

**Date :** March 28, 2018

**CERTIFICATE OF ANALYSIS - GC PROFILING**

**SAMPLE IDENTIFICATION**

**Internal code :** 18C16-CHS2-1-CC

**Customer identification :** Grapefruit - USA - MD66302ORG

**Type :** Essential oil

**Source :** *Citrus x paradisi* cv. Red

**Customer :** American College of Healthcare Sciences

**ANALYSIS**

**Method:** PC-PA-014-17J19 - Analysis of the composition of an essential oil, or other volatile liquid, by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Sarah-Eve Tremblay, M. Sc. A., Chimiste

**Analysis date :** March 22, 2018

Checked and approved by :

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

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## PYHSICOCHEMICAL DATA

**Physical aspect:** Bright yellow liquid

**Refractive index:**  $1.4743 \pm 0.0003$  (20 °C)

## COMPLIANCE WITH ISO 3053:2005 (*CITRUS X PARADISI*)

Compound	Min. Content	Max. Content	Observed %	Complies?
α-Pinene	0.2	0.6	0.5	Yes
Sabinene	0.1	0.6	0.5	Yes
β-Pinene	0.05	0.2	0.04	No
Myrcene	1.5	2.5	1.7	Yes
Limonene	92	96	92.1	Yes
Octanal	0.2	0.8	0.4	Yes
Nonanal	0.04	0.1	0.06	Yes
Decanal	0.1	0.6	0.3	Yes
Neral	0.02	0.04	0.02	Yes
β-Caryophyllene	0.2	0.5	0.3	Yes
Nootkatone	0.01	0.8	0.2	Yes
Refractive index	1.474	1.479	1.4743	Yes

## CONCLUSION

No adulterant, contaminant or diluent has been detected using this method. The oil marginally does not comply with the ISO standard, but nevertheless corresponds to the expectations for the species.

## ANALYSIS SUMMARY

Identification	DB-5 (%)	DB-WAX (%)	Classe
Ethanol	0.03	0.03	Aliphatic alcohol
Heptanal	tr	tr	Aliphatic aldehyde
$\alpha$ -Thujene	tr	tr	Monoterpene
$\alpha$ -Pinene	0.45	0.46	Monoterpene
Camphene	tr	tr	Monoterpene
Sabinene	0.48*	0.45	Monoterpene
$\beta$ -Pinene	[0.48]*	0.04	Monoterpene
Heptanol	tr	tr	Aliphatic alcohol
Myrcene	1.75	1.78	Monoterpene
$\alpha$ -Phellandrene	0.01	0.02	Monoterpene
Octanal	0.41	0.41	Aliphatic aldehyde
para-Cymene	90.91*	0.01	Monoterpene
Limonene	[90.91]*	92.14	Monoterpene
1,8-Cineole	[90.91]*	0.23*	Monoterpnic ether
$\beta$ -Phellandrene	[90.91]*	[0.23]*	Monoterpene
(Z)- $\beta$ -Ocimene	0.14	[0.23]*	Monoterpene
(E)- $\beta$ -Ocimene	0.18	0.15	Monoterpene
$\gamma$ -Terpinene	tr	0.01	Monoterpene
cis-Sabinene hydrate	0.01	0.01	Monoterpnic alcohol
Octanol	0.02	0.03	Aliphatic alcohol
Terpinolene	0.01	tr	Monoterpene
6,7-Epoxymyrcene	tr	tr	Monoterpnic ether
Linalool	0.09	0.10	Monoterpnic alcohol
Nonanal	0.06	0.05	Aliphatic aldehyde
Heptyl acetate	tr	tr	Aliphatic ester
(E)-4,8-Dimethylnona-1,3,7-triene	0.03	0.03	Terpene derivative
trans-para-Mentha-2,8-dien-1-ol	0.01	tr	Monoterpnic alcohol
cis-Limonene oxide	0.02	0.02	Monoterpnic ether
(Z)-Myroxide	0.02*	tr	Monoterpnic ether
cis-para-Mentha-2,8-dien-1-ol	[0.02]*	0.06*	Monoterpnic alcohol
(E)-Myroxide	0.01	0.04*	Monoterpnic ether
Citronellal	0.08	0.08	Monoterpnic aldehyde
Terpinen-4-ol	tr	tr	Monoterpnic alcohol
Cryptone	tr	tr	Normonoterpenic ketone
$\alpha$ -Terpineol	0.05	0.06	Monoterpnic alcohol
trans-Isopiperitenol	0.01	0.02	Monoterpnic alcohol
Decanal	0.32	0.31	Aliphatic aldehyde
Octyl acetate	0.03	[0.04]*	Aliphatic ester
trans-Carveol	0.01	0.01	Monoterpnic alcohol
cis-Carveol	tr	0.01	Monoterpnic alcohol
Citronellol	0.01	0.01	Monoterpnic alcohol
Neral	0.06*	[0.06]*	Monoterpnic aldehyde
Carvone	[0.06]*	0.04*	Monoterpnic ketone
Geraniol	tr	0.02	Monoterpnic alcohol
Isopiperitenone	tr	tr	Monoterpnic ketone
Geranial	0.11	0.13*	Monoterpnic aldehyde
Unknown	0.02	0.01*	Oxygenated monoterpene
Undecanal	0.02	0.01	Aliphatic aldehyde

<i>cis</i> -para-Mentha-2,8-diene-1-hydroperoxide	0.02		Monoterpenic peroxide
para-Mentha-1,8-diene-4-hydroperoxide	0.01		Monoterpenic peroxide
$\alpha$ -Terpinyl acetate	0.01	0.01	Monoterpenic ester
Limonene hydroperoxide IV	0.02		Monoterpenic peroxide
Neryl acetate	0.01	0.02	Monoterpenic ester
$\alpha$ -Copaene	0.13*	0.11	Sesquiterpene
<i>trans</i> -para-Mentha-6,8-diene-2-hydroperoxide	[0.13]*		Monoterpenic peroxide
Geranyl acetate	0.19*	0.10	Monoterpenic ester
<i>cis</i> -para-Mentha-6,8-diene-2-hydroperoxide	[0.19]*		Monoterpenic peroxide
$\beta$ -Cubebene	[0.19]*	0.10	Sesquiterpene
$\beta$ -Elemene	0.02	0.32*	Sesquiterpene
Dodecanal	0.03	0.02	Aliphatic aldehyde
$\beta$ -Caryophyllene	0.31	[0.32]*	Sesquiterpene
$\alpha$ -Humulene	0.04	0.05	Sesquiterpene
(E)- $\beta$ -Farnesene	0.02	0.02	Sesquiterpene
Germacrene D	0.09	0.09	Sesquiterpene
Bicyclogermacrene	0.03	[0.13]*	Sesquiterpene
$\alpha$ -Muurolene	0.01	[0.04]*	Sesquiterpene
Cubebol	tr	0.01	Sesquiterpenic alcohol
$\delta$ -Cadinene	0.12	0.12	Sesquiterpene
$\alpha$ -Elemol	0.04	0.04	Sesquiterpenic alcohol
(E)-Nerolidol	0.02	0.02	Sesquiterpenic alcohol
Germacrene D-4-ol	0.02	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	[0.01]*	Sesquiterpenic ether
$\beta$ -Sinensal	0.02	0.03	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	0.01	0.02	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	0.03	Sesquiterpenic aldehyde
Myristic acid	0.05	0.06	Aliphatic acid
Nootkatone	0.17	0.16	Sesquiterpenic ketone
Hexadecanal	0.02		Aliphatic aldehyde
Palmitic acid	0.10	0.10	Aliphatic acid
Bergapten	0.01		Furanocoumarin
Osthole	0.04		Coumarin
Linoleic acid	0.12	0.11	Aliphatic acid
Oleic acid	0.07	0.09*	Aliphatic acid
<i>cis</i> -Vaccenic acid?	0.02	[0.09]*	Aliphatic acid
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	0.03		Coumarin
Meranzin	0.14		Coumarin
Auraptenol	0.03		Coumarin
Unknown	tr		Coumarin
Auraptene	0.73		Coumarin
Epoxyaurapten	0.24		Coumarin
Tangeretin	0.03		Flavonoid
<b>Total identified</b>	<b>98.32%</b>	<b>98.46%</b>	

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken account in the identified total

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

Essential oil, *Citrus x paradisi* cv. Red  
Internal code: 18C16-CHS2-1-CC

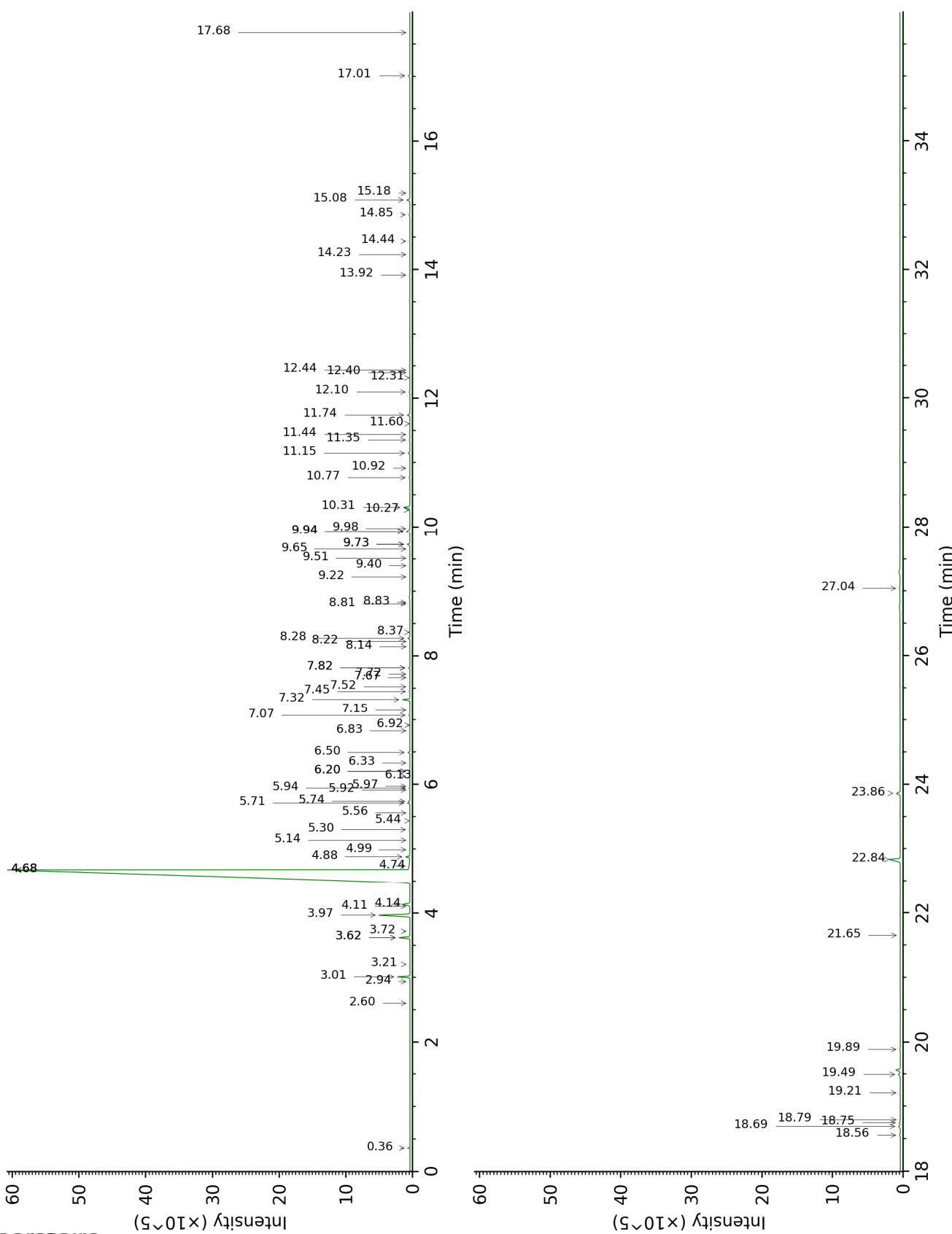
Grapefruit - USA - MD66302ORG

Report prepared for  
American College of Healthcare Sciences

Note: no correction factor was applied

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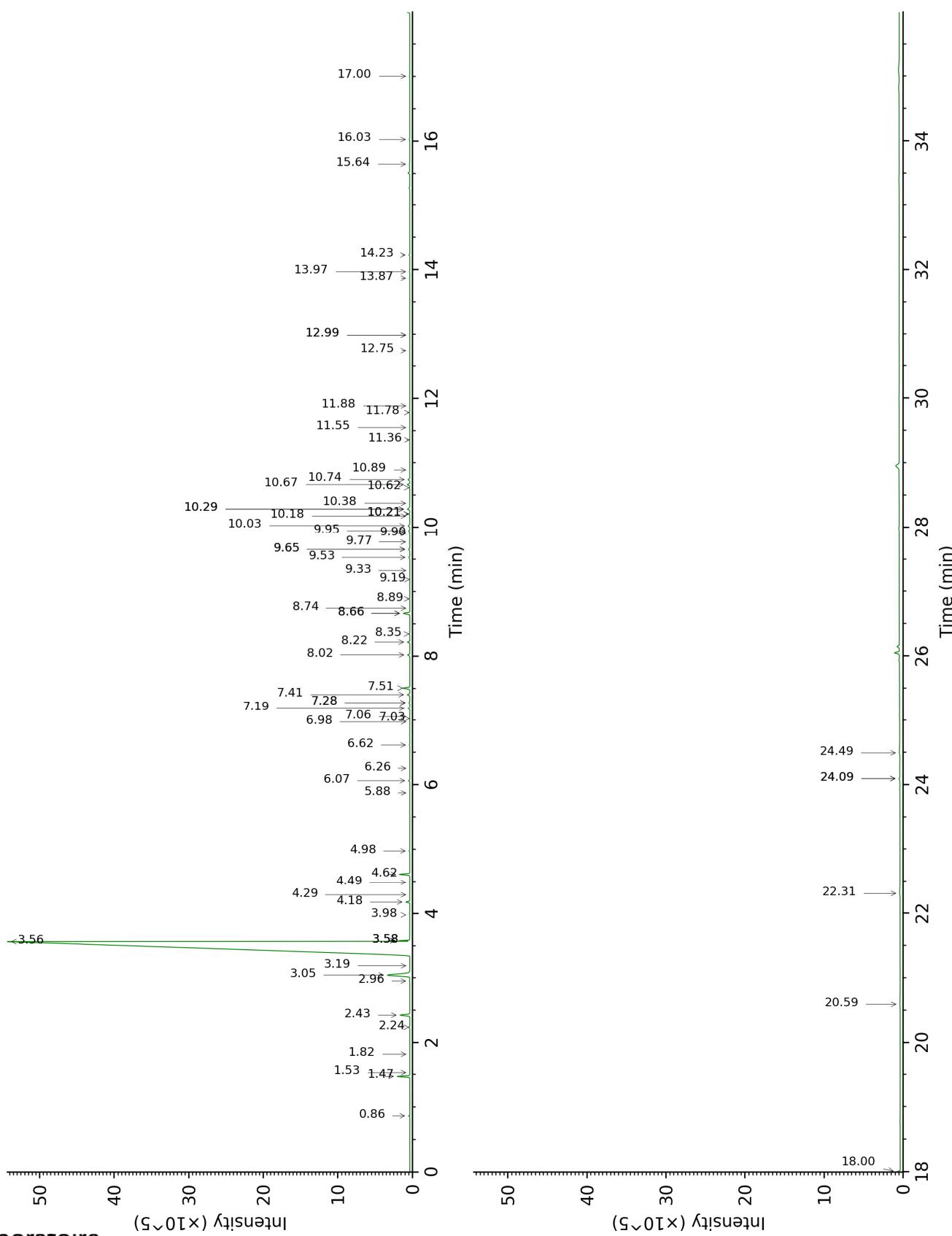
DB-5



Laboratoire  
**PhytoChemia**

Plus que des analyses... des conseils

DB-WAX



Laboratoire  
**PhytoChemia**

Plus que des analyses... des conseils

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Ethanol	0.36	496	0.03	0.86	903	0.03
Heptanal	2.60	899	tr	3.19	1148	tr
α-Thujene	2.94	922	tr	1.53	1002	tr
α-Pinene	3.01	927	0.45	1.47	996	0.46
Camphene	3.21	940	tr	1.82	1030	tr
Sabinene	3.62*	968	0.48	2.43	1088	0.45
β-Pinene	3.62*	968	[0.48]	2.24	1070	0.04
Heptanol	3.72	974	tr	6.98	1423	tr
Myrcene	3.97	991	1.75	3.05	1137	1.78
α-Phellandrene	4.10	1000	0.01	2.96	1130	0.02
Octanal	4.14	1002	0.41	4.62	1253	0.41
para-Cymene	4.68*	1036	90.91	4.29	1230	0.01
Limonene	4.68*	1036	[90.91]	3.56	1177	92.14
1,8-Cineole	4.68*	1036	[90.91]	3.58*	1178	0.23
β-Phellandrene	4.68*	1036	[90.91]	3.58*	1178	[0.23]
(Z)-β-Ocimene	4.74	1040	0.14	3.58*	1178	[0.23]
(E)-β-Ocimene	4.88	1049	0.18	4.18	1222	0.15
γ-Terpinene	4.99	1056	tr	3.98	1208	0.01
cis-Sabinene hydrate	5.14	1065	0.01	7.06	1429	0.01
Octanol	5.30	1075	0.02	8.34	1525	0.03
Terpinolene	5.44	1084	0.01	4.49	1244	tr
6,7-Epoxymyrcene	5.56	1092	tr	6.26	1370	tr
Linalool	5.71	1102	0.09	8.22	1516	0.10
Nonanal	5.74	1103	0.06	6.06	1357	0.05
Heptyl acetate	5.92	1114	tr	5.88	1343	tr
(E)-4,8-Dimethylnona-1,3,7-triene	5.94	1116	0.03	4.98	1279	0.03
trans-para-Mentha-2,8-dien-1-ol	5.97	1118	0.01	9.19	1590	tr
cis-Limonene oxide	6.13	1128	0.02	6.62	1396	0.02
(Z)-Myroxide	6.20*	1133	0.02	7.03	1426	tr
cis-para-Mentha-2,8-dien-1-ol	6.20*	1133	[0.02]	9.66*	1628	0.06
(E)-Myroxide	6.33	1141	0.01	7.28*	1445	0.04
Citronellal	6.50	1152	0.08	7.19	1438	0.08
Terpinen-4-ol	6.83	1173	tr	8.74	1556	tr
Cryptone	6.92	1179	tr	9.33	1601	tr
α-Terpineol	7.07	1188	0.05	9.95	1651	0.06
trans-Isopiperitenol	7.15	1194	0.01	10.62	1706	0.02
Decanal	7.32	1205	0.32	7.51	1462	0.31
Octyl acetate	7.45	1213	0.03	7.28*	1445	[0.04]
trans-Carveol	7.52	1218	0.01	11.55	1785	0.01
cis-Carveol	7.67	1228	tr	11.88	1814	0.01
Citronellol	7.72	1231	0.01	10.89	1729	0.01
Neral	7.82*	1238	0.06	9.66*	1628	[0.06]
Carvone	7.82*	1238	[0.06]	10.21*	1673	0.04
Geraniol	8.14	1260	tr	11.78	1805	0.02
Isopiperitenone	8.22	1265	tr	11.36	1768	tr

Geranal	8.28	1268	0.11	10.29*	1679	0.13
Unknown [m/z 43, 43 (84), 72 (81), 97 (90), 95 (60)... 150 (4)]	8.37	1274	0.02	12.99*	1912	0.01
Undecanal	8.81	1304	0.02	8.89	1567	0.01
cis-para-Mentha-2,8-diene-1-hydroperoxide	8.83	1306	0.02			
para-Mentha-1,8-diene-4-hydroperoxide	9.22	1333	0.01			
α-Terpinyl acetate	9.40	1346	0.01	9.90	1648	0.01
Limonene hydroperoxide IV	9.51	1354	0.02			
Neryl acetate	9.66	1364	0.01	10.38	1686	0.02
α-Copaene	9.73*	1369	0.13	7.40	1454	0.11
trans-para-Mentha-6,8-diene-2-hydroperoxide	9.73*	1369	[0.13]			
Geranyl acetate	9.94*	1384	0.19	10.74	1717	0.10
cis-para-Mentha-6,8-diene-2-hydroperoxide	9.94*	1384	[0.19]			
β-Cubebene	9.94*	1384	[0.19]	8.02	1500	0.10
β-Elemene	9.98	1387	0.02	8.66*	1550	0.32
Dodecanal	10.27	1407	0.03	10.18	1670	0.02
β-Caryophyllene	10.31	1410	0.31	8.66*	1550	[0.32]
α-Humulene	10.77	1445	0.04	9.53	1618	0.05
(E)-β-Farnesene	10.92	1456	0.02	9.77	1637	0.02
Germacrene D	11.15	1473	0.09	10.03	1658	0.09
Bicyclogermacrene	11.35	1488	0.03	10.29*	1679	[0.13]
α-Murolene	11.44	1494	0.01	10.21*	1673	[0.04]
Cubebol	11.60	1507	tr	12.75	1890	0.01
δ-Cadinene	11.74	1518	0.12	10.67	1710	0.12
α-Elemol	12.10	1546	0.04	14.23	2028	0.04
(E)-Nerolidol	12.32	1563	0.02	13.97	2003	0.02
Germacrene D-4-ol	12.40	1569	0.02	13.87	1993	0.01
Caryophyllene oxide	12.44	1572	0.01	12.99*	1912	[0.01]
β-Sinensal	13.92	1693	0.02	15.64	2167	0.03
(2E,6E)-Farnesol	14.23	1720	0.01	17.00	2308	0.02
(2E,6E)-Farnesal	14.44	1738	0.02	16.03	2206	0.03
Myristic acid	14.85	1773	0.05	20.59	2719	0.06
Nootkatone	15.08	1793	0.17	18.00	2416	0.16
Hexadecanal	15.18	1802	0.02			
Palmitic acid	17.01	1971	0.10	22.31	2937	0.10
Bergapten	17.68	2036	0.01			
Osthole	18.56	2124	0.04			
Linoleic acid	18.69	2138	0.12	24.49	3238	0.11
Oleic acid	18.75	2144	0.07	24.09*	3181	0.09
cis-Vaccenic acid?	18.79	2148	0.02	24.09*	3181	[0.09]
7-Methoxy-8-(2-formyl-2-methylpropyl)coumarin	19.21	2191	0.03			
Meranzin	19.49	2221	0.14			
Auraptenol	19.89	2264	0.03			
Unknown [m/z 219, 247]	21.65	2462	tr			

(85), 217 (61), 161 (48), 189 (33), 232 (23)... 290 (18)]		
Auraptene	22.84	2603
Epoxyaurapten	23.86	2732
Tangeretin	27.04	3146
<b>Total identified</b>	<b>98.32%</b>	<b>98.46%</b>
<b>Total reported</b>	<b>98.34%</b>	<b>98.46%</b>

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken account in the identified 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