Date : March 15, 2022

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 22C01-PTH01
Customer identification : Nerolina - Australia - NB1100218R
Type : Essential oil
Source : *Melaleuca quinquenervia* ct. Nerolina (linalool/nerolidol)
Customer : Plant Therapy

Analysis

Method: PC-MAT-014 ISO - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.
Analyst : Seydou Ka, Ph. D.
Analysis date : March 14, 2022

Checked and approved by :

Alexis St-Gelais, Ph. D., 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid
Refractive index: 1.4703 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

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

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Analysis summary – Consolidated contents

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
Ethanol	0.20	Aliphatic alcohol
Ethyl acetate	0.01	Aliphatic ester
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Pentanone	0.01	Aliphatic ketone
Methyl 2-methylbutyrate	0.03	Aliphatic ester
Hexanal	0.01	Aliphatic aldehyde
(3*Z*)-Hexenol	0.23	Aliphatic alcohol
Hexanol	0.03	Aliphatic alcohol
Nonene	0.01	Alkene
α-Pinene	0.30	Monoterpene
Benzaldehyde	0.47	Simple phenolic
Geranic oxide	0.01	Monoterpenic ether
β-Pinene	0.02	Monoterpene
6-Methyl-5-hepten-2-one	0.06	Aliphatic ketone
trans-Dehydroxylinalool oxide	0.07	Monoterpenic ether
6-Methyl-5-hepten-2-ol	0.01	Aliphatic alcohol
cis-Dehydroxylinalool oxide	0.03	Monoterpenic ether
α-Terpinene	0.01	Monoterpene
para-Cymene	0.02	Monoterpene
Limonene	0.21	Monoterpene
1,8-Cineole	0.14	Monoterpenic ether
(*Z*)-β-Ocimene	0.06	Monoterpene
(*E*)-β-Ocimene	0.17	Monoterpene
γ-Terpinene	0.03	Monoterpene
cis-Linalool oxide (fur.)	0.22	Monoterpenic alcohol
trans-Linalool oxide (fur.)	0.23	Monoterpenic alcohol
Terpinolene	0.05	Monoterpene
Linalool	46.38	Monoterpenic alcohol
Hotrienol	0.11	Monoterpenic alcohol
cis-Linalool oxide (pyr.)	0.01	Monoterpenic alcohol
Ethyl benzoate	0.01	Phenolic ester
Terpinen-4-ol	0.05	Monoterpenic alcohol
α-Terpineol	0.41	Monoterpenic alcohol
Hodiendiol	0.01	Monoterpenic alcohol
Nerol	0.10	Monoterpenic alcohol
Geraniol	0.30	Monoterpenic alcohol
Methyl thiobenzoate?	0.03	Simple phenolic
Eugenol	0.04	Phenylpropanoid
Isocaryophyllene	tr	Sesquiterpene
β-Caryophyllene	1.85	Sesquiterpene
α-Humulene	0.29	Sesquiterpene
Cabreuva oxide A?	0.03	Sesquiterpenic ether
allo-Aromadendrene	0.04	Sesquiterpene
(*E*)-β-Farnesene	0.08	Sesquiterpene

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(3*Z*,6*E*)-α-Farnesene	0.04	Sesquiterpene
(*Z*)-α-Bisabolene	0.03	Sesquiterpene
β-Bisabolene	0.10	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	0.03	Sesquiterpene
(*Z*)-γ-Bisabolene	0.01	Sesquiterpene
δ-Cadinene	0.02	Sesquiterpene
(*E*)-γ-Bisabolene	0.02	Sesquiterpene
(*E*)-α-Bisabolene	0.02	Sesquiterpene
(*E*)-Nerolidol	44.88	Sesquiterpenic alcohol
Unknown	0.26	Unknown
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Caryophyllene oxide	0.35	Sesquiterpenic ether
Globulol	0.02	Sesquiterpenic alcohol
Viridiflorol	0.05	Sesquiterpenic alcohol
Humulene epoxide II	0.08	Sesquiterpenic ether
Unknown	0.01	Unknown
α-Bisabolol	0.03	Sesquiterpenic alcohol
Cedroxyde	0.03	Synthetic
(2*E*,6*E*)-Farnesol	0.09	Sesquiterpenic alcohol
Consolidated total	**98.44%**	

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.

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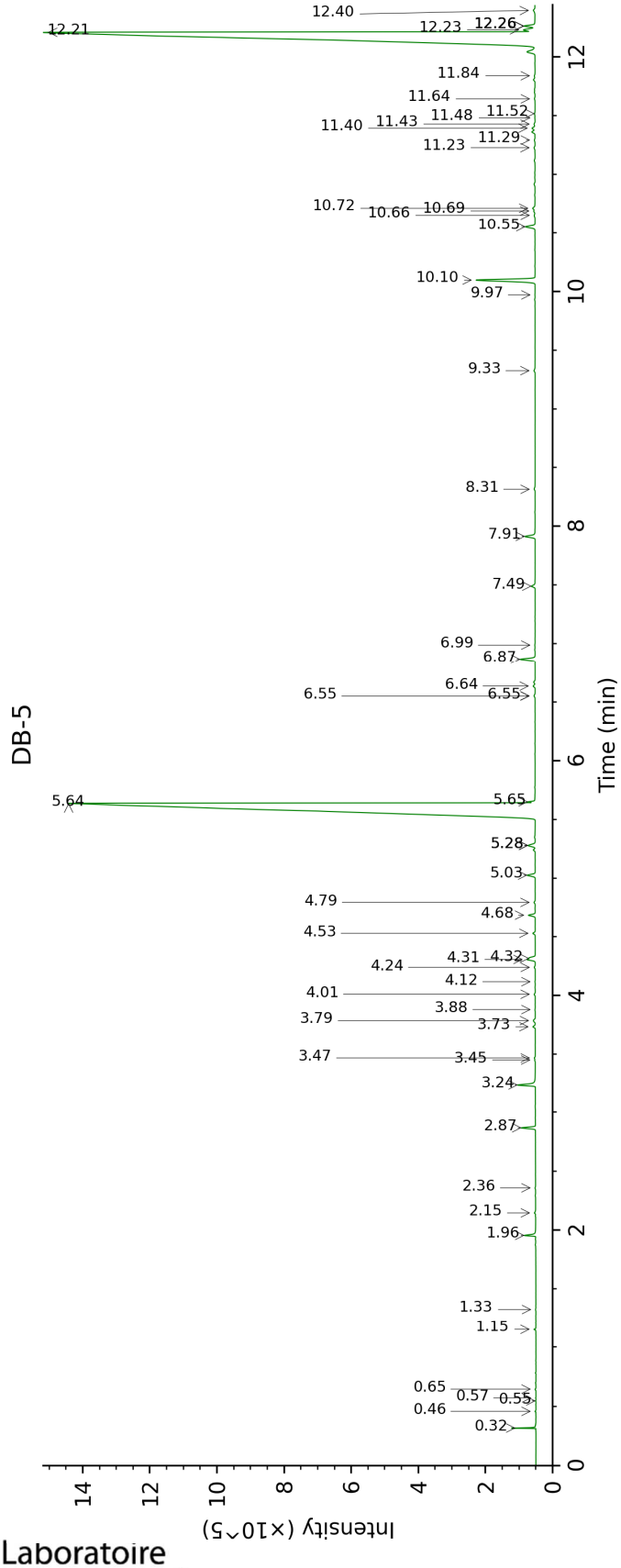
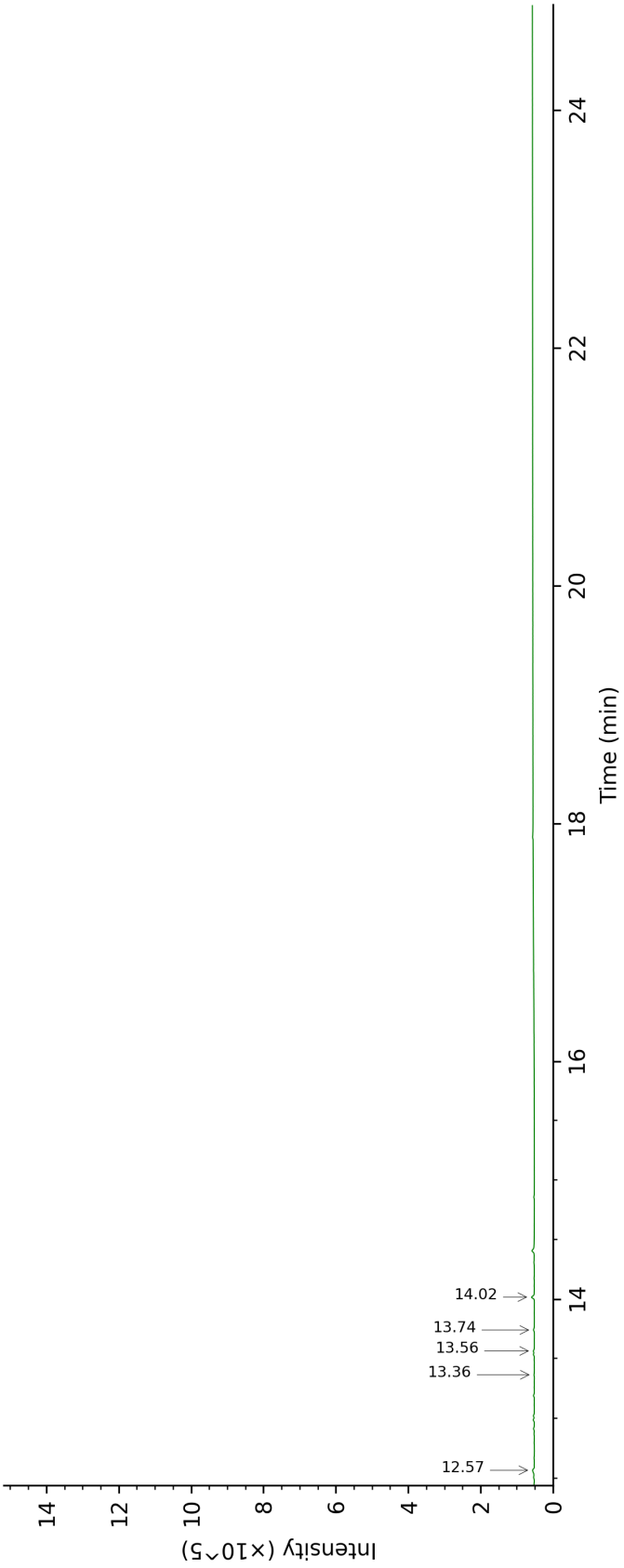
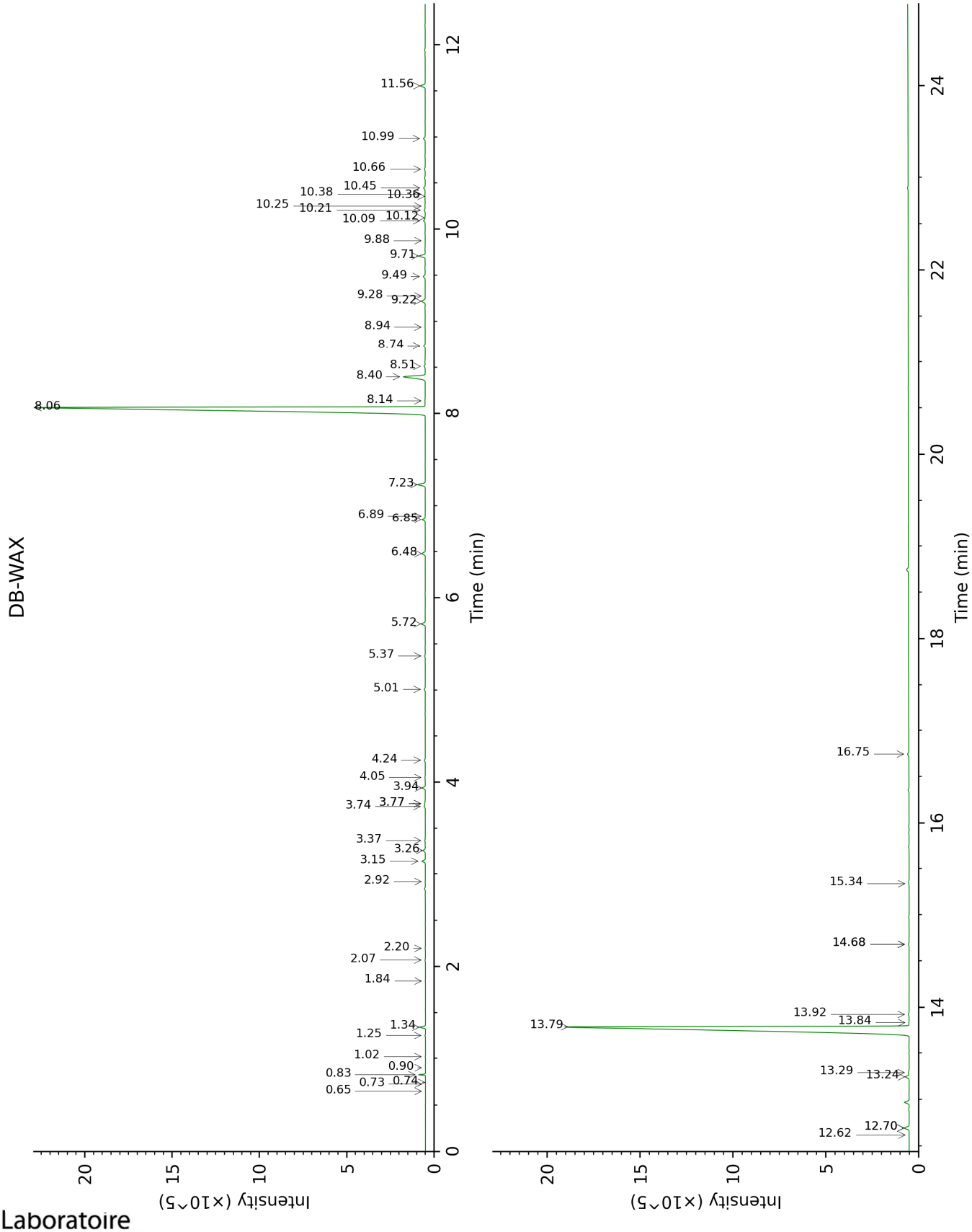

DB-5
12.40
12.21
12.23
12.26
11.84
11.64
11.40
11.43
11.48
11.52
11.29
11.23
10.72
10.66
10.69
10.55
10.10
9.97
9.33
8.31
7.91
7.49
6.99
6.87
6.64
6.55
6.55
5.64
5.65
5.28
5.03
4.79
4.68
4.53
4.24
4.31
4.32
4.12
4.01
3.88
3.79
3.73
3.47
3.45
3.24
2.87
2.36
2.15
1.96
1.33
1.15
0.65
0.57
0.55
0.46
0.32
Intensity (×10^5)
Time (min)


14.02
13.74
13.56
13.36
12.57
Intensity (×10^5)
Time (min)


DB-WAX
Intensity (×10^5)
Time (min)
0
5
10
15
20
0
2
4
6
8
10
12
14
16
18
20
22
24
0.65
0.73
0.74
0.83
0.90
1.02
1.25
1.34
1.84
2.07
2.20
2.92
3.15
3.26
3.37
3.74
3.77
3.94
4.05
4.24
5.01
5.37
5.72
6.48
6.85
6.89
7.23
8.06
8.14
8.40
8.51
8.74
8.94
9.22
9.28
9.49
9.71
9.88
10.09
10.12
10.21
10.25
10.36
10.38
10.45
10.66
10.99
11.56
12.62
12.70
13.24
13.29
13.79
13.84
13.92
14.68
15.34
16.75

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Ethanol	0.32	499	0.20	0.83	908	0.20
Ethyl acetate	0.46	605	0.01	0.65	852	tr
Isovaleral	0.55	640	tr	0.74	886	tr
2-Methylbutyral	0.57	650	tr	0.73	880	tr
2-Pentanone	0.65	679	0.01	1.02	939	0.01
Methyl 2-methylbutyrate	1.15	772	0.03	1.26	976	0.03
Hexanal	1.33	800	0.01	1.84	1044	0.01
(3*Z*)-Hexenol	1.96	856	0.23	5.72	1348	0.25
Hexanol	2.15	873	0.03	5.37	1323	0.03
Nonene	2.36	892	0.01	0.90	920	tr
α-Pinene	2.87	929	0.30	1.34	991	0.30
Benzaldehyde	3.24	954	0.47	7.23	1458	0.51
Geranic oxide	3.45	968	0.01	2.20	1078	0.02
β-Pinene	3.47	970	0.02	2.07	1066	0.02
6-Methyl-5-hepten-2-one	3.74	988	0.06	5.01	1299	0.07
trans-Dehydroxylinalool oxide	3.79	991	0.07	3.37	1175	0.04
6-Methyl-5-hepten-2-ol	3.88	998	0.01	6.89	1433	0.01
cis-Dehydroxylinalool oxide	4.01	1006	0.03	3.77*	1206	0.06
α-Terpinene	4.12	1013	0.01	2.92	1140	0.01
para-Cymene	4.24	1021	0.02	4.05	1227	0.03
Limonene	4.31†	1025	0.33	3.15	1158	0.21
1,8-Cineole	4.32†	1025	[0.33]	3.26	1167	0.14
(*Z*)-β-Ocimene	4.53	1039	0.06	3.74	1204	0.07
(*E*)-β-Ocimene	4.68	1049	0.17	3.94	1219	0.18
γ-Terpinene	4.79	1056	0.03	3.77*	1206	[0.06]
cis-Linalool oxide (fur.)	5.03	1071	0.22	6.48	1402	0.22
trans-Linalool oxide (fur.)	5.28*	1087	0.23	6.85	1430	0.23
Terpinolene	5.28*	1087	[0.23]	4.24	1241	0.05
Linalool	5.64	1109	46.38	8.06	1521	46.14
Hotrienol	5.65	1110	0.11	8.74	1573	0.10
cis-Linalool oxide (pyr.)	6.55*	1168	0.03	10.25	1695	0.01
Ethyl benzoate	6.55*	1168	[0.03]	9.28	1616	0.01
Terpinen-4-ol	6.64	1173	0.05	8.51	1556	0.07
α-Terpineol	6.87	1188	0.41	9.71	1651	0.42
Hodiendiol	6.99	1196	0.01	12.70*	1908	0.36
Nerol	7.49	1229	0.10	10.99	1757	0.13
Geraniol	7.91	1258	0.30	11.56	1806	0.33

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Methyl thiobenzoate?	8.31	1285	0.03			
Eugenol	9.33	1355	0.04	14.68*	2097	0.04
Isocaryophyllene	9.97	1401	tr	8.14	1526	0.02
β-Caryophyllene	10.10	1410	1.85	8.40	1547	1.84
α-Humulene	10.55	1444	0.29	9.22	1611	0.27
Cabreuva oxide A?	10.66	1452	0.03			
allo-Aromadendrene	10.69	1454	0.04	8.94	1589	0.01
(*E*)-β-Farnesene	10.72	1456	0.08	9.49	1633	0.14
(3*Z*,6*E*)-α-Farnesene	11.23	1495	0.04	10.21	1691	0.07
(*Z*)-α-Bisabolene	11.30	1500	0.03	10.12	1684	0.02
β-Bisabolene	11.40	1507	0.10	10.09	1682	0.12
(3*E*,6*E*)-α-Farnesene	11.43	1510	0.03	10.45	1711	0.13
(*Z*)-γ-Bisabolene	11.48	1514	0.01	9.88	1664	tr
δ-Cadinene	11.52	1517	0.02	10.38	1705	0.02
(*E*)-γ-Bisabolene	11.64	1527	0.02	10.36	1703	0.02
(*E*)-α-Bisabolene	11.84	1542	0.02	10.66	1729	0.06
(*E*)-Nerolidol	12.21†	1571	45.95	13.79	2010	44.88
Unknown [m/z 109, 69 (60), 43 (40), 93 (28), 41 (25), 111 (22)...]	12.23†	1573	[45.95]	13.24	1959	0.26
Caryophyllene oxide isomer	12.26*†	1575	[45.95]	12.62	1901	0.01
Caryophyllene oxide	12.26*†	1575	[45.95]	12.70*	1908	[0.36]
Globulol	12.26*†	1575	[45.95]	13.84	2014	0.02
Viridiflorol	12.40	1586	0.05	13.92	2023	0.07
Humulene epoxide II	12.57	1600	0.08	13.29	1963	0.08
Unknown [m/z 91, 93 (81), 79 (81), 41 (79), 69 (76), 105 (66)...]	13.36	1665	0.01			
α-Bisabolol	13.56	1682	0.03	15.34	2163	0.02
Cedroxyde	13.74	1697	0.03	14.68*	2097	[0.04]
(2*E*,6*E*)-Farnesol	14.02	1720	0.09	16.74	2310	0.09
Total identified		**98.81%**			**98.21%**	
Total reported		**98.82%**			**98.47%**	

*: 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

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