



## GC/MS BATCH NUMBER: OQ0100

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**ESSENTIAL OIL:** ORANGE ESSENCE

**BOTANICAL NAME:** CITRUS SINENSIS

KEY CONSTITUENTS PRESENT IN THIS BATCH OF ORANGE ESSENCE OIL	%
LIMONENE	93.5
MYRCENE	1.7

Date : September 24, 2018

## CERTIFICATE OF ANALYSIS – GC PROFILING

### SAMPLE IDENTIFICATION

**Internal code :** 18I17-PTH1-1-CC

**Customer identification :** Orange Essence - OQ010088R

**Type :** Essential oil

**Source :** *Citrus sinensis*

**Customer :** Plant Therapy

### 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 :** Sylvain Mercier, M. Sc., Chimiste

**Analysis date :** September 18, 2018

Checked and approved by :

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

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#### *P*HYSICO*C*HEMICAL *D*ATA

**Physical aspect:** Clear liquid

**Refractive index:**  $1.4718 \pm 0.0003$  (20 °C)

#### *C*ONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

## ANALYSIS SUMMARY

Identification	DB-5 (%)	DB-WAX (%)	Classe
Ethyl acetate	tr	tr	Aliphatic ester
Heptane	0.01	0.01	Alkane
Toluene	tr	0.05*	Simple phenolic
Hexanal	0.01	0.01	Aliphatic aldehyde
Ethyl butyrate	0.05	[0.05]*	Aliphatic ester
(2E)-Hexenal	0.01	93.63*	Aliphatic aldehyde
Heptanal	0.01*	tr	Aliphatic aldehyde
Nonane	[0.01]*	tr	Alkane
α-Thujene	0.01	0.01	Monoterpene
α-Pinene	0.45	0.45	Monoterpene
Camphene	tr	tr	Monoterpene
Unknown	tr		Unknown
Unknown	tr		Unknown
Sabinene	0.33*	0.31	Monoterpene
β-Pinene	[0.33]*	0.04	Monoterpene
Heptanol	0.01	0.01*	Aliphatic alcohol
6-Methyl-5-hepten-2-one	tr	tr	Aliphatic ketone
Myrcene	1.69	1.70	Monoterpene
α-Phellandrene	0.31*	0.01	Monoterpene
Pseudolimonene	[0.31]*	0.01	Monoterpene
Octanal	[0.31]*	0.29	Aliphatic aldehyde
Δ3-Carene	0.13	0.12	Monoterpene
para-Cymene	93.73*	0.02	Monoterpene
Limonene	[93.73]*	[93.63]*	Monoterpene
1,8-Cineole	[93.73]*	0.18	Monoterpenic ether
(Z)-β-Ocimene	tr	tr	Monoterpene
(E)-β-Ocimene	0.02	0.02	Monoterpene
γ-Terpinene	0.01	0.02	Monoterpene
cis-Sabinene hydrate	0.01	[0.01]*	Monoterpenic alcohol
Octanol	0.07	0.07	Aliphatic alcohol
Isoterpinolene	tr	tr	Monoterpene
Terpinolene	0.02*	0.02	Monoterpene
para-Cymenene	[0.02]*	tr	Monoterpene
6,7-Epoxy-myrcene	0.01	0.01	Monoterpenic ether
Linalool	0.52	0.53*	Monoterpenic alcohol
Nonanal	0.06	0.05	Aliphatic aldehyde
(E)-4,8-Dimethyl-1,3,7-nonatriene	0.01	0.01	Monoterpene
trans-para-Mentha-2,8-dien-1-ol	0.05	0.06	Monoterpenic alcohol
Limona ketone	tr	tr	Normonoterpenic ketone
cis-Limonene oxide	0.13	0.13	Monoterpenic ether
(Z)-Ocimene epoxide?	0.12*	tr	Monoterpenic ether
trans-Limonene oxide	[0.12]*	0.08	Monoterpenic ether
cis-para-Mentha-2,8-dien-1-ol	[0.12]*	0.08	Monoterpenic alcohol
neoiso-Thujol	0.01	0.07*	Monoterpenic alcohol
Citronellal	0.05	0.05	Monoterpenic aldehyde
Unknown	0.01		Unknown
Unknown	tr	tr	Unknown
Terpinen-4-ol	0.04*	0.01	Monoterpenic alcohol

Unknown	[0.04]*	[0.07]*	Oxygenated monoterpene
<i>trans</i> -Isocarveol	0.01	tr	Monoterpenic alcohol
$\alpha$ -Terpineol	0.09	0.10	Monoterpenic alcohol
Unknown	0.03	0.03	Unknown
Unknown	0.05*	[0.53]*	Unknown
<i>trans</i> -Isopiperitenol	[0.05]*	0.02	Monoterpenic alcohol
Decanal	0.23	0.22	Aliphatic aldehyde
Octyl acetate	0.02	0.02	Aliphatic ester
<i>trans</i> -Carveol	0.08*	0.08	Monoterpenic alcohol
Unknown	[0.08]*	tr	Oxygenated monoterpene
<i>cis</i> -Carveol	0.07*	0.06	Monoterpenic alcohol
Citronellol	[0.07]*	0.03*	Monoterpenic alcohol
Nerol	[0.07]*	0.01	Monoterpenic alcohol
Neral	0.13*	0.01	Monoterpenic aldehyde
Carvone	[0.13]*	0.13	Monoterpenic ketone
(2Z)-Decenal	tr		Aliphatic aldehyde
Geraniol	0.01	0.02	Monoterpenic alcohol
(2E)-Decenal	0.01	tr	Aliphatic aldehyde
Isopiperitenone	0.01	0.01	Monoterpenic ketone
Perillaldehyde	0.02	[0.03]*	Monoterpenic aldehyde
Geranial	0.08	0.12*	Monoterpenic aldehyde
Limonen-10-ol	0.02	0.01	Monoterpenic alcohol
Undecanal	0.01	0.01	Aliphatic aldehyde
<i>cis</i> -para-Mentha-2,8-diene-1-hydroperoxide	0.08		Monoterpenic peroxide
Limonene hydroperoxide I	tr		Monoterpenic peroxide
<i>trans</i> -para-Mentha-2,8-diene-1-hydroperoxide	0.07		Monoterpenic peroxide
para-Mentha-1,8-diene-4-hydroperoxide	0.04		Monoterpenic peroxide
$\alpha$ -Cubebene	0.01	0.01	Sesquiterpene
Limonene hydroperoxide IV	0.01		Monoterpenic peroxide
<i>trans</i> -para-Mentha-6,8-diene-2-hydroperoxide	0.08*		Monoterpenic peroxide
Neryl acetate	[0.08]*	0.02	Monoterpenic ester
$\alpha$ -Copaene	0.03	0.03	Sesquiterpene
Geranyl acetate	0.07*	0.03	Monoterpenic ester
<i>cis</i> -para-Mentha-6,8-diene-2-hydroperoxide	[0.07]*		Monoterpenic peroxide
$\beta$ -Cubebene	0.02	0.02	Sesquiterpene
$\beta$ -Elemene	0.02	0.04*	Sesquiterpene
Unknown	tr		Sesquiterpene
Dodecanal	0.03	0.04	Aliphatic aldehyde
$\beta$ -Caryophyllene	0.03	[0.04]*	Sesquiterpene
$\beta$ -Copaene	0.03	0.02	Sesquiterpene
$\alpha$ -Humulene	0.01	0.01	Sesquiterpene
( <i>E</i> )- $\beta$ -Farnesene	tr	[0.07]*	Sesquiterpene
$\gamma$ -Muurolene	tr	[0.07]*	Sesquiterpene
Germacrene D	0.01	0.02	Sesquiterpene
Valencene	0.24*	0.23	Sesquiterpene
Bicyclogermacrene	[0.24]*	[0.12]*	Sesquiterpene
$\alpha$ -Muurolene	0.02*	[0.12]*	Sesquiterpene

(3Z,6E)- $\alpha$ -Farnesene	[0.02]*	tr	Sesquiterpene
$\gamma$ -Cadinene	0.02*	0.04	Sesquiterpene
7-epi- $\alpha$ -Selinene	[0.02]*	[0.04]*	Sesquiterpene
$\delta$ -Cadinene	0.02	[0.04]*	Sesquiterpene
$\alpha$ -Elemol	tr	0.01	Sesquiterpenic alcohol
Spathulenol	tr	tr	Sesquiterpenic alcohol
Caryophyllene oxide	0.01*	0.01	Sesquiterpenic ether
Caryophyllene oxide isomer	[0.01]*	tr	Sesquiterpenic ether
$\beta$ -Sinensal	0.01	0.01	Sesquiterpenic aldehyde
$\alpha$ -Sinensal	tr	0.01	Sesquiterpenic aldehyde
Nootkatone	tr	tr	Sesquiterpenic ketone
<b>Total identified</b>	<b>99.58%</b>	<b>99.48%</b>	

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

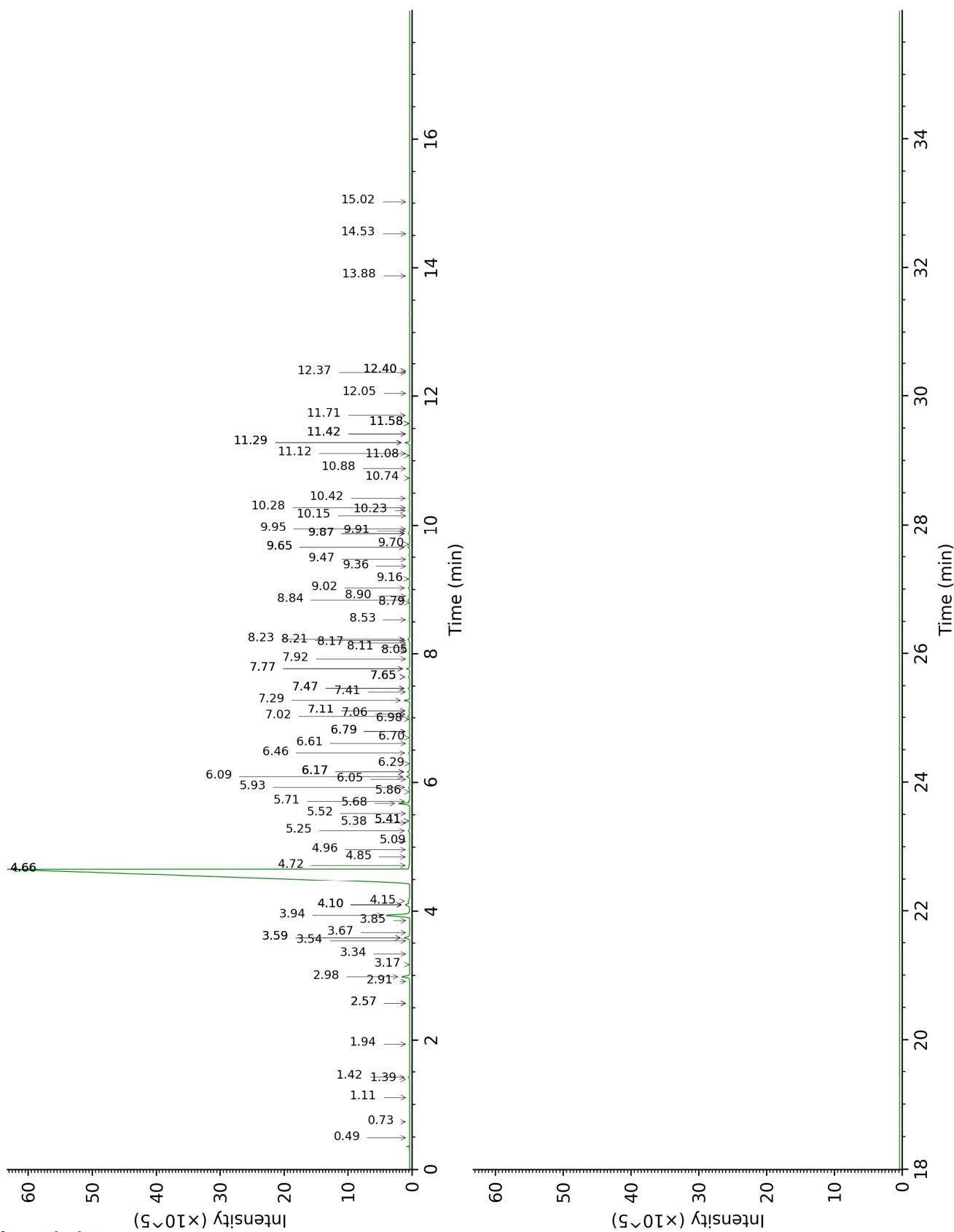
[xx]: Duplicate percentage due to coelutions, not taken account in the identified total

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

Note: no correction factor was applied

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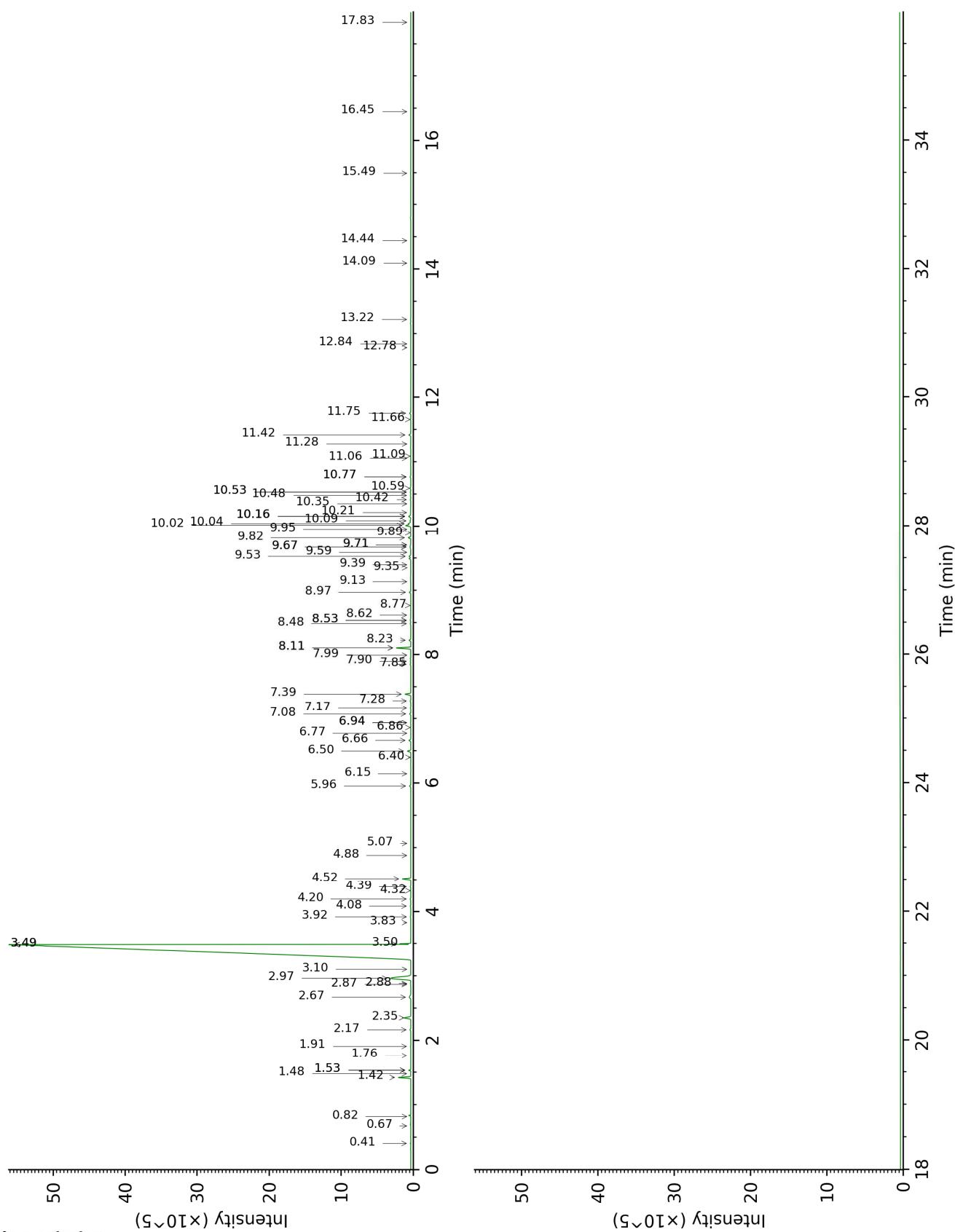
DB-5



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DB-WAX



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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Ethyl acetate	0.49	606	tr	0.67	850	tr
Heptane	0.74	696	0.01	0.41	690	0.01
Toluene	1.11	755	tr	1.53*	1008	0.05
Hexanal	1.39	797	0.01	1.91	1045	0.01
Ethyl butyrate	1.42	802	0.05	1.53*	1008	[0.05]
(2E)-Hexenal	1.94	846	0.01	3.49*	1180	93.63
Heptanal	2.57*	900	0.01	3.10	1150	tr
Nonane	2.57*	900	[0.01]	0.82	899	tr
$\alpha$ -Thujene	2.91	923	0.01	1.48	1002	0.01
$\alpha$ -Pinene	2.98	928	0.45	1.42	996	0.45
Camphene	3.17	941	tr	1.76	1030	tr
Unknown [m/z 55, 70 (27), 43 (25), 83 (22), 84 (20)...]	3.34	952	tr			
Unknown [m/z 43, 41 (71), 57 (70), 82 (63), 69 (58), 56 (49), 85 (45)...]	3.54	966	tr			
Sabinene	3.59*	969	0.33	2.35	1089	0.31
$\beta$ -Pinene	3.59*	969	[0.33]	2.17	1070	0.04
Heptanol	3.67	974	0.01	6.94*	1428	0.01
6-Methyl-5-hepten-2-one	3.85	986	tr	5.07	1293	tr
Myrcene	3.94	992	1.69	2.97	1140	1.70
$\alpha$ -Phellandrene	4.10*	1003	0.31	2.87	1132	0.01
Pseudolimonene	4.10*	1003	[0.31]	2.88	1133	0.01
Octanal	4.10*	1003	[0.31]	4.52	1254	0.29
$\Delta^3$ -Carene	4.15	1006	0.13	2.67	1117	0.12
para-Cymene	4.66*	1038	93.73	4.20	1231	0.02
Limonene	4.66*	1038	[93.73]	3.49*	1180	[93.63]
1,8-Cineole	4.66*	1038	[93.73]	3.50	1181	0.18
(Z)- $\beta$ -Ocimene	4.72	1042	tr	3.83	1205	tr
(E)- $\beta$ -Ocimene	4.85	1050	0.02	4.08	1224	0.02
$\gamma$ -Terpinene	4.96	1058	0.01	3.92	1212	0.02
cis-Sabinene hydrate	5.09	1066	0.01	6.94*	1428	[0.01]
Octanol	5.26	1076	0.07	8.23	1524	0.07
Isoterpinolene	5.38	1084	tr	4.32	1241	tr
Terpinolene	5.41*	1086	0.02	4.39	1245	0.02
para-Cymenene	5.41*	1086	[0.02]	6.40	1388	tr
6,7-Epoxymyrcene	5.52	1093	0.01	6.15	1370	0.01
Linalool	5.68	1103	0.52	8.11*	1515	0.53
Nonanal	5.71	1105	0.06	5.96	1357	0.05
(E)-4,8-Dimethyl-1,3,7-nonatriene	5.86	1114	0.01	4.88	1280	0.01
trans-para-Mentha-2,8-dien-1-ol	5.93	1118	0.05	8.97	1581	0.06

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Limona ketone	6.05	1126	tr	7.99	1506	tr
<i>cis</i> -Limonene oxide	6.09	1129	0.13	6.50	1395	0.13
(Z)-Ocimene epoxide?	6.17*	1134	0.12	6.77	1416	tr
<i>trans</i> -Limonene oxide	6.17*	1134	[0.12]	6.66	1408	0.08
<i>cis</i> -para-Menth-2,8-dien-1-ol	6.17*	1134	[0.12]	9.53	1626	0.08
neoiso-Thujol	6.29	1142	0.01	9.67*†	1638	0.07
Citronellal	6.46	1153	0.05	7.08	1438	0.05
Unknown [m/z 79, 56 (53), 55 (53), 136 (50), 41 (49), 80 (42)...]	6.61	1162	0.01			
Unknown [m/z 55, 96 (88), 67 (43), 41 (25), 43 (22)... 154 (1)]	6.70	1168	tr	9.95	1660	tr
Terpinen-4-ol	6.79*†	1174	0.04	8.62	1554	0.01
Unknown [m/z 69, 84 (62), 41 (30), 123 (26), 97 (24), 109 (23)...]	6.79*†	1174	[0.04]	9.70*†	1640	[0.07]
<i>trans</i> -Isocarveol	6.98	1186	0.01	11.06	1752	tr
α-Terpineol	7.02	1189	0.09	9.82	1649	0.10
Unknown [m/z 121, 79 (98), 93 (87), 94 (73), 91 (63), 105 (45)...]	7.06	1191	0.03	7.85	1495	0.03
Unknown [m/z 121, 79 (61), 93 (55), 94 (40), 91 (39), 84 (37)...]	7.11*†	1194	0.05	8.11*	1515	[0.53]
<i>trans</i> -Isopiperitenol	7.11*†	1194	[0.05]	10.42	1698	0.02
Decanal	7.28	1206	0.23	7.39	1461	0.22
Octyl acetate	7.41	1214	0.02	7.17	1445	0.02
<i>trans</i> -Carveol	7.47*	1218	0.08	11.42	1783	0.08
Unknown [m/z 122, 91 (56), 79 (33), 95 (33), 107 (31), 43 (30), 77 (30), 135 (27)... 150 (9)]	7.47*	1218	[0.08]	9.35	1611	tr
<i>cis</i> -Carveol	7.65*†	1230	0.07	11.75	1812	0.06
Citronellol	7.65*†	1230	[0.07]	10.77*	1728	0.03
Nerol	7.65*†	1230	[0.07]	11.09	1755	0.01
Neral	7.77*	1239	0.13	9.59	1631	0.01
Carvone	7.77*	1239	[0.13]	10.04	1667	0.13
(2Z)-Decenal	7.92	1249	tr			
Geraniol	8.05	1257	0.01	11.66	1803	0.02

(2E)-Decenal	8.10	1261	0.01	9.13	1594	tr
Isopiperitenone	8.17	1265	0.01	11.28	1771	0.01
Perillaldehyde	8.21	1268	0.02	10.77*	1728	[0.03]
Geranal	8.23	1269	0.08	10.16*	1677	0.12
Limonen-10-ol	8.53	1289	0.02	13.22	1944	0.01
Undecanal	8.80	1307	0.01	8.77	1566	0.01
<i>cis</i> -para-Mentha-2,8-diene-1-hydroperoxide	8.84	1310	0.08			
Limonene hydroperoxide I	8.90	1314	tr			
<i>trans</i> -para-Mentha-2,8-diene-1-hydroperoxide	9.02	1323	0.07			
para-Mentha-1,8-diene-4-hydroperoxide	9.16	1333	0.04			
$\alpha$ -Cubebene	9.36	1347	0.01	6.86	1422	0.01
Limonene hydroperoxide IV	9.47	1355	0.01			
<i>trans</i> -para-Mentha-6,8-diene-2-hydroperoxide	9.65*	1368	0.08			
Neryl acetate	9.65*	1368	[0.08]	10.22	1682	0.02
$\alpha$ -Copaene	9.70	1371	0.03	7.28	1453	0.03
Geranyl acetate	9.87*	1383	0.07	10.59	1713	0.03
<i>cis</i> -para-Mentha-6,8-diene-2-hydroperoxide	9.87*	1383	[0.07]			
$\beta$ -Cubebene	9.91	1386	0.02	7.90	1499	0.02
$\beta$ -Elemene	9.95	1389	0.02	8.53*	1548	0.04
Unknown [m/z 106, 119 (99), 43 (78), 91 (74), 105 (60), 134 (55)... 204 (19)]	10.15	1403	tr			
Dodecanal	10.23	1409	0.03	10.09	1671	0.04
$\beta$ -Caryophyllene	10.28	1412	0.03	8.53*	1548	[0.04]
$\beta$ -Copaene	10.42	1423	0.03	8.48	1544	0.02
$\alpha$ -Humulene	10.74	1447	0.01	9.40	1615	0.01
(E)- $\beta$ -Farnesene	10.88	1458	tr	9.67*†	1638	[0.07]
$\gamma$ -Muurolene	11.08	1473	tr	9.70*†	1640	[0.07]
Germacrene D	11.12	1475	0.01	9.89	1656	0.02
Valencene	11.28*	1488	0.24	10.02	1665	0.23
Bicyclogermacrene	11.28*	1488	[0.24]	10.16*	1677	[0.12]
$\alpha$ -Muurolene	11.42*	1498	0.02	10.16*	1677	[0.12]
(3Z,6E)- $\alpha$ -Farnesene	11.42*	1498	[0.02]	10.35	1692	tr
$\gamma$ -Cadinene	11.58*	1510	0.02	10.48†	1703	0.04
7-epi- $\alpha$ -Selinene	11.58*	1510	[0.02]	10.53*†	1708	[0.04]
$\delta$ -Cadinene	11.71	1520	0.02	10.53*†	1708	[0.04]
$\alpha$ -Elemol	12.05	1547	tr	14.09	2025	0.01

Spathulenol	12.37	1572	tr	14.44	2059	tr
Caryophyllene oxide	12.40*	1574	0.01	12.84	1909	0.01
Caryophyllene oxide isomer	12.40*	1574	[0.01]	12.78	1903	tr
$\beta$ -Sinensal	13.88	1695	0.01	15.50	2163	0.01
$\alpha$ -Sinensal	14.53	1751	tr	16.45	2261	0.01
Nootkatone	15.02	1794	tr	17.83	2410	tr
<b>Total identified</b>	<b>99.58%</b>			<b>99.48%</b>		
<b>Total reported</b>	<b>99.64%</b>			<b>99.52%</b>		

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

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

t: 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