien-1-ol	0.03	Monoterpenic alcohol
trans-Limonene oxide	0.06	Monoterpenic ether
Citronellal	0.05	Monoterpenic aldehyde
Terpinen-4-ol	0.01	Monoterpenic alcohol
Cryptone	0.01	Normonoterpenic ketone
para-Cymen-8-ol	0.03	Monoterpenic alcohol
$\alpha$ -Terpineol	0.04	Monoterpenic alcohol
Decanal	0.23	Aliphatic aldehyde
Octyl acetate	0.01	Aliphatic ester
trans-Carveol	0.05	Monoterpenic alcohol
2,3-Epoxyneral?	0.01	Monoterpenic aldehyde
Nerol	0.01	Monoterpenic alcohol
cis-Carveol	0.03	Monoterpenic alcohol
Neral	0.03	Monoterpenic aldehyde
Carvone	0.03	Monoterpenic ketone
Geranial	0.07	Monoterpenic aldehyde
Perillaldehyde	0.01	Monoterpenic aldehyde
Limonen-10-ol	0.02	Monoterpenic alcohol
Undecanal	0.01	Aliphatic aldehyde
cis-para-Mentha-2,8-diene-1-hydroperoxide	0.03	Monoterpenic peroxide
trans-para-Mentha-2,8-diene-1-hydroperoxide	0.04	Monoterpenic peroxide
para-Mentha-1,8-diene-4-hydroperoxide	0.02	Monoterpenic peroxide

$\alpha$ -Cubebene	0.01	Sesquiterpene
<i>trans</i> -para-Mentha-6,8-diene-2-hydroperoxide	0.04	Monoterpenic peroxide
$\alpha$ -Copaene	0.03	Sesquiterpene
$\beta$ -Cubebene	0.03	Sesquiterpene
$\beta$ -Elemene	0.01	Sesquiterpene
Dodecanal	0.05	Aliphatic aldehyde
$\beta$ -Caryophyllene	0.02	Sesquiterpene
$\beta$ -Copaene	0.02	Sesquiterpene
$\alpha$ -Humulene	0.01	Sesquiterpene
( <i>E</i> )- $\beta$ -Farnesene	0.01	Sesquiterpene
Germacrene D	0.02	Sesquiterpene
Valencene	0.06	Sesquiterpene
$\gamma$ -Cadinene	0.02	Sesquiterpene
$\delta$ -Cadinene	0.03	Sesquiterpene
$\alpha$ -Elemol	0.01	Sesquiterpenic alcohol
Spathulenol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
$\beta$ -Sinensal	0.03	Sesquiterpenic aldehyde
$\alpha$ -Sinensal	0.02	Sesquiterpenic aldehyde
Myristic acid	0.02	Aliphatic acid
Nootkatone	0.01	Sesquiterpenic ketone
meta-Camphorene	0.01	Diterpene
Palmitic acid	0.07	Aliphatic acid
Linoleic acid	0.03	Aliphatic acid
Oleic acid	0.02	Aliphatic acid
<i>cis</i> -Vaccenic acid?	0.02	Aliphatic acid
Stearic acid	0.09	Aliphatic acid
Tetramethoxyflavone isomer	0.03	Flavonoid
Tangeretin	0.06	Flavonoid
3,5,6,7,8,3',4'-Heptamethoxyflavone?	0.02	Flavonoid
3,3',4',5,6,7,8-Heptamethoxyflavone	0.08	Flavonoid
Nobiletin	0.04	Flavonoid
<b>Consolidated total</b>	<b>99.72%</b>	

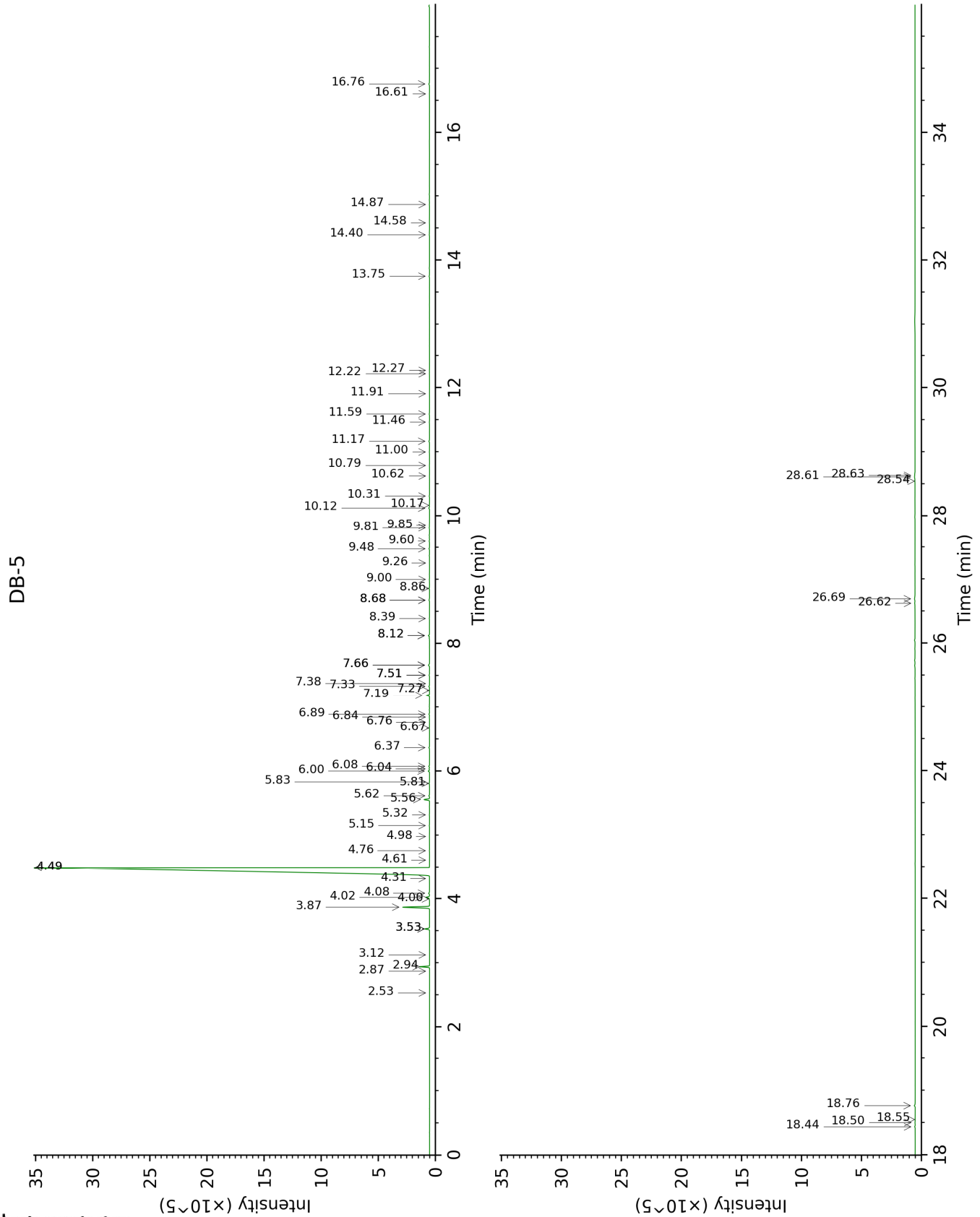
tr: The compound has been detected below 0.005% of total signal.

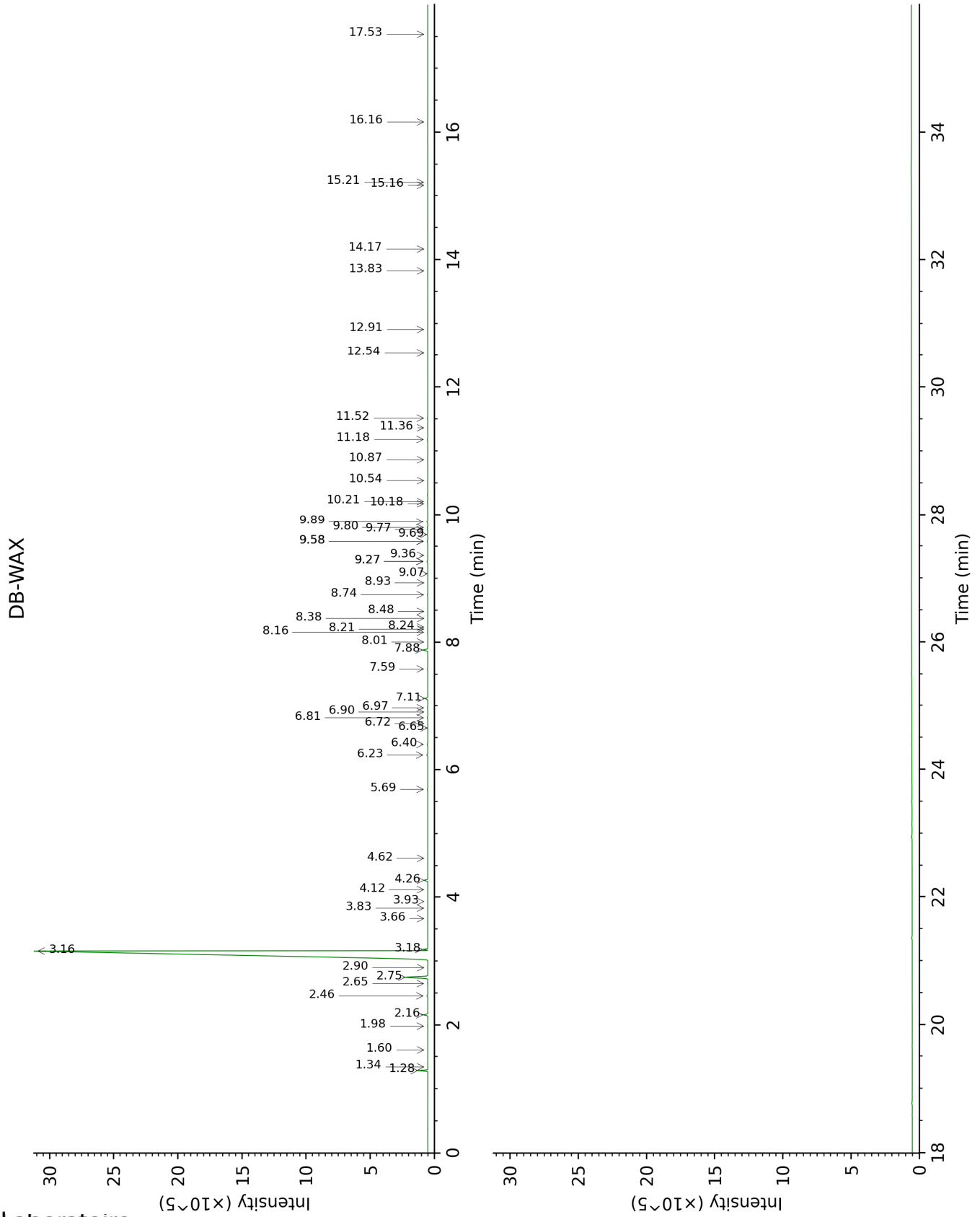
Note: no correction factor was applied

**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	%
Heptanal	2.53	904	tr	2.90	1146	tr
$\alpha$ -Thujene	2.87	927	tr	1.34	1001	0.01
$\alpha$ -Pinene	2.94	932	0.53	1.28	992	0.54
Camphene	3.12	944	tr	1.60	1027	0.01
$\beta$ -Pinene	3.53*	972	0.30	1.98	1066	0.02
Sabinene	3.53*	972	[0.30]	2.16	1084	0.28
Myrcene	3.87	994	1.77	2.75	1134	1.78
$\alpha$ -Phellandrene	4.00	1003	0.02	2.65	1126	0.02
Octanal	4.02	1005	0.26	4.26	1251	0.25
$\Delta^3$ -Carene	4.08	1009	0.06	2.46	1111	0.07
para-Cymene	4.31	1023	tr	3.93	1227	0.02
Limonene	4.49*	1035	93.74	3.16	1167	94.15
$\beta$ -Phellandrene	4.49*	1035	[93.74]	3.18	1169	0.24
(Z)- $\beta$ -Ocimene	4.61	1042	tr	3.66	1207	0.01
(E)- $\beta$ -Ocimene	4.76	1052	0.01	3.83	1219	0.02
cis-Sabinene hydrate	4.98	1066	0.01	6.72	1429	0.01
Octanol	5.15	1076	0.02	8.01	1526	0.02
Terpinolene	5.32	1087	0.02	4.12	1240	0.02
Linalool	5.56	1102	0.36	7.88	1517	0.36
Nonanal	5.62	1106	0.05	5.69	1354	0.04
trans-para-Mentha-2,8-dien-1-ol	5.81	1118	0.04	8.74	1584	0.03
(E)-4,8-Dimethyl-1,3,7-nonatriene	5.83	1120	tr	4.62	1278	0.01
cis-Limonene oxide	6.00	1131	0.09	6.23	1392	0.09
cis-para-Mentha-2,8-dien-1-ol	6.04	1133	0.03	9.26*	1626	0.07
trans-Limonene oxide	6.08	1135	0.06	6.40	1405	0.05
Citronellal	6.37	1154	0.05	6.81	1436	0.04
Terpinen-4-ol	6.67	1174	0.01	8.38	1555	0.01
Cryptone	6.76	1180	0.01	8.93	1599	0.01
para-Cymen-8-ol	6.84	1185	0.03	11.36	1802	0.02
$\alpha$ -Terpineol	6.89	1188	0.04	9.58*	1652	0.07
Decanal	7.19	1207	0.23	7.11	1458	0.20
Octyl acetate	7.27	1213	0.01	6.90	1443	0.01
trans-Carveol	7.33	1217	0.05	11.18	1786	0.04
2,3-Epoxyneral?	7.38	1220	0.01			
Nerol	7.51*†	1228	0.05	10.86	1759	0.01
cis-Carveol	7.51*†	1228	[0.05]	11.52	1815	0.03
Neral	7.66*	1239	0.10	9.26*	1626	[0.07]
Carvone	7.66*	1239	[0.10]	9.80	1669	0.03
Geranial	8.12*	1270	0.08	9.89	1677	0.07
Perillaldehyde	8.12*	1270	[0.08]	10.54	1731	0.01
Limonen-10-ol	8.39	1288	0.02	12.91	1941	0.02
Undecanal	8.68*	1307	0.04	8.48	1564	0.01
cis-para-Mentha-2,8-diene-1-hydroperoxide	8.68*	1307	[0.04]			



<i>trans</i> -para-Mentha-2,8-diene-1-hydroperoxide	8.86	1320	0.04			
para-Mentha-1,8-diene-4-hydroperoxide	9.00	1330	0.02			
$\alpha$ -Cubebene	9.26	1348	0.01	6.65	1424	0.01
<i>trans</i> -para-Mentha-6,8-diene-2-hydroperoxide	9.48	1364	0.04			
$\alpha$ -Copaene	9.60	1373	0.03	6.97	1448	0.03
$\beta$ -Cubebene	9.81	1387	0.03	7.59	1494	0.04
$\beta$ -Elemene	9.84	1390	0.01	8.24	1545	0.01
Dodecanal	10.12	1410	0.05	9.77	1667	0.05
$\beta$ -Caryophyllene	10.17	1413	0.02	8.21	1542	0.02
$\beta$ -Copaene	10.31	1424	0.02	8.16	1538	0.03
$\alpha$ -Humulene	10.62	1447	0.01	9.07	1610	0.01
( <i>E</i> )- $\beta$ -Farnesene	10.79	1460	0.01	9.36	1634	0.01
Germacrene D	11.00	1475	0.02	9.58*	1652	[0.07]
Valencene	11.17	1488	0.06	9.69	1660	0.05
$\gamma$ -Cadinene	11.46	1510	0.02	10.18	1700	0.03
$\delta$ -Cadinene	11.59	1520	0.03	10.21	1703	0.03
$\alpha$ -Elemol	11.91	1545	0.01	13.83	2028	0.01
Spathulenol	12.22	1570	0.01	14.17	2061	0.01
Caryophyllene oxide	12.27	1574	0.02	12.54	1906	0.01
$\beta$ -Sinensal	13.75	1695	0.03	15.21	2164	0.03
$\alpha$ -Sinensal	14.40	1750	0.02	16.16	2263	0.01
Myristic acid	14.58	1767	0.02			
Nootkatone	14.87	1792	0.01	17.53	2410	0.01
meta-Camphorene	16.61	1951	0.01	15.16	2159	0.01
Palmitic acid	16.76	1966	0.07			
Linoleic acid	18.44	2132	0.03			
Oleic acid	18.50	2139	0.02			
<i>cis</i> -Vaccenic acid?	18.55	2144	0.02			
Stearic acid	18.76	2166	0.09			
Tetramethoxyflavone isomer	26.62	3130	0.03			
Tangeretin	26.69	3138	0.06			
3,5,6,7,8,3',4'-Heptamethoxyflavone?	28.54	3319	0.02			
3,3',4',5,6,7,8-Heptamethoxyflavone	28.61	3324	0.08			
Nobiletin	28.63	3326	0.04			
<b>Total identified</b>		<b>99.10%</b>			<b>99.09%</b>	
<b>Total reported</b>		<b>99.10%</b>			<b>99.09%</b>	

\*: 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