

Date : May 04, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

**Internal code** : 21D20-ORA13

**Customer identification** : Lime - Brazil - 3 years - 012103A

**Type** : Essential oil

**Source** : *Citrus latifolia*

**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 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*Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.*

*PHYSICOCHEMICAL DATA*

**Physical aspect:** Yellow greenish liquid

**Refractive index:**  $1.4844 \pm 0.0003$  (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
Tricyclene	0.01	Monoterpene
$\alpha$ -Thujene	0.53	Monoterpene
$\alpha$ -Pinene	2.10	Monoterpene
Camphene	0.07	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
Sabinene	1.92	Monoterpene
$\beta$ -Pinene	11.69	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	1.40	Monoterpene
$\alpha$ -Phellandrene	0.05	Monoterpene
Octanal	0.02	Aliphatic aldehyde
$\Delta^3$ -Carene	0.01	Monoterpene
$\alpha$ -Terpinene	0.26	Monoterpene
para-Cymene	0.68	Monoterpene
1,8-Cineole	0.12	Monoterpenic ether
Limonene	52.63	Monoterpene
$\beta$ -Phellandrene	0.36	Monoterpene
(Z)- $\beta$ -Ocimene	0.07	Monoterpene
(E)- $\beta$ -Ocimene	0.13	Monoterpene
$\gamma$ -Terpinene	11.79	Monoterpene
cis-Sabinene hydrate	0.05	Monoterpenic alcohol
Terpinolene	0.59	Monoterpene
trans-Sabinene hydrate	0.06	Monoterpenic alcohol
Linalool	0.21	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
cis-Limonene oxide	0.02	Monoterpenic ether
1-Terpineol	0.01	Monoterpenic alcohol
trans-Limonene oxide	0.01	Monoterpenic ether
Camphor	0.01	Monoterpenic ketone
Epoxyterpinolene	0.01	Monoterpenic ether
Citronellal	0.06	Monoterpenic aldehyde
Borneol	0.02	Monoterpenic alcohol
Isoneral	0.01	Monoterpenic aldehyde
$\alpha$ -Phellandren-8-ol	0.01	Monoterpenic alcohol
Terpinen-4-ol	0.10	Monoterpenic alcohol
para-Cymen-8-ol	0.01	Monoterpenic alcohol
Isogeranial	0.01	Monoterpenic aldehyde
$\alpha$ -Terpineol	0.32	Monoterpenic alcohol
Unknown	0.01	Unknown
$\gamma$ -Terpineol	0.01	Monoterpenic alcohol
Decanal	0.08	Aliphatic aldehyde
trans-Carveol	tr	Monoterpenic alcohol
2,3-Epoxyneral?	0.02	Monoterpenic aldehyde
Nerol	0.15	Monoterpenic alcohol
2,3-Epoxygeranial?	0.04	Monoterpenic aldehyde

Neral	1.77	Monoterpenic aldehyde
Geraniol	0.05	Monoterpenic alcohol
Unknown	0.01	Unknown
<i>trans</i> -Ascaridole glycol	0.03	Monoterpenic alcohol
Geranial	2.93	Monoterpenic aldehyde
Unknown	0.02	Oxygenated monoterpene
<i>cis</i> -Ascaridole glycol	0.01	Monoterpenic alcohol
Undecanal	0.02	Aliphatic aldehyde
$\delta$ -Elemene	0.01	Sesquiterpene
Neryl acetate	1.16	Monoterpenic ester
Geranyl acetate	0.29	Monoterpenic ester
$\beta$ -Elemene	0.14	Sesquiterpene
Dodecanal	0.05	Aliphatic aldehyde
<i>cis</i> - $\alpha$ -Bergamotene	0.08	Sesquiterpene
$\beta$ -Caryophyllene	0.64	Sesquiterpene
$\alpha$ -Santalene	0.02	Sesquiterpene
$\gamma$ -Elemene	0.02	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	1.10	Sesquiterpene
$\alpha$ -Humulene	0.07	Sesquiterpene
$\beta$ -Santalene	0.01	Sesquiterpene
( <i>E</i> )- $\beta$ -Farnesene	0.15	Sesquiterpene
Germacrene D	0.08	Sesquiterpene
$\gamma$ -Curcumene	0.05	Sesquiterpene
<i>trans</i> - $\beta$ -Bergamotene	0.07	Sesquiterpene
Bicyclogermacrene	0.05	Sesquiterpene
(3 <i>Z</i> ,6 <i>E</i> )- $\alpha$ -Farnesene	0.09	Sesquiterpene
( <i>Z</i> )- $\alpha$ -Bisabolene	0.13	Sesquiterpene
$\beta$ -Bisabolene	1.66	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i> )- $\alpha$ -Farnesene	0.14	Sesquiterpene
( <i>Z</i> )- $\gamma$ -Bisabolene	0.04	Sesquiterpene
$\delta$ -Cadinene	0.01	Sesquiterpene
Selina-4(15),7(11)-diene	0.01	Sesquiterpene
Unknown	0.02	Sesquiterpene
( <i>E</i> )- $\alpha$ -Bisabolene	0.06	Sesquiterpene
Germacrene B	0.19	Sesquiterpene
Caryophyllenyl alcohol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Caryophyllene oxide	0.02	Sesquiterpenic ether
Alismol	0.05	Sesquiterpenic alcohol
Unknown	0.03	Sesquiterpenic alcohol
Unknown	0.06	Oxygenated sesquiterpene
Unknown	0.06	Oxygenated sesquiterpene
$\alpha$ -Bisabolol	0.10	Sesquiterpenic alcohol
Herniarin	0.38	Coumarin
(2 <i>E</i> ,6 <i>Z</i> )-Farnesal	0.02	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>E</i> )-Farnesal	0.03	Sesquiterpenic aldehyde
Myristic acid	0.03	Aliphatic acid
Hexadecanal	0.01	Aliphatic aldehyde
Citropten	0.37	Furanocoumarin
Palmitic acid	0.10	Aliphatic acid
Bergapten	0.18	Furanocoumarin
Stearic acid	0.01	Aliphatic acid

Isopimpinellin	0.15	Furanocoumarin
Oxypeucedanin	0.01	Furanocoumarin
Heraclenin	0.23	Furanocoumarin
Pseudolimonene	0.01	Monoterpene
<b>Consolidated total</b>	<b>98.72%</b>	

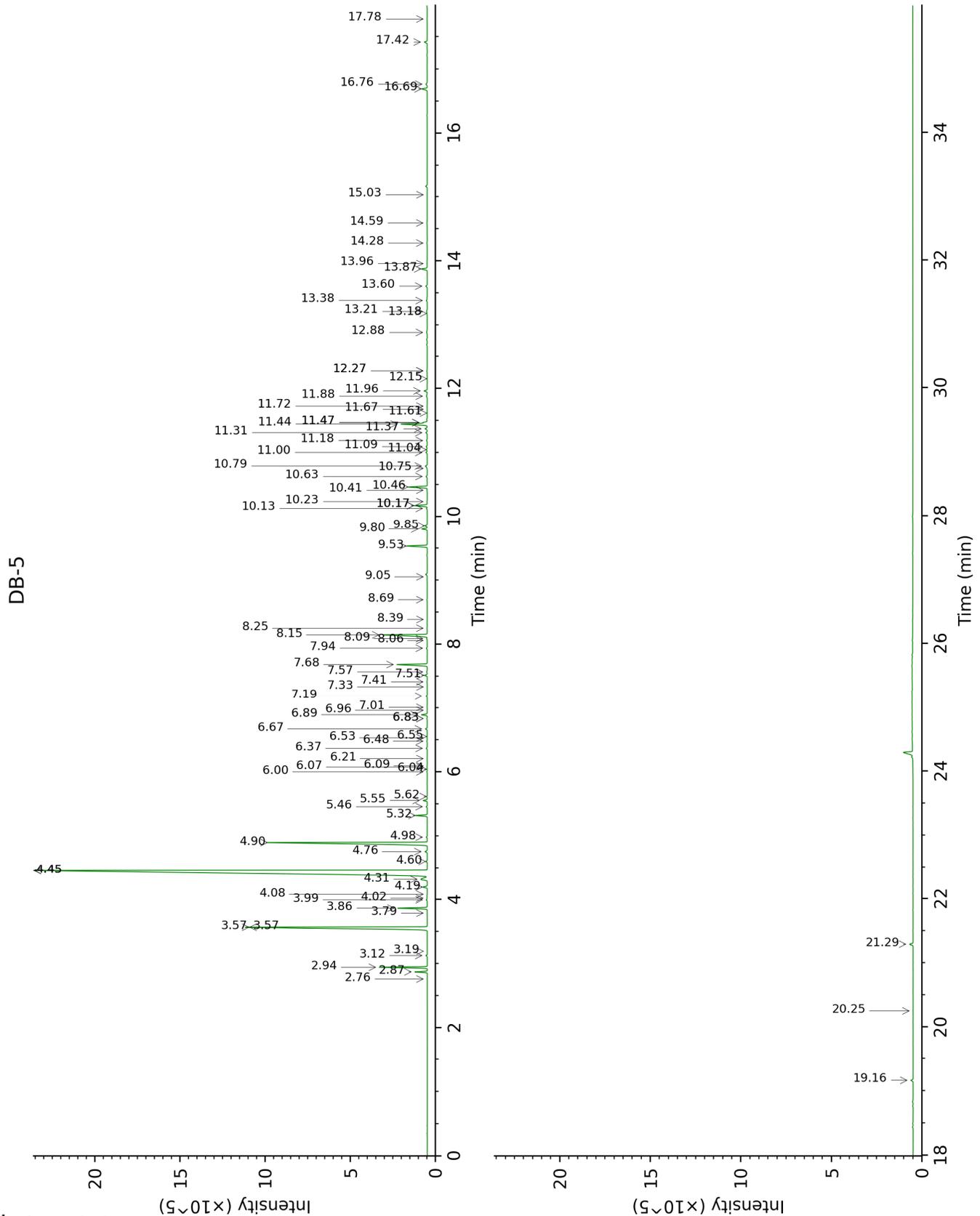
tr: The compound has been detected below 0.005% of total signal.

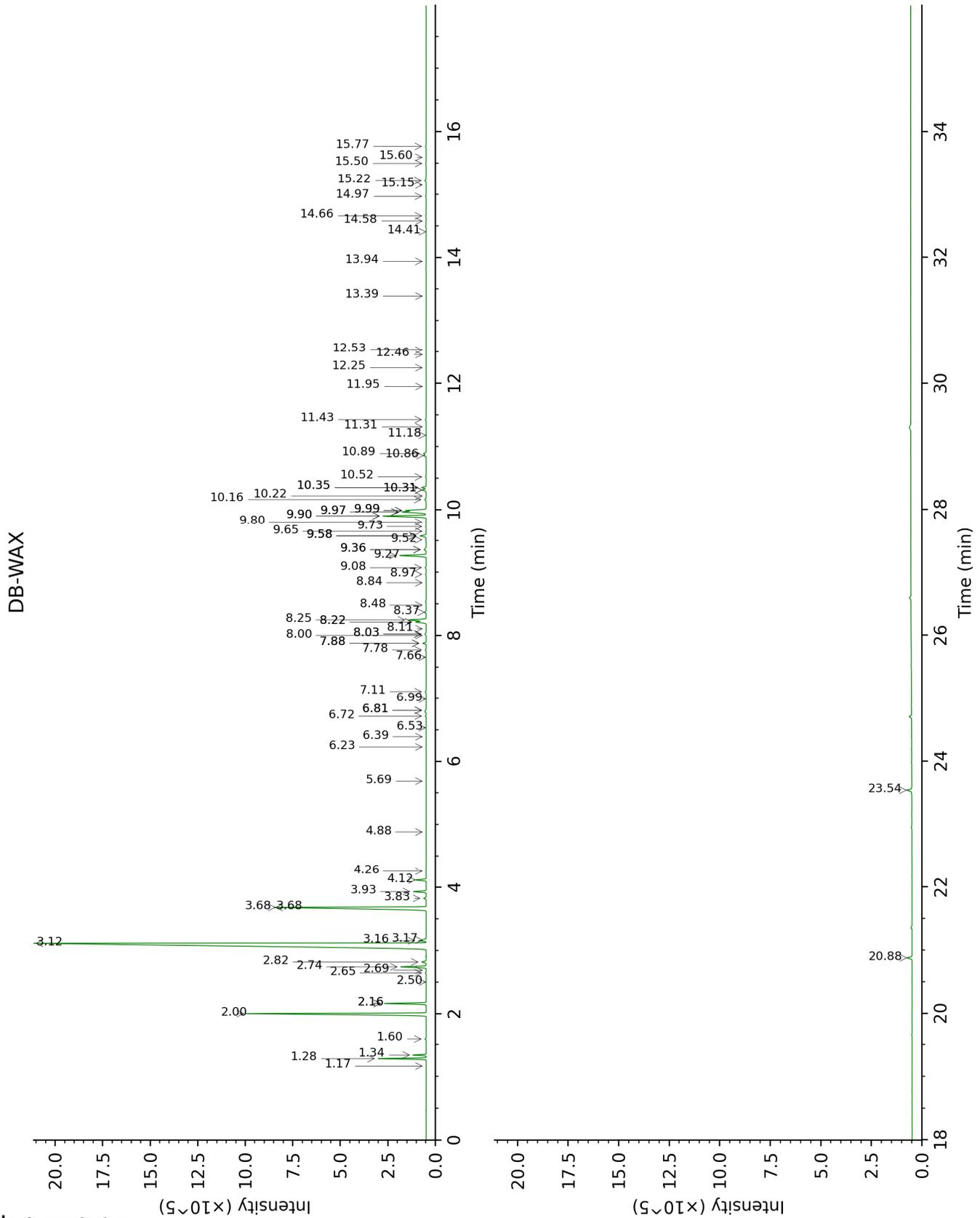
Note: no correction factor was applied

**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	%
Tricyclene	2.76	920	0.01	1.17	972	0.01
α-Thujene	2.87	927	0.53	1.34	1001	0.53
α-Pinene	2.94	932	2.10	1.28	992	2.12
Camphene	3.12	944	0.07	1.60	1027	0.07
Thuja-2,4(10)-diene	3.19	949	0.01	2.16*	1084	2.05
Sabinene	3.57*	974	13.62	2.16*	1084	[2.05]
β-Pinene	3.57*	974	[13.62]	2.00	1068	11.69
6-Methyl-5-hepten-2-one	3.79	989	0.01	4.88	1298	0.01
Myrcene	3.86	994	1.40	2.74	1134	1.41
α-Phellandrene	3.99	1003	0.05	2.65	1126	0.05
Octanal	4.02	1005	0.02	4.26	1251	0.02
Δ <sup>3</sup> -Carene	4.08	1009	0.01	2.50	1114	0.01
α-Terpinene	4.19	1016	0.26	2.82	1140	0.27
para-Cymene	4.31	1023	0.68	3.93	1227	0.70
1,8-Cineole	4.45*	1032	52.56	3.17	1168	0.12
Limonene	4.45*	1032	[52.56]	3.12	1163	52.63
β-Phellandrene	4.45*	1032	[52.56]	3.16	1167	0.36
(Z)-β-Ocimene	4.60	1042	0.07	3.68*	1208	11.98
(E)-β-Ocimene	4.76	1051	0.13	3.83	1219	0.14
γ-Terpinene	4.90	1060	11.79	3.68*	1208	[11.98]
cis-Sabinene hydrate	4.98	1066	0.05	6.72	1429	0.05
Terpinolene	5.32	1087	0.59	4.12	1241	0.59
trans-Sabinene hydrate	5.46	1096	0.06	7.78	1508	0.06
Linalool	5.55	1102	0.21	7.88*	1516	0.20
Nonanal	5.62	1106	0.02	5.69	1353	0.02
cis-Limonene oxide	6.00	1130	0.02	6.23	1392	0.02
1-Terpineol	6.04	1133	0.01	8.11	1534	0.01
trans-Limonene oxide	6.07	1135	0.01	6.39	1404	0.01
Camphor	6.09	1136	0.01	6.99	1449	0.01
Epoxyterpinolene	6.20	1144	0.01	6.53	1415	0.01
Citronellal	6.36	1154	0.06	6.81*†	1436	0.14
Borneol	6.48	1161	0.02	9.58*	1651	0.43
Isoneral	6.53	1165	0.01	7.66	1499	0.02
α-Phellandren-8-ol	6.55	1166	0.01	9.97*	1683	1.78
Terpinen-4-ol	6.67	1174	0.10	8.37	1555	0.10
para-Cymen-8-ol	6.83*	1184	0.02	11.31	1797	0.01
Isogeranial	6.83*	1184	[0.02]	8.00	1526	0.01
α-Terpineol	6.89	1188	0.32	9.58*	1651	[0.43]
Unknown [m/z 121, 79 (61), 93 (55), 94 (40), 91 (39), 84 (37)...]	6.96	1192	0.01	7.88*	1516	[0.20]

γ-Terpineol	7.01	1195	0.01	9.65	1657	0.02
Decanal	7.19	1207	0.08	7.11	1458	0.06
<i>trans</i> -Carveol	7.33	1217	tr	11.18	1786	0.01
2,3-Epoxyneral?	7.41	1222	0.02			
Nerol	7.52	1229	0.15	10.86	1758	0.15
2,3-Epoxygeranial?	7.57	1233	0.04			
Neral	7.68	1240	1.77	9.27	1626	1.72
Geraniol	7.94	1258	0.05	11.43	1807	0.06
Unknown [m/z 43, 128 (61), 79 (60), 127 (52), 58 (50)...]	8.06	1266	0.01	11.95	1854	0.01
<i>trans</i> -Ascaridole glycol	8.09	1268	0.03	13.94	2038	0.01
Geranial	8.15	1272	2.93	9.90*	1678	2.85
Unknown [m/z 95, 67 (45), 41 (42), 110 (42), 43 (41), 59 (36)]	8.25	1278	0.02	12.25	1881	0.02
<i>cis</i> -Ascaridole glycol	8.39	1288	0.01	14.58	2100	0.01
Undecanal	8.69	1308	0.02	8.48	1564	0.02
δ-Elemene	9.05	1334	0.01	6.81*†	1436	[0.14]
Neryl acetate	9.53	1368	1.16	9.99*	1685	1.16
Geranyl acetate	9.80	1387	0.29	10.35*	1715	0.29
β-Elemene	9.85	1390	0.14	8.22*†	1543	1.87
Dodecanal	10.13	1410	0.05	9.80	1670	0.04
<i>cis</i> -α-Bergamotene	10.17*	1414	0.78	8.03*	1528	0.10
β-Caryophyllene	10.17*	1414	[0.78]	8.22*†	1543	[1.87]
α-Santalene	10.23	1418	0.02	8.03*	1528	[0.10]
γ-Elemene	10.41	1431	0.02	8.84	1591	0.02
<i>trans</i> -α-Bergamotene	10.46	1435	1.10	8.25†	1545	[1.87]
α-Humulene	10.63	1447	0.07	9.08	1610	0.07
β-Santalene	10.75	1457	0.01	8.97	1602	0.06
( <i>E</i> )-β-Farnesene	10.79	1460	0.15	9.36*	1634	0.20
Germacrene D	11.00	1475	0.08	9.58*	1651	[0.43]
γ-Curcumene	11.04	1479	0.05	9.52	1646	0.05
<i>trans</i> -β-Bergamotene	11.09	1482	0.07	9.36*	1634	[0.20]
Bicyclogermacrene	11.18	1489	0.05	9.90*	1678	[2.85]
(3 <i>Z</i> ,6 <i>E</i> )-α-Farnesene	11.31	1498	0.09	9.99*	1685	[1.16]
( <i>Z</i> )-α-Bisabolene	11.37	1503	0.13	10.16	1699	0.10
β-Bisabolene	11.44	1509	1.66	9.97*	1683	[1.78]
(3 <i>E</i> ,6 <i>E</i> )-α-Farnesene	11.47*	1510	0.18	10.31*	1712	0.28
( <i>Z</i> )-γ-Bisabolene	11.47*	1510	[0.18]	9.73	1664	0.04
δ-Cadinene	11.61	1522	0.01	10.22	1704	0.01
Selina-4(15),7(11)-diene	11.67	1527	0.01	10.35*	1715	[0.29]
Unknown [m/z 189, 204 (92), 161	11.72	1531	0.02	10.31*	1712	[0.28]

(65), 133 (51), 105 (51), 91 (51), 119 (45)]						
(E)- $\alpha$ -Bisabolene	11.88	1543	0.06	10.52	1730	0.05
Germacrene B	11.96	1549	0.19	10.89	1761	0.18
Caryophyllenyl alcohol	12.15	1564	0.01	13.39	1986	0.01
Caryophyllene oxide isomer	12.27*	1574	0.03	12.46	1899	0.01
Caryophyllene oxide	12.27*	1574	[0.03]	12.53	1906	0.02
Alismol	12.88	1623	0.05	15.50	2193	0.06
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	13.18	1647	0.03	14.97	2140	0.05
Unknown [m/z 94, 43 (89), 41 (67), 122 (46), 69 (41)...222]	13.21	1650	0.06	14.66	2108	0.05
Unknown [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	13.38	1664	0.06	15.77	2221	0.06
$\alpha$ -Bisabolol	13.60	1683	0.10	15.22	2165	0.10
Herniarin	13.87	1705	0.38	20.88	2806	0.35
(2E,6Z)-Farnesal	13.96	1712	0.02	15.15	2158	0.02
(2E,6E)-Farnesal	14.28	1740	0.03	15.60	2203	0.02
Myristic acid	14.59	1767	0.03			
Hexadecanal	15.03	1805	0.01	14.41	2084	0.01
Citropten	16.69	1959	0.37	23.54	3162	0.39
Palmitic acid	16.76	1966	0.10			
Bergapten	17.42	2030	0.18			
Stearic acid	17.78	2066	0.01			
Isopimpinellin	19.16	2207	0.15			
Oxypeucedanin	20.25	2326	0.01			
Heraclenin	21.29	2444	0.23			
Pseudolimonene				2.69	1129	0.01
<b>Total identified</b>		<b>98.02%</b>			<b>98.10%</b>	
<b>Total reported</b>		<b>98.22%</b>			<b>98.29%</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