

Date : October 05, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21I21-PTH04


Customer identification : Citronella - Indonesia - CE0106204R

Type : Essential oil

Source : *Cymbopogon winterianus*

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

Analysis date : October 04, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.4690 ± 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
3-Methylcyclopentene	tr	Alkene
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	tr	Aliphatic alcohol
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Tricyclene	tr	Monoterpene
α -Thujene	0.01	Monoterpene
α -Pinene	0.03	Monoterpene
Camphene	0.02	Monoterpene
β -Pinene	0.01	Monoterpene
Sabinene	0.02	Monoterpene
6-Methyl-5-hepten-2-one	0.08	Aliphatic ketone
Myrcene	0.06	Monoterpene
α -Phellandrene	0.02	Monoterpene
Octanal	0.01	Aliphatic aldehyde
α -Terpinene	0.01	Monoterpene
para-Cymene	0.01	Monoterpene
β -Phellandrene	0.04	Monoterpene
Limonene	2.98	Monoterpene
(Z)- β -Ocimene	0.08	Monoterpene
(E)- β -Ocimene	0.04	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.07	Aliphatic aldehyde
γ -Terpinene	0.02	Monoterpene
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.06	Monoterpene
Linalool	0.60	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
cis-Rose oxide	0.01	Monoterpenic ether
Unknown	0.01	Oxygenated monoterpene
trans-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
trans-Rose oxide	0.01	Monoterpenic ether
Unknown	0.02	Unknown
Isopulegol	0.81	Monoterpenic alcohol
Menthone	0.17	Monoterpenic ketone
Citronellal	35.84	Monoterpenic aldehyde
iso-Isopulegol	0.25	Monoterpenic alcohol
Borneol	0.03	Monoterpenic alcohol
neoiso-Isopulegol	0.05	Monoterpenic alcohol
Isopulegol isomer	0.02	Monoterpenic alcohol
Rosefuran oxide	0.02	Monoterpenic ether
Terpinen-4-ol	0.01	Monoterpenic alcohol
α -Terpineol	0.05	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde

(4Z)-Decenal	0.03	Aliphatic aldehyde
Decanal	0.10	Aliphatic aldehyde
2,3-Epoxyneral?	0.07	Monoterpenic aldehyde
Nerol	0.20	Monoterpenic alcohol
Citronellol	11.44	Monoterpenic alcohol
Neral	0.49	Monoterpenic aldehyde
Piperitone	0.02	Monoterpenic ketone
Geraniol	22.82	Monoterpenic alcohol
Geranial	0.70	Monoterpenic aldehyde
Citronellyl formate	0.03	Monoterpenic ester
Geranyl formate	0.03	Monoterpenic ester
Unknown	0.02	Norsesquiterpene
Citronellic acid	0.01	Monoterpenic acid
8-Hydroxy-neo-menthol	0.16	Monoterpenic alcohol
α -Cubebene	0.02	Sesquiterpene
Citronellyl acetate	2.27	Monoterpenic ester
Eugenol	0.66	Phenylpropanoid
Neryl acetate	0.05	Monoterpenic ester
α -Copaene	0.03	Sesquiterpene
β -Bourbonene	0.09	Sesquiterpene
<i>cis</i> - β -Elemene	0.06	Sesquiterpene
Geranyl acetate	3.62	Monoterpenic ester
β -Elemene	1.33	Sesquiterpene
Methyleugenol	0.01	Phenylpropanoid
Dodecanal	0.01	Aliphatic aldehyde
β -Caryophyllene	0.19	Sesquiterpene
β -Copaene	0.03	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.06	Sesquiterpene
Isogermacrene D	0.02	Sesquiterpene
α -Humulene	0.10	Sesquiterpene
(<i>E</i>)-Isoeugenol	0.02	Phenylpropanoid
<i>trans</i> -Cadina-1(6),4-diene	0.04	Sesquiterpene
γ -Muurolene	0.13	Sesquiterpene
Germacrene D	1.83	Sesquiterpene
β -Selinene	0.03	Sesquiterpene
α -Selinene	0.02	Sesquiterpene
epi-Cubebol	0.11	Sesquiterpenic alcohol
Germacrene A	1.02	Sesquiterpene
α -Muurolene	0.08	Sesquiterpene
γ -Cadinene	0.41	Sesquiterpene
Cubebol	0.10	Sesquiterpenic alcohol
<i>trans</i> -Calamenene	0.02	Sesquiterpene
δ -Cadinene	1.41	Sesquiterpene
Unknown	0.05	Sesquiterpene
α -Cadinene	0.10	Sesquiterpene
α -Elemol	2.41	Sesquiterpenic alcohol
Geranyl butyrate	0.06	Monoterpenic ester
(<i>E</i>)-Nerolidol	0.03	Sesquiterpenic alcohol
Germacrene D-4-ol	1.09	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	Sesquiterpenic ether
10-epi-Cubebol	0.04	Sesquiterpenic alcohol
γ -Eudesmol	0.21	Sesquiterpenic alcohol

τ-Cadinol	0.18	Sesquiterpenic alcohol
τ-Muurolol	0.41	Sesquiterpenic alcohol
α-Muurolol	0.11	Sesquiterpenic alcohol
β-Eudesmol	0.24	Sesquiterpenic alcohol
α-Eudesmol	0.27	Sesquiterpenic alcohol
α-Cadinol	0.56	Sesquiterpenic alcohol
Unknown	0.93	Oxygenated sesquiterpene
(2E,6Z)-Farnesal	0.06	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	0.10	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.03	Sesquiterpenic aldehyde
Cryptomeridiol	0.02	Sesquiterpenic alcohol
Geranyl caprylate	0.02	Monoterpenic ester
Unknown	0.07	Oxygenated diterpene
Unknown	0.01	Unknown
Unknown	0.02	Unknown
Unknown	0.06	Unknown
Consolidated total	98.53%	

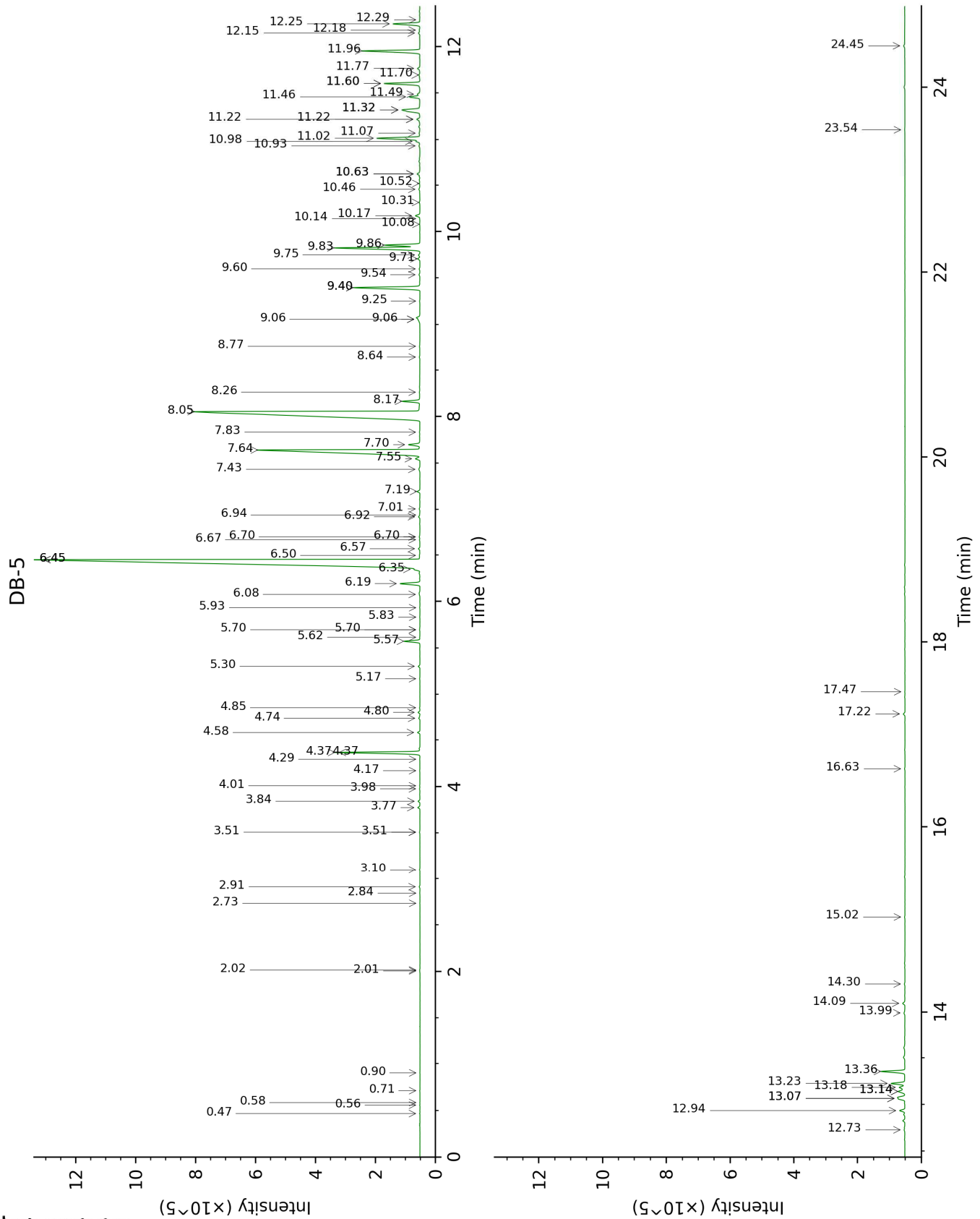
tr: The compound has been detected below 0.005% of total signal.

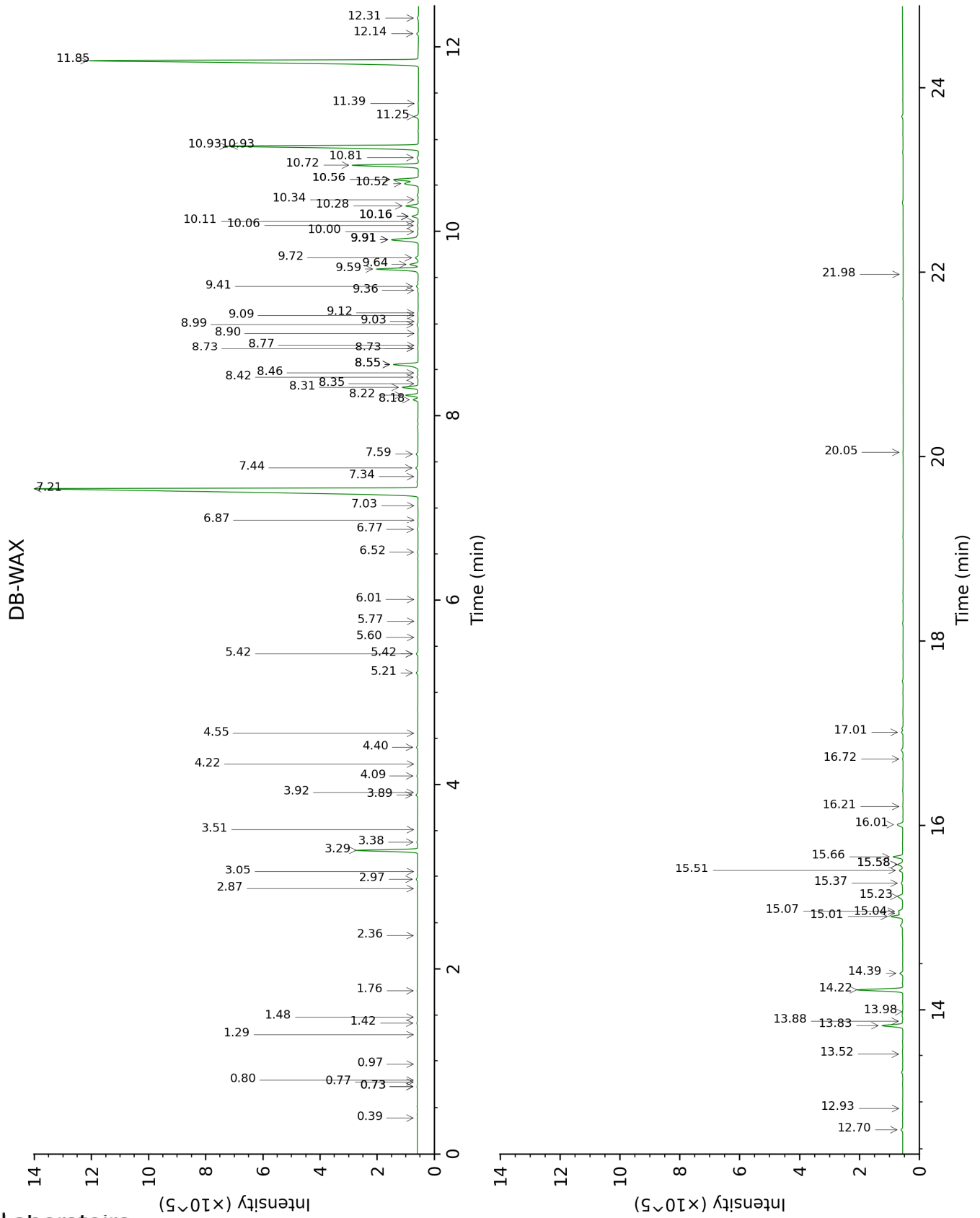
Note: no correction factor was applied

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	%
3-Methylcyclopentene	0.47	607	tr	0.39	669	tr
Isovaleral	0.56	642	tr	0.80	890	tr
2-Methylbutyral	0.58	653	tr	0.77	882	tr
2-Ethylfuran	0.71	702	tr	0.97	918	tr
Isoamyl alcohol	0.90	732	tr	3.51	1176	tr
Unknown [m/z 55, 83 (89), 82 (70), 67 (66), 41 (55), 69 (46), 111 (37)... 126 (2)]	2.01	859	0.01	0.73*	865	0.02
Unknown [m/z 55, 83 (79), 67 (65), 41 (63), 82 (60), 69 (58)... 111 (27), 126 (9)]	2.02	860	0.01	0.73*	865	[0.02]
Tricyclene	2.74	918	tr	1.29	970	0.01
α -Thujene	2.84	925	0.01	1.48	996	0.01
α -Pinene	2.91	930	0.03	1.42	990	0.03
Camphene	3.10	943	0.02	1.76	1024	0.02
β -Pinene	3.51*	970	0.02			
Sabinene	3.51*	970	[0.02]	2.36	1083	0.02
6-Methyl-5-hepten-2-one	3.77	988	0.08	5.22	1297	0.08
Myrcene	3.84	993	0.06	2.97	1133	0.06
α -Phellandrene	3.98	1002	0.02	2.87	1125	0.01
Octanal	4.01	1004	0.01	4.56	1254	0.01
α -Terpinene	4.17	1014	0.01	3.05	1139	0.01
para-Cymene	4.29	1022	0.01	4.22	1229	tr
β -Phellandrene	4.37*	1026	2.97	3.38	1165	0.04
Limonene	4.37*	1026	[2.97]	3.29	1158	2.98
(Z)- β -Ocimene	4.58	1040	0.08	3.89	1204	0.09
(E)- β -Ocimene	4.74	1050	0.04	4.09	1220	0.05
2,6-Dimethyl-5-heptenal (melonal)	4.80	1054	0.07	5.42*	1312	0.08
γ -Terpinene	4.85	1057	0.02	3.92	1206	0.01
Octanol	5.17	1077	0.01	8.35	1527	0.02
Terpinolene	5.30	1085	0.06	4.40	1243	0.06
Linalool	5.57	1102	0.60	8.22	1517	0.60
Nonanal	5.62	1105	0.02	6.01	1354	0.01
cis-Rose oxide	5.70*	1110	0.02	5.42*	1312	[0.08]
Unknown [m/z 111, 69 (70), 41 (68), 55 (53), 43 (51)... 154 (7)]	5.70*	1110	[0.02]	5.77	1337	0.01
trans-para-Mentha-2,8-dien-1-ol	5.83	1119	0.01	9.12	1586	0.01
trans-Rose oxide	5.93	1126	0.01	5.60	1325	0.01

Unknown [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	6.08	1135	0.02	7.03	1428	0.01
Isopulegol	6.19	1142	0.81	8.31	1524	0.82
Menthone	6.35	1152	0.17	6.77	1409	0.04
Citronellal	6.45*	1159	36.24	7.21	1442	35.84
iso-Isopulegol	6.45*	1159	[36.24]	8.18	1514	0.25
Borneol	6.50	1162	0.03	9.91*	1650	1.90
neoiso-Isopulegol	6.57	1166	0.05	8.99	1576	0.07
Isopulegol isomer	6.67	1172	0.02	8.73*	1556	0.03
Rosefuran oxide	6.70*	1174	0.04	8.73*	1556	[0.03]
Terpinen-4-ol	6.70*	1174	[0.04]	8.77	1559	0.01
α -Terpineol	6.92	1189	0.05	9.91*	1650	[1.90]
Myrtenal	6.94	1190	0.01	8.90	1569	0.01
(4Z)-Decenal	7.01	1194	0.03			
Decanal	7.19	1206	0.10	7.44	1458	0.12
2,3-Epoxyneral?	7.43	1222	0.07			
Nerol	7.55	1230	0.20	11.25	1760	0.25
Citronellol	7.64	1236	11.44	10.93*	1733	11.65
Neral	7.70	1240	0.49	9.64	1628	0.46
Piperitone	7.83	1249	0.02	10.06	1662	0.06
Geraniol	8.05	1264	22.82	11.85	1812	23.01
Geranial	8.17	1271	0.70	10.28	1679	0.65
Citronellyl formate	8.26	1278	0.03	9.09	1584	0.02
Geranyl formate	8.64	1303	0.03	10.11	1665	0.02
Unknown [m/z 135, 121 (81), 177 (78), 107 (60), 192 (42), 149 (35)]	8.77	1312	0.02	6.52	1390	0.03
Citronellic acid	9.06*†	1332	0.25	16.21	2220	0.01
8-Hydroxy-neomenthol	9.06*†	1332	[0.25]	14.40	2042	0.16
α -Cubebene	9.25	1346	0.02	6.87	1417	0.02
Citronellyl acetate	9.40*	1356	2.83	9.59	1624	2.27
Eugenol	9.40*	1356	[2.83]	15.01	2101	0.66
Neryl acetate	9.54	1366	0.05	10.34	1684	0.03
α -Copaene	9.60	1370	0.03	7.34	1451	0.02
β -Bourbonene	9.71	1378	0.09	7.59	1469	0.09
<i>cis</i> - β -Elemene	9.75	1381	0.06	8.42	1532	0.06
Geranyl acetate	9.83	1386	3.62	10.72	1716	3.63
β -Elemene	9.86	1388	1.33	8.56*	1543	1.55
Methyleugenol	10.08	1404	0.01	13.52	1960	0.01
Dodecanal	10.14	1409	0.01	10.16*	1670	0.35
β -Caryophyllene	10.17	1411	0.19	8.56*	1543	[1.55]
β -Copaene	10.32	1422	0.03	8.46	1536	0.03
<i>trans</i> - α -Bergamotene	10.46	1432	0.06	8.56*	1543	[1.55]
Isogermacrene D	10.52	1437	0.02	9.03	1579	0.01
α -Humulene	10.63*	1445	0.13	9.41	1609	0.10
(<i>E</i>)-Isoeugenol	10.63*	1445	[0.13]	16.72	2273	0.02

<i>trans</i> -Cadina-1(6),4-diene	10.93	1468	0.04	9.36	1606	0.04
γ -Muurolene	10.98	1471	0.13	9.72	1634	0.17
Germacrene D	11.02	1474	1.83	9.91*	1650	[1.90]
β -Selinene	11.07	1478	0.03	10.00	1656	0.06
α -Selinene	11.22*†	1489	0.14	10.16*	1670	[0.35]
epi-Cubebol	11.22*†	1489	[0.14]	12.14	1837	0.11
Germacrene A	11.32*	1496	1.09	10.52	1698	1.02
α -Muurolene	11.32*	1496	[1.09]	10.16*	1670	[0.35]
γ -Cadinene	11.46†	1507	0.51	10.56*	1702	1.42
Cubebol	11.49†	1510	[0.51]	12.70	1886	0.10
<i>trans</i> -Calamenene	11.60*	1518	1.43	11.39	1772	0.02
δ -Cadinene	11.60*	1518	[1.43]	10.56*	1702	[1.42]
Unknown [m/z 119, 105 (53), 161 (33), 93 (28), 91 (25), 40 (20)...204]	11.70	1526	0.05	10.81	1723	0.08
α -Cadinene	11.77	1531	0.10	10.93*	1733	[11.65]
α -Elemol	11.96	1546	2.41	14.22	2025	2.45
Geranyl butyrate	12.15	1561	0.06	12.31	1852	0.10
(<i>E</i>)-Nerolidol	12.18	1564	0.03	13.98	2003	0.02
Germacrene D-4-ol	12.25	1569	1.09	13.83	1989	1.15
Caryophyllene oxide	12.29	1572	0.01	12.93	1907	0.01
10-epi-Cubebol	12.73	1607	0.04	13.88	1993	0.03
γ -Eudesmol	12.94	1624	0.21	15.07	2107	0.24
τ -Cadinol	13.07*†	1635	0.50	15.04	2104	0.18
τ -Muurolol	13.07*†	1635	[0.50]	15.23	2122	0.41
α -Muurolol	13.14*	1641	0.36	15.37	2136	0.11
β -Eudesmol	13.14*	1641	[0.36]	15.58*	2157	0.33
α -Eudesmol	13.18	1644	0.27	15.51	2150	0.20
α -Cadinol	13.23	1648	0.56	15.66	2165	0.55
Unknown [suspected m/z 59, 93 (79), 161 (61), 107 (47), 81 (44), 121 (37)...]	13.36	1659	0.93			
(2 <i>E</i> ,6 <i>Z</i>)-Farnesal	13.99	1712	0.06	15.58*	2157	[0.33]
(2 <i>E</i> ,6 <i>E</i>)-Farnesol	14.09	1720	0.10	17.01	2303	0.10
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	14.30	1738	0.03	16.01	2200	0.39
Cryptomeridiol	15.02	1801	0.02	20.05	2642	0.02
Geranyl caprylate	16.63	1949	0.02			
Unknown [m/z 41, 69 (98), 55 (55), 81 (46), 109 (46)... 290 (8)]	17.22	2005	0.07			
Unknown [m/z 69, 41 (96), 55 (53), 109 (48), 95 (43), 67 (35)...]	17.47	2029	0.01			
Unknown [m/z 69, 81 (79), 81 (70), 137	23.54	2712	0.02	21.98	2878	0.01

(53), 139 (35), 95 (30)...			
Unknown [m/z 69, 81 (64), 95 (29), 137 (19), 41 (19)...	24.45	2830	0.06
Total identified	97.34%		97.72%
Total reported	98.53%		97.87%

*: 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