

Date : April 14, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23D06-PTH01


Customer identification : Key Lime - Mexico - K30101R

Type : Essential oil

Source : *Citrus aurantifolia*

Customer : Plant Therapy

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 2014-005

Analysis date : April 12, 2023

Checked and approved by :

Alexis St-Gelais, Ph. D., Chimiste 2013-174

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PHYSICOCHEMICAL DATA

Physical aspect: Yellow green liquid

Refractive index: 1.4851 ± 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
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Heptanal	0.01	Aliphatic aldehyde
Tricyclene	0.02	Monoterpene
α -Thujene	0.40	Monoterpene
α -Pinene	2.41	Monoterpene
Camphene	0.11	Monoterpene
α -Fenchene	tr	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
Sabinene	2.50	Monoterpene
β -Pinene	20.15	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	1.24	Monoterpene
α -Phellandrene	0.05	Monoterpene
Octanal	0.03	Aliphatic aldehyde
Pseudolimonene	0.01	Monoterpene
Δ^3 -Carene	0.01	Monoterpene
α -Terpinene	0.27	Monoterpene
para-Cymene	0.25	Monoterpene
β -Phellandrene	0.53	Monoterpene
Limonene	45.33	Monoterpene
(Z)- β -Ocimene	0.15	Monoterpene
(E)- β -Ocimene	0.37	Monoterpene
γ -Terpinene	7.39	Monoterpene
cis-Sabinene hydrate	0.04	Monoterpenic alcohol
Terpinolene	0.42	Monoterpene
trans-Sabinene hydrate	0.04	Monoterpenic alcohol
Linalool	0.15	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
endo-Fenchol	0.01	Monoterpenic alcohol
trans-para-Mentha-2,8-dien-1-ol	0.02	Monoterpenic alcohol
1-Terpineol	0.02	Monoterpenic alcohol
cis- β -Terpineol	0.01	Monoterpenic alcohol
Citronellal	0.02	Monoterpenic aldehyde
Borneol	0.02	Monoterpenic alcohol
Isoneral	0.02	Monoterpenic aldehyde
Isopinocampone	0.02	Monoterpenic ketone
Terpinen-4-ol	0.50	Monoterpenic alcohol
para-Cymen-8-ol	0.01	Monoterpenic alcohol
Isogeranial	0.01	Monoterpenic aldehyde
α -Terpineol	0.25	Monoterpenic alcohol
Decanal	0.18	Aliphatic aldehyde
2,3-Epoxyneral?	0.02	Monoterpenic aldehyde
Nerol	0.04	Monoterpenic alcohol
2,3-Epoxygeranial?	0.04	Monoterpenic aldehyde
Neral	1.48	Monoterpenic aldehyde

Geraniol	0.05	Monoterpenic alcohol
Geranial	2.33	Monoterpenic aldehyde
<i>trans</i> -Ascaridole glycol	0.01	Monoterpenic alcohol
Unknown	0.01	Unknown
Undecanal	0.03	Aliphatic aldehyde
δ -Elemene	0.47	Sesquiterpene
Citronellyl acetate	0.01	Monoterpenic ester
Neryl acetate	0.09	Monoterpenic ester
Geranyl acetate	0.18	Monoterpenic ester
β -Elemene	0.24	Sesquiterpene
Dodecanal	0.12	Aliphatic aldehyde
β -Caryophyllene	1.22	Sesquiterpene
<i>cis</i> - α -Bergamotene	0.12	Sesquiterpene
α -Santalene	0.02	Sesquiterpene
γ -Elemene	0.06	Sesquiterpene
<i>trans</i> - α -Bergamotene	1.51	Sesquiterpene
α -Humulene	0.16	Sesquiterpene
β -Santalene	0.01	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.22	Sesquiterpene
Selina-4,11-diene	0.02	Sesquiterpene
Germacrene D	0.33	Sesquiterpene
γ -Curcumene	0.05	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.05	Sesquiterpene
Unknown	0.06	Sesquiterpene
δ -Selinene	0.01	Sesquiterpene
Bicyclogermacrene	0.02	Sesquiterpene
α -Selinene	0.03	Sesquiterpene
(3 <i>Z</i> ,6 <i>E</i>)- α -Farnesene	0.19	Sesquiterpene
(<i>Z</i>)- α -Bisabolene	0.21	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i>)- α -Farnesene	1.31	Sesquiterpene
γ -Cadinene	0.21	Sesquiterpene
β -Bisabolene	1.79	Sesquiterpene
(<i>Z</i>)- γ -Bisabolene	0.03	Sesquiterpene
δ -Cadinene	0.02	Sesquiterpene
Selina-4(15),7(11)-diene	0.02	Sesquiterpene
Selina-3,7(11)-diene	0.01	Sesquiterpene
(<i>E</i>)- α -Bisabolene	0.07	Sesquiterpene
Germacrene B	0.66	Sesquiterpene
Caryophyllenyl alcohol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	Sesquiterpenic ether
Tetradecanal?	0.06	Aliphatic aldehyde
Alismol	0.05	Sesquiterpenic alcohol
Unknown	0.08	Oxygenated sesquiterpene
Unknown	0.09	Oxygenated sesquiterpene
α -Bisabolol	0.12	Sesquiterpenic alcohol
(2 <i>E</i> ,6 <i>Z</i>)-Farnesal	0.04	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	0.03	Sesquiterpenic aldehyde
Myristic acid	0.01	Aliphatic acid
Citropten	0.26	Furanocoumarin
Palmitic acid	0.04	Aliphatic acid
Bergapten	0.08	Furanocoumarin
Linoleic acid	0.07	Aliphatic acid

Oleic acid	0.02	Aliphatic acid
<i>cis</i> -Vaccenic acid?	0.01	Aliphatic acid
Isopimpinellin	0.22	Furanocoumarin
Oxypeucedanin	0.01	Furanocoumarin
Consolidated total	97.76%	

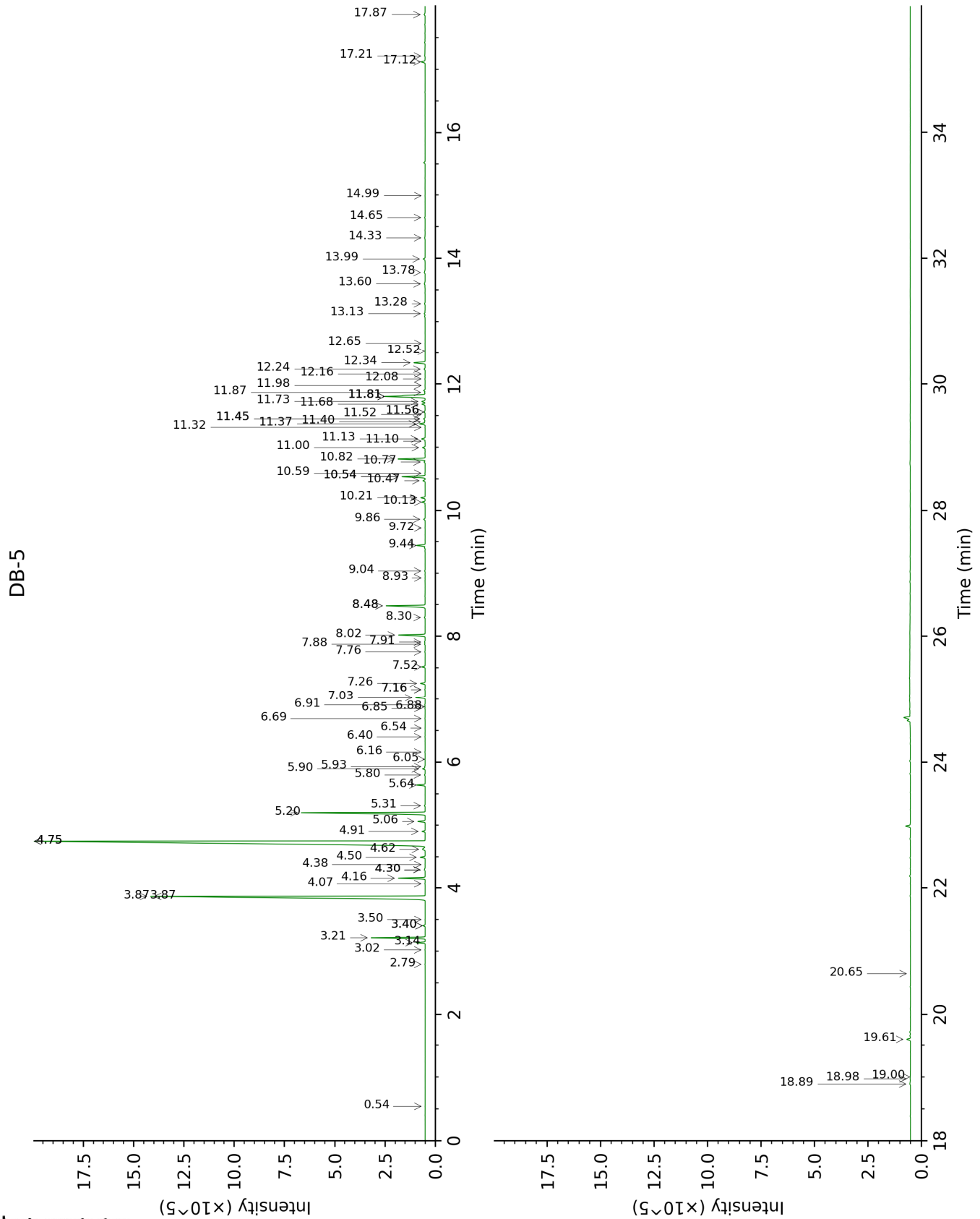
tr: The compound has been detected below 0.005% of total signal.

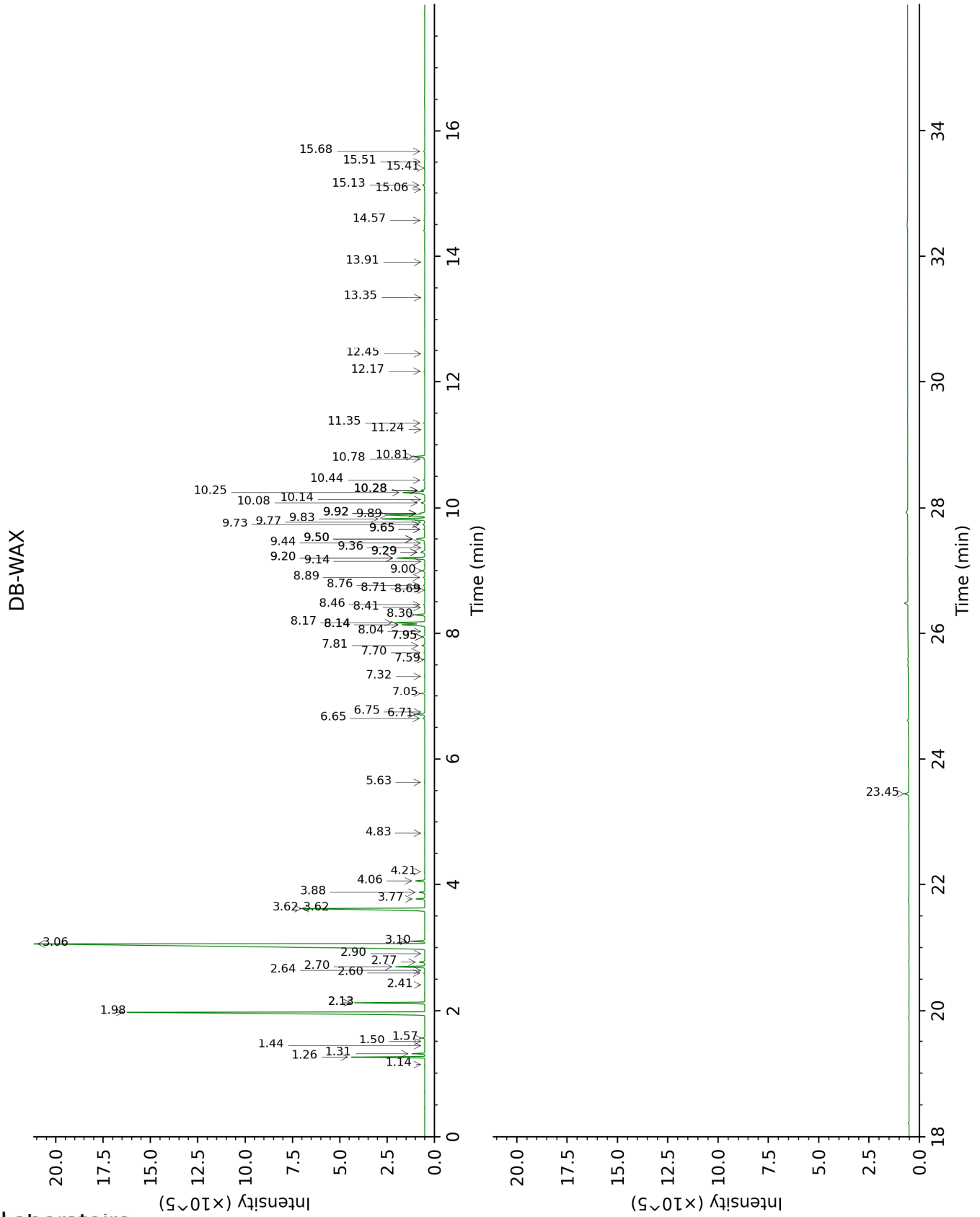
Note: no correction factor was applied

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	%
2-Methyl-3-buten-2-ol	0.54	606	tr	1.44	1012	tr
Heptanal	2.79	904	0.01	2.90	1151	0.01
Tricyclene	3.02	919	0.02	1.14	971	0.01
α -Thujene	3.14	926	0.40	1.31	999	0.40
α -Pinene	3.21	931	2.41	1.26	991	2.42
Camphene	3.40*	944	0.12	1.57	1026	0.11
α -Fenchene	3.40*	944	[0.12]	1.50	1019	tr
Thuja-2,4(10)-diene	3.50	950	0.01	2.13*	1084	2.75
Sabinene	3.87*	974	22.66	2.13*	1084	[2.75]
β -Pinene	3.87*	974	[22.66]	1.98	1068	20.15
6-Methyl-5-hepten-2-one	4.07	988	0.02	4.83	1302	0.01
Myrcene	4.16	993	1.24	2.70	1134	1.27
α -Phellandrene	4.30*	1002	0.08	2.60	1126	0.05
Octanal	4.30*	1002	[0.08]	4.21	1254	0.03
Pseudolimonene	4.30*	1002	[0.08]	2.64	1129	0.01
Δ^3 -Carene	4.38	1008	0.01	2.41	1110	0.01
α -Terpinene	4.50	1015	0.27	2.77	1140	0.27
para-Cymene	4.62	1023	0.25	3.88	1229	0.26
β -Phellandrene	4.75*	1031	45.34	3.10	1167	0.53
Limonene	4.75*	1031	[45.34]	3.06	1164	45.33
(Z)- β -Ocimene	4.91	1041	0.15	3.62*	1209	7.63
(E)- β -Ocimene	5.06	1050	0.37	3.77	1221	0.39
γ -Terpinene	5.20	1059	7.39	3.62*	1209	[7.63]
cis-Sabinene hydrate	5.31	1066	0.04	6.65	1428	0.08
Terpinolene	5.64	1086	0.42	4.06	1243	0.42
trans-Sabinene hydrate	5.80	1096	0.04	7.70	1507	0.04
Linalool	5.90	1102	0.15	7.81	1516	0.14
Nonanal	5.93	1105	0.02	5.63	1354	0.02
endo-Fenchol	6.05	1112	0.01	8.14*†	1542	2.98
trans-para-Mentha-2,8-dien-1-ol	6.16	1119	0.02	8.69	1585	0.01
1-Terpineol	6.40	1135	0.02	8.04	1534	0.01
cis- β -Terpineol	6.54	1143	0.01	8.71	1586	0.01
Citronellal	6.69	1153	0.02	6.75	1436	0.01
Borneol	6.85	1163	0.02	9.50*	1651	0.62
Isoneral	6.88	1165	0.02	7.59	1499	0.02
Isopinocampone	6.91	1167	0.02	7.32	1479	0.02
Terpinen-4-ol	7.03	1174	0.50	8.30	1554	0.50
para-Cymen-8-ol	7.16*	1183	0.02	11.24	1797	0.01
Isogeranial	7.16*	1183	[0.02]	7.95*	1527	0.15
α -Terpineol	7.26	1189	0.25	9.50*	1651	[0.62]
Decanal	7.52	1206	0.18	7.05	1458	0.17

2,3-Epoxyneral?	7.76	1222	0.02			
Nerol	7.88	1230	0.04	10.78	1758	0.04
2,3-Epoxygeranial?	7.91	1232	0.04			
Neral	8.02	1239	1.48	9.20*	1626	1.50
Geraniol	8.30	1258	0.05	11.35	1806	0.06
Geranial	8.48*	1270	2.33	9.83	1678	2.33
<i>trans</i> -Ascaridole glycol	8.48*	1270	[2.33]	13.91	2042	0.01
Unknown [m/z 112, 97 (93), 83 (60), 43 (46), 41 (20), 69 (19)...]	8.93	1300	0.01			
Undecanal	9.04	1307	0.03	8.42	1564	0.03
δ-Elemene	9.44	1336	0.47	6.71	1433	0.47
Citronellyl acetate	9.72	1355	0.01	9.20*	1626	[1.50]
Neryl acetate	9.86	1366	0.09	9.92*†	1685	[2.46]
Geranyl acetate	10.14	1385	0.18	10.28*	1715	0.19
β-Elemene	10.20	1390	0.24	8.14*†	1542	[2.98]
Dodecanal	10.47	1409	0.12	9.73	1669	0.11
β-Caryophyllene	10.54*	1413	1.39	8.14*†	1542	[2.98]
<i>cis</i> -α-Bergamotene	10.54*	1413	[1.39]	7.95*	1527	[0.15]
α-Santalene	10.59	1417	0.02	7.95*	1527	[0.15]
γ-Elemene	10.77	1431	0.06	8.76	1591	0.06
<i>trans</i> -α-Bergamotene	10.82	1434	1.51	8.17†	1545	[2.98]
α-Humulene	11.00	1448	0.16	9.00	1609	0.15
β-Santalene	11.10	1455	0.01	8.89	1601	0.08
(<i>E</i>)-β-Farnesene	11.14	1458	0.22	9.29*	1633	0.29
Selina-4,11-diene	11.32	1472	0.02	9.14	1622	tr
Germacrene D	11.37	1476	0.33	9.50*	1651	[0.62]
γ-Curcumene	11.40	1478	0.05	9.44	1645	0.04
<i>trans</i> -β-Bergamotene	11.45*	1481	0.12	9.29*	1633	[0.29]
Unknown [m/z 41, 69 (90), 79 (78), 93 (72), 91 (70)...204]	11.45*	1481	[0.12]	8.46	1567	0.06
δ-Selinene	11.52	1486	0.01	9.36	1639	0.01
Bicyclogermacrene	11.56*	1490	0.07	9.77	1672	0.02
α-Selinene	11.56*	1490	[0.07]	9.65*	1663	0.06
(3 <i>Z</i> ,6 <i>E</i>)-α-Farnesene	11.68	1499	0.19	9.92*†	1685	[2.46]
(<i>Z</i>)-α-Bisabolene	11.73	1502	0.21	9.92*†	1685	[2.46]
(3 <i>E</i> ,6 <i>E</i>)-α-Farnesene	11.81*	1508	3.31	10.25	1712	1.31
γ-Cadinene	11.81*	1508	[3.31]	10.08	1698	0.21
β-Bisabolene	11.81*	1508	[3.31]	9.89†	1683	2.46
(<i>Z</i>)-γ-Bisabolene	11.87	1513	0.03	9.65*	1663	[0.06]
δ-Cadinene	11.98	1522	0.02	10.14	1703	0.01
Selina-4(15),7(11)-diene	12.08	1530	0.02	10.28*	1715	[0.19]
Selina-3,7(11)-diene	12.16	1536	0.01	10.28*	1715	[0.19]

(E)- α -Bisabolene	12.24	1542	0.07	10.44	1729	0.08
Germacrene B	12.34	1550	0.66	10.82	1761	0.66
Caryophyllenyl alcohol	12.52	1564	0.01	13.35	1988	0.01
Caryophyllene oxide	12.66	1574	0.01	12.45	1904	0.01
Tetradecanal?	13.13	1612	0.06	12.17	1880	0.05
Alismol	13.28	1625	0.05	15.41	2191	0.03
Unknown [m/z 94, 43 (89), 41 (67), 122 (46), 69 (41)...222]	13.60	1651	0.08	14.57	2106	0.05
Unknown [m/z 69, 95 (100), 41 (89), 109 (68), 67 (61)...222]	13.78	1666	0.09	15.68	2219	0.06
α -Bisabolol	13.99	1683	0.12	15.13	2163	0.13
(2E,6Z)-Farnesal	14.33	1711	0.04	15.06	2156	0.02
(2E,6E)-Farnesal	14.65	1739	0.03	15.51	2201	0.03
Myristic acid	14.99	1769	0.01			
Citropten	17.12	1963	0.26	23.45	3158	0.27
Palmitic acid	17.21	1972	0.04			
Bergapten	17.87	2035	0.08			
Linoleic acid	18.89	2138	0.07			
Oleic acid	18.98	2147	0.02			
cis-Vaccenic acid?	19.00	2150	0.01			
Isopimpinellin	19.61	2212	0.22			
Oxypeucedanin	20.65	2325	0.01			
Total identified		97.14%			97.58%	
Total reported		97.32%			97.75%	

*: 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