

Date : 2024-08-29

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 24H16-PTH04

**Customer Identification :** Citronella - Indonesia - CE0110R

**Type :** Essential Oil

**Source :** *Cymbopogon winterianus*

**Customer :** Plant Therapy

Checked and approved by:

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

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## GAS CHROMATOGRAPHIC ANALYSIS

**Method :** PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID



**Results :** See analysis summary (next page)

**Analyst :** Sylvain Mercier, M. Sc., Chimiste 2014-005

**Date :** 2024-08-26

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.4676 \pm 0.0003$  (20 °C)

**Method :** PC-MAT-016 - Measure of the refractive index of a liquid.

**Analyst :** Kassandra Baker

**Date :** 2024-08-19

## 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
Methylcyclopentane	tr	Alkane
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	tr	Aliphatic alcohol
(3Z)-Hexenol	tr	Aliphatic alcohol
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Tricyclene	0.03	Monoterpene
$\alpha$ -Thujene	0.01	Monoterpene
$\alpha$ -Pinene	0.09	Monoterpene
Camphene	0.09	Monoterpene
Sabinene	0.02	Monoterpene
$\beta$ -Pinene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	0.07	Aliphatic ketone
Myrcene	0.07	Monoterpene
$\alpha$ -Phellandrene	0.01	Monoterpene
Octanal	0.01	Aliphatic aldehyde
$\Delta$ 3-Carene	0.01	Monoterpene
$\alpha$ -Terpinene	0.01	Monoterpene
para-Cymene	0.01	Monoterpene
$\beta$ -Phellandrene	0.05	Monoterpene
Limonene	3.60	Monoterpene
Unknown	0.04	Unknown
(Z)- $\beta$ -Ocimene	0.02	Monoterpene
(E)- $\beta$ -Ocimene	0.03	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.07	Aliphatic aldehyde
$\gamma$ -Terpinene	0.02	Monoterpene
4-Nonanone	0.02	Aliphatic ketone
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.07	Monoterpene
Rosefuran	0.02	Monoterpenic ether
Linalool	0.71	Monoterpenic alcohol
Unknown	0.02	Oxygenated monoterpene
cis-Rose oxide	0.01	Monoterpenic ether
trans-para-Mentha-2,8-dien-1-ol	0.01	Monoterpenic alcohol
trans-Rose oxide	0.01	Monoterpenic ether
Melonol ?	0.02	Normonoterpene
Unknown	0.02	Unknown

Unknown	0.02	Unknown
Isopulegol	0.97	Monoterpenic alcohol
Menthone	0.05	Monoterpenic ketone
Citronellal	42.67	Monoterpenic aldehyde
Borneol	0.04	Monoterpenic alcohol
neoiso-Isopulegol	0.06	Monoterpenic alcohol
Isopulegol isomer	0.03	Monoterpenic alcohol
Terpinen-4-ol	[0.05]	Monoterpenic alcohol
Rosefuran oxide	[0.05]	Monoterpenic ether
Isogeranial	0.01	Monoterpenic aldehyde
para-Cymen-8-ol	tr	Monoterpenic alcohol
α-Terpineol	0.08	Monoterpenic alcohol
(4Z)-Decenal	0.04	Aliphatic aldehyde
(4E)-Decenal	0.01	Aliphatic aldehyde
Decanal	0.13	Aliphatic aldehyde
2,3-Epoxyneral?	0.02	Monoterpenic aldehyde
Nerol	0.15	Monoterpenic alcohol
Citronellol	10.98	Monoterpenic alcohol
Neral	0.57	Monoterpenic aldehyde
Piperitone	0.02	Monoterpenic ketone
Geraniol	18.54	Monoterpenic alcohol
Geranial	0.75	Monoterpenic aldehyde
Citronellyl formate	0.02	Monoterpenic ester
Bornyl acetate	0.01	Monoterpenic ester
Geranyl formate	0.02	Monoterpenic ester
Unknown	0.02	Norsesquiterpene
Citronellic acid	0.25	Monoterpenic acid
8-Hydroxy-neo-menthol	0.05	Monoterpenic alcohol
α-Terpinyl acetate	0.01	Monoterpenic ester
Citronellyl acetate	1.59	Monoterpenic ester
Eugenol	0.87	Phenylpropanoid
Neryl acetate	0.03	Monoterpenic ester
α-Copaene	0.04	Sesquiterpene
β-Bourbonene	0.09	Sesquiterpene
cis-β-Elemene	0.05	Sesquiterpene
Geranyl acetate	2.37	Monoterpenic ester
β-Elemene	1.23	Sesquiterpene
Methyleugenol	0.01	Phenylpropanoid
Dodecanal	0.01	Aliphatic aldehyde
β-Caryophyllene	0.39	Sesquiterpene
β-Ylangene	0.04	Sesquiterpene
β-Copaene	0.03	Sesquiterpene
trans-α-Bergamotene	0.02	Sesquiterpene
Isogermacrene D	0.02	Sesquiterpene
α-Humulene	0.17	Sesquiterpene

(E)-Isoeugenol	0.02	Phenylpropanoid
Methyl (Z)-isoeugenol	0.05	Phenylpropanoid
(E)- $\beta$ -Farnesene	0.01	Sesquiterpene
trans-Cadina-1(6),4-diene	0.04	Sesquiterpene
$\gamma$ -Muurolene	0.16	Sesquiterpene
Germacrene D	1.71	Sesquiterpene
$\beta$ -Selinene	0.04	Sesquiterpene
$\gamma$ -Amorphene	0.05	Sesquiterpene
$\alpha$ -Selinene	0.04	Sesquiterpene
epi-Cubebol	0.09	Sesquiterpenic alcohol
Methyl (E)-isoeugenol	0.02	Phenylpropanoid
$\alpha$ -Muurolene	0.33	Sesquiterpene
Germacrene A	0.48	Sesquiterpene
$\gamma$ -Cadinene	0.61	Sesquiterpene
Cubebol	0.09	Sesquiterpenic alcohol
trans-Calamenene	0.02	Sesquiterpene
$\delta$ -Cadinene	1.39	Sesquiterpene
Unknown	0.05	Sesquiterpene
$\alpha$ -Cadinene	0.10	Sesquiterpene
$\alpha$ -Elemol	1.95	Sesquiterpenic alcohol
Germacrene B	0.01	Sesquiterpene
Geranyl butyrate	0.02	Monoterpenic ester
(E)-Nerolidol	0.02	Sesquiterpenic alcohol
Germacrene D-4-ol	0.96	Sesquiterpenic alcohol
Caryophyllene oxide	0.02	Sesquiterpenic ether
Unknown	0.03	Unknown
1,10-diepi-Cubenol	0.05	Sesquiterpenic alcohol
$\gamma$ -Eudesmol	0.19	Sesquiterpenic alcohol
$\tau$ -Cadinol	0.06	Sesquiterpenic alcohol
Cubenol	0.03	Sesquiterpenic alcohol
$\tau$ -Muurolol	0.29	Sesquiterpenic alcohol
$\alpha$ -Muurolol	0.09	Sesquiterpenic alcohol
$\beta$ -Eudesmol	0.19	Sesquiterpenic alcohol
$\alpha$ -Eudesmol	0.19	Sesquiterpenic alcohol
$\alpha$ -Cadinol	0.54	Sesquiterpenic alcohol
(E)-Isoelemicin	0.01	Phenylpropanoid
Unknown	0.69	Oxygenated sesquiterpene
7-epi- $\gamma$ -Eudesmol	0.03	Sesquiterpenic alcohol
(3Z)-Caryophylla-3,8(13)-dien-5 $\beta$ -ol	0.01	Sesquiterpenic alcohol
(2Z,6Z)-Farnesol	tr	Sesquiterpenic alcohol
(2E,6Z)-Farnesal	0.02	Sesquiterpenic aldehyde
(2E,6E)-Farnesol	0.08	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
Cryptomeridiol	0.02	Sesquiterpenic alcohol
Unknown	0.01	Oxygenated diterpene

Unknown	0.06	Oxygenated diterpene
Unknown	0.01	Unknown
Unknown	0.02	Unknown
Unknown	0.07	Unknown
Unknown	0.08	Unknown
<b>Consolidated total</b>	<b>98.77</b>	

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

Note: no correction factor was applied

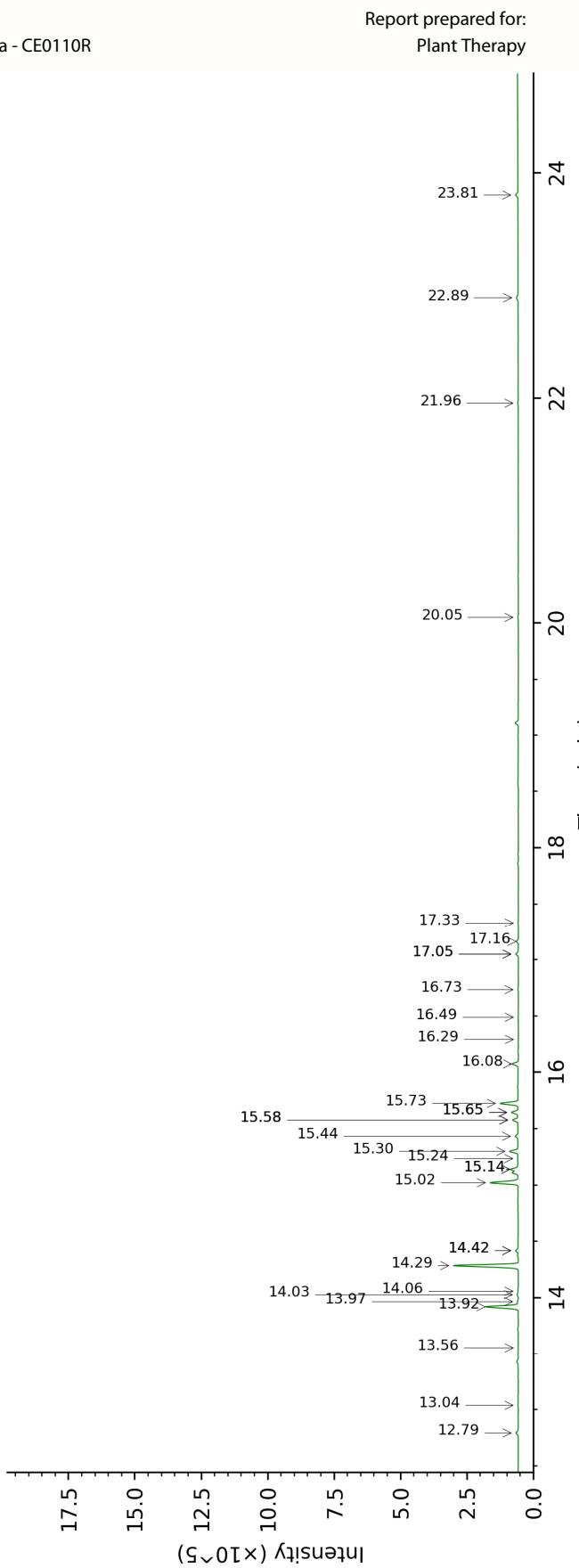
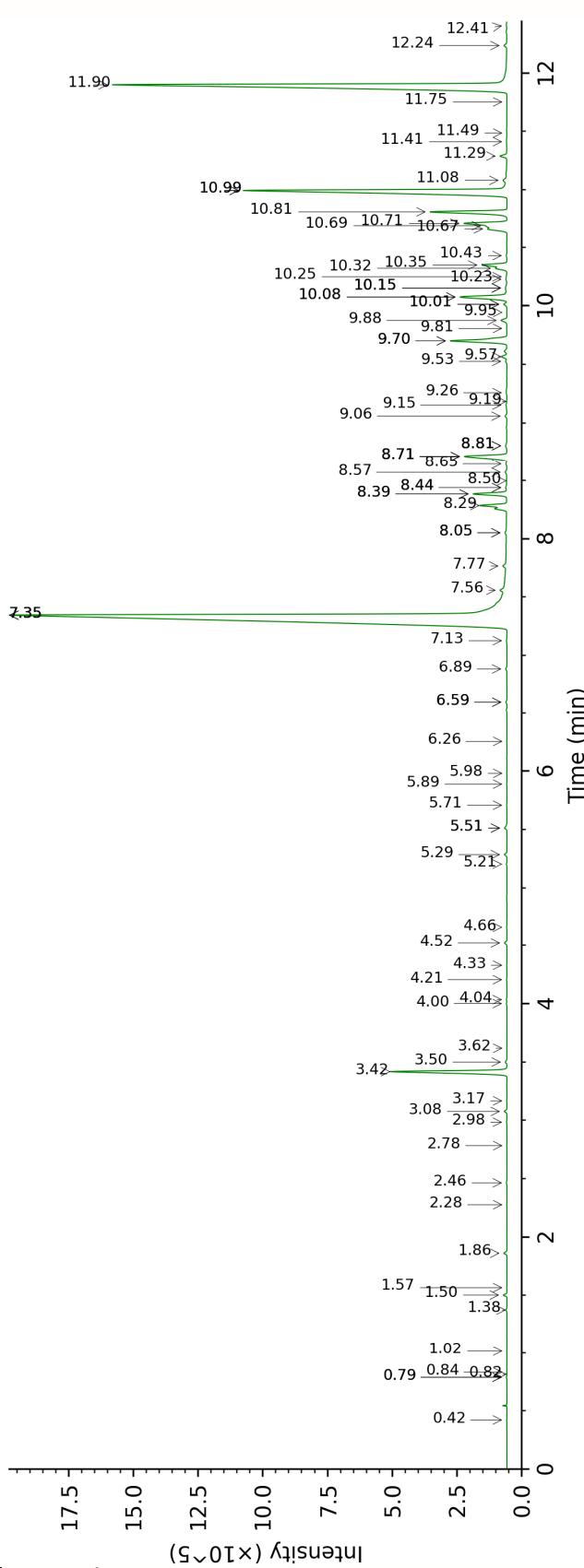
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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.

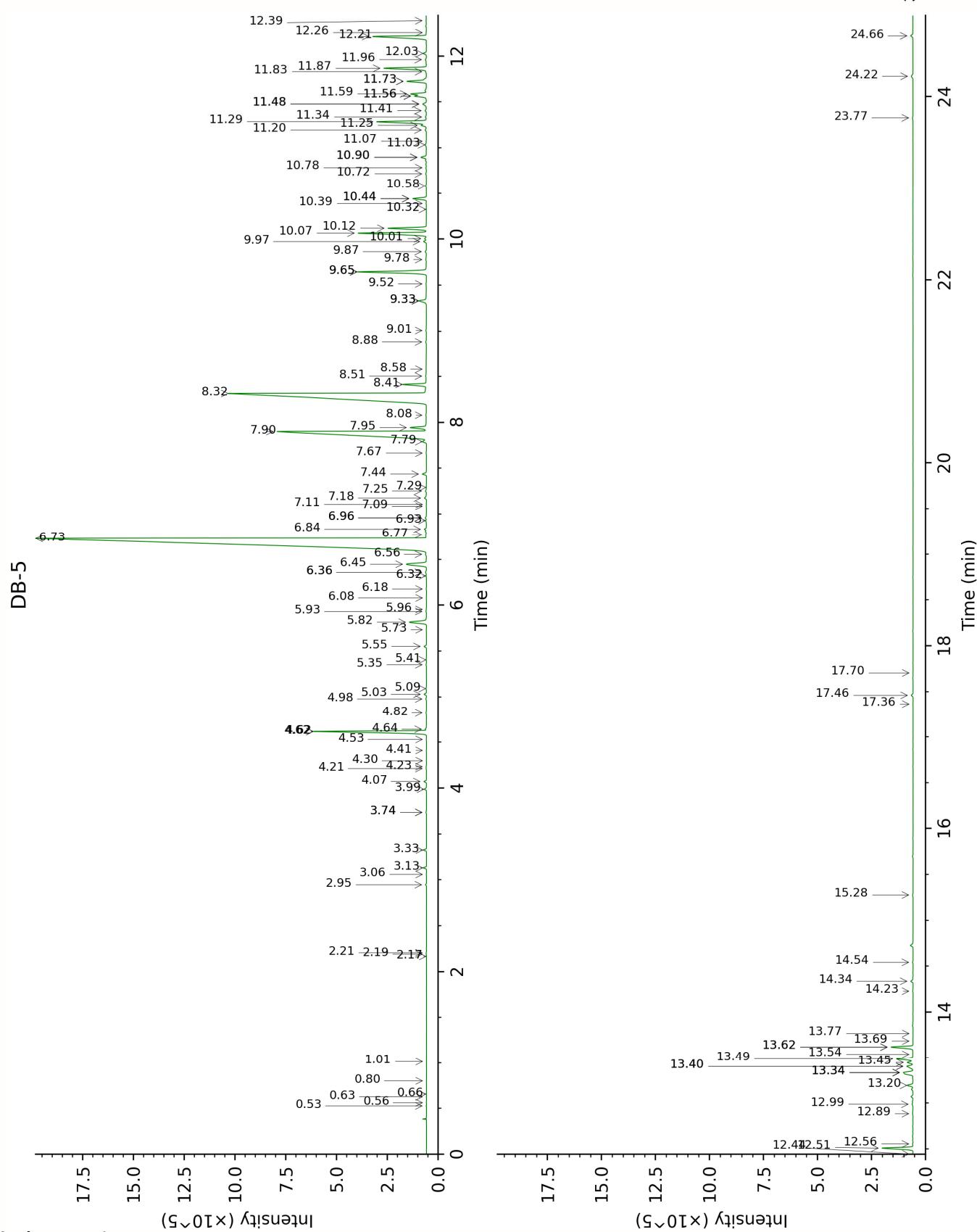
**Unknowns:** Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

**Bracketed value ([xx]):** A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

This page was intentionally left blank. The following pages present the complete data of the analysis.

DB-WAX





FULL ANALYSIS DATA

2-Methyl-3-butene-2-ol	Column DB-WAX			Column DB-5		
				0.53	606.2	tr
Methylcyclopentane	0.42	660.8	tr	0.56	618.3	tr
Isovaleral	0.84	884.2	tr	0.63	640.5	tr
2-Methylbutyral	0.82	877.8	tr	0.66	650.8	tr
2-Ethylfuran	1.02	917.8	tr	0.80	701.0	tr
Isoamyl alcohol	3.62	1174.9	tr	1.02	732.5	tr
(3Z)-Hexenol	5.98	1345.0	0.01	2.17	857.0	tr
Unknown COCI I [m/z 55, 83 (89), 82 (70), 67 (66), 41 (55), 69 (46), 111 (37)... 126 (2)]	0.79*	869.0	[0.01]	2.19	859.0	0.01
Unknown COCI II [m/z 55, 83 (79), 67 (65), 41 (63), 82 (60), 69 (58)... 111 (27), 126 (9)]	0.79*	869.0	[0.01]	2.21	860.3	0.01
Tricyclene	1.38	972.6	0.03	2.95	917.9	0.03
$\alpha$ -Thujene	1.57	999.2	0.01	3.06	925.3	0.01
$\alpha$ -Pinene	1.50	992.2	0.08	3.13	930.1	0.09
Camphene	1.86	1027.3	0.09	3.33	942.9	0.09
Sabinene	2.46	1084.8	0.02	3.74*	969.9	[0.02]
$\beta$ -Pinene	2.28	1066.9	0.01	3.74*	969.9	[0.02]
6-Methyl-5-hepten-2-one	5.29	1295.4	0.07	3.99	986.6	0.07
Myrcene	3.08	1133.5	0.07	4.07	992.2	0.07
$\alpha$ -Phellandrene	2.98	1126.5	0.02	4.21	1001.5	0.01
Octanal	4.66	1250.2	0.01	4.23	1002.8	0.01
$\Delta$ 3-Carene	2.78	1111.1	0.01	4.30	1006.9	0.01
$\alpha$ -Terpinene	3.17	1140.5	0.01	4.41	1013.9	0.01
para-Cymene	4.33	1227.0	0.01	4.53	1021.5	0.01
$\beta$ -Phellandrene	3.50	1165.9	0.05	4.62*	1026.9	[3.59]
Limonene	3.42	1159.6	3.60	4.62*	1026.9	[3.59]
Unknown COCI XLIV [m/z 59, 43 (12), 109 (11), 41 (10), 127 (8)...]	6.59*	1388.5	[0.03]	4.64	1028.4	0.04
(Z)- $\beta$ -Ocimene	4.00	1203.5	0.02	4.82	1039.6	0.02
(E)- $\beta$ -Ocimene	4.21	1218.1	0.02	4.98	1049.4	0.03
2,6-Dimethyl-5-heptenal (melonal)	5.51*	1311.6	[0.09]	5.03	1052.7	0.07
$\gamma$ -Terpinene	4.04	1205.9	0.02	5.09	1056.5	0.02
4-Nonanone	5.20	1289.5	0.02	5.35	1072.8	0.02

Octanol	8.44*	1525.7	[0.04]	5.41	1076.1	0.01
Terpinolene	4.52	1240.6	0.07	5.55	1085.3	0.07
Rosefuran	6.26	1364.5	0.01	5.73	1096.7	0.02
Linalool	8.29	1513.9	0.74	5.82	1101.8	0.71
Unknown COCI VII [m/z 111, 69 (70), 41 (68), 55 (53), 43 (51)... 154 (7)]	5.89	1338.4	0.01	5.93	1109.2	0.02
cis-Rose oxide	5.51*	1311.6	[0.09]	5.96	1110.7	0.01
trans-para-Mentha- 2,8-dien-1-ol	9.18	1583.0	0.01	6.08	1118.7	0.01
trans-Rose oxide	5.71	1325.5	0.01	6.18	1124.9	0.01
Melonol ?				6.32	1134.0	0.02
Unknown CYFL III [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43) ...]	7.13	1427.7	0.02	6.36*	1136.4	[0.04]
Unknown MEOF V [m/z 70, 81 (94), 67 (52), 69 (45), 109 (44), 82 (35) ...]	7.35*	1443.8	[41.64]	6.36*	1136.4	[0.04]
Isopulegol	8.39*	1521.6	[0.98]	6.45	1142.1	0.97
Menthone	6.89	1409.8	0.04	6.56	1149.0	0.05
Citronellal	7.35*	1443.8	[41.64]	6.73	1160.1	42.67
Borneol	10.01*	1649.3	[0.09]	6.77	1162.8	0.04
neoiso-Isopulegol	9.06	1573.3	0.05	6.84	1166.8	0.06
Isopulegol isomer	8.81*	1553.8	[0.05]	6.93	1172.8	0.03
Terpinen-4-ol	8.81*	1553.8	[0.05]	6.96*	1174.8	[0.05]
Rosefuran oxide	8.81*	1553.8	[0.05]	6.96*	1174.8	[0.05]
Isogeranial	8.44*	1525.7	[0.04]	7.09	1182.8	0.01
para-Cymen-8-ol	11.75	1794.0	tr	7.11	1184.1	tr
α-Terpineol	10.01*	1649.3	[0.09]	7.18	1188.5	0.08
(4Z)-Decenal	8.05*	1495.9	[0.06]	7.25	1193.5	0.04
(4E)-Decenal	8.05*	1495.9	[0.06]	7.29	1195.9	0.01
Decanal	7.56	1459.5	0.68	7.44	1205.3	0.13
2,3-Epoxyneral?				7.67	1220.6	0.02
Nerol	11.29	1754.8	0.21	7.79	1228.9	0.15
Citronellol	11.00*	1729.9	[11.14]	7.90	1236.3	10.98
Neral	9.70*	1624.1	[2.11]	7.94	1239.2	0.57
Piperitone	10.15*	1660.5	[0.09]	8.08	1248.2	0.02
Geraniol	11.90	1806.9	18.94	8.32	1264.0	18.54
Geranal	10.35	1676.2	0.75	8.42	1270.5	0.75
Citronellyl formate	9.15	1580.6	0.03	8.51	1276.6	0.02
Bornyl acetate	8.50	1530.2	0.01	8.58	1281.7	0.01
Geranyl formate	10.15*	1660.5	[0.09]	8.88	1301.9	0.02

Unknown CYSC II [m/z 135, 121 (81), 177 (78), 107 (60), 192 (42), 149 (35)]	6.59*	1388.5	[0.03]	9.01	1310.7	0.02
Citronellic acid				9.33*	1333.3	[0.30]
8-Hydroxy-neo- menthol	14.42*	2036.6	[0.10]	9.33*	1333.3	[0.30]
$\alpha$ -Terpinyl acetate	9.94	1643.7	0.01	9.52	1346.3	0.01
Citronellyl acetate	9.70*	1624.1	[2.11]	9.65*	1355.5	[2.46]
Eugenol	15.02	2094.6	0.87	9.65*	1355.5	[2.46]
Neryl acetate	10.43	1682.7	0.02	9.78	1364.9	0.03
$\alpha$ -Copaene	7.35*	1443.8	[41.64]	9.86	1370.9	0.04
$\beta$ -Bourbonene	7.77	1474.8	0.25	9.97	1378.6	0.09
cis- $\beta$ -Elemene	8.57	1535.9	0.05	10.01	1380.9	0.05
Geranyl acetate	10.81	1714.5	2.47	10.07	1385.0	2.37
$\beta$ -Elemene	8.71*	1546.8	[1.65]	10.12	1388.8	1.23
Methyleugenol	13.56	1955.4	0.01	10.32	1403.3	0.01
Dodecanal	10.25	1668.2	0.02	10.39	1408.1	0.01
$\beta$ -Caryophyllene	8.71*	1546.8	[1.65]	10.44*	1412.0	[0.43]
$\beta$ -Ylangene	8.39*	1521.6	[0.98]	10.44*	1412.0	[0.43]
$\beta$ -Copaene	8.65	1541.5	0.03	10.58	1422.4	0.03
trans- $\alpha$ - Bergamotene	8.71*	1546.8	[1.65]	10.72	1432.5	0.02
Isogermacrene D	9.26	1588.7	0.02	10.78	1437.5	0.02
$\alpha$ -Humulene	9.57	1613.3	0.17	10.90*	1445.9	[0.18]
(E)-Isoeugenol	16.74	2268.1	0.02	10.90*	1445.9	[0.18]
Methyl (Z)- isoeugenol	14.42*	2036.6	[0.10]	11.03	1456.0	0.05
(E)- $\beta$ -Farnesene	9.81	1632.7	0.01	11.07	1458.9	0.01
trans-Cadina-1(6),4- diene	9.53	1610.1	0.04	11.20	1468.0	0.04
$\gamma$ -Muurolene	9.88	1638.2	0.19	11.25	1471.8	0.16
Germacrene D	10.08*	1654.2	[1.78]	11.29	1474.7	1.71
$\beta$ -Selinene	10.15*	1660.5	[0.09]	11.34	1478.6	0.04
$\gamma$ -Amorphene	10.08*	1654.2	[1.78]	11.41	1483.6	0.05
$\alpha$ -Selinene	10.23	1666.4	0.04	11.48*	1489.0	[0.15]
epi-Cubebol	12.24	1836.6	0.09	11.48*	1489.0	[0.15]
Methyl (E)- isoeugenol	15.24	2115.9	0.02	11.56*	1495.5	[0.38]
$\alpha$ -Muurolene	10.32	1674.0	0.33	11.56*	1495.5	[0.38]
Germacrene A	10.69*†	1704.5	[0.47]	11.59	1497.2	0.48
$\gamma$ -Cadinene	10.67	1702.2	0.61	11.73*	1507.7	[0.70]
Cubebol	12.79	1885.5	0.09	11.73*	1507.7	[0.70]
trans-Calamenene	11.49	1771.4	tr	11.83	1516.0	0.02
$\delta$ -Cadinene	10.71*†	1706.2	[1.38]	11.87	1518.9	1.39

Unknown OCSA II [m/z 119, 105 (53), 161 (33), 93 (28), 91 (25), 40 (20)...204]	11.00*	1729.9	[11.14]	11.96	1526.3	0.05
$\alpha$ -Cadinene	11.08	1737.2	0.16	12.03	1531.6	0.10
$\alpha$ -Elemol	14.29	2023.9	1.96	12.21	1546.0	1.95
Germacrene B	11.41	1765.1	0.01	12.26	1549.3	0.01
Geranyl butyrate	12.41	1851.9	0.02	12.39	1559.6	0.02
(E)-Nerolidol	14.06	2002.2	0.02	12.44	1563.9	0.02
Germacrene D-4-ol	13.92	1989.0	1.01	12.51	1569.2	0.96
Caryophyllene oxide	13.04	1908.0	0.01	12.56	1572.7	0.02
Unknown PEFR I [m/z 107, 135 (87), 93 (51), 91 (38), 41 (35), 43 (31), 105 (23), 204 (20)]				12.89	1598.6	0.03
1,10-diepi-Cubenol	14.03	1999.2	0.04	12.99	1607.0	0.05
$\gamma$ -Eudesmol	15.14*	2106.4	[0.25]	13.20	1623.9	0.19
$\tau$ -Cadinol	15.14*	2106.4	[0.25]	13.34*	1635.5	[0.51]
Cubenol	13.97	1993.3	0.03	13.34*	1635.5	[0.51]
$\tau$ -Muurolol	15.30	2122.3	0.29	13.34*	1635.5	[0.51]
$\alpha$ -Muurolol	15.44	2135.6	0.09	13.40*	1641.1	[0.28]
$\beta$ -Eudesmol	15.65*	2156.6	[0.22]	13.40*	1641.1	[0.28]
$\alpha$ -Eudesmol	15.58*	2149.9	[0.17]	13.45	1644.7	0.19
$\alpha$ -Cadinol	15.73	2164.5	0.55	13.49	1648.1	0.54
(E)-Isoelemicin	17.33	2331.5	0.01	13.54	1652.3	0.01
Unknown CYWI V [suspected m/z 59, 93 (79), 161 (61), 107 (47), 81 (44), 121 (37)...]				13.62*	1658.9	[0.71]
7-epi- $\gamma$ -Eudesmol	15.65*	2156.6	[0.22]	13.62*	1658.9	[0.71]
(3Z)-Caryophylla-3,8(13)-dien-5 $\beta$ -ol	17.05*	2301.3	[0.09]	13.68	1664.3	0.01
(2Z,6Z)-Farnesol	16.29	2222.4	0.01	13.77	1671.1	tr
(2E,6Z)-Farnesal	15.58*	2149.9	[0.17]	14.23	1709.6	0.02
(2E,6E)-Farnesol	17.05*	2301.3	[0.09]	14.34	1719.0	0.08
(2E,6E)-Farnesal	16.08	2199.9	0.20	14.54	1736.9	0.02
Cryptomeridiol	20.05	2639.7	0.02	15.28	1800.3	0.02
Unknown COCI XXIX [m/z 81, 137 (70), 95 (46), 69 (45), 41 (39), 55 (29)...]	16.49	2242.8	0.01	17.36	1993.6	0.01
Unknown COCI XXX	17.16	2313.5	0.06	17.46	2002.9	0.06

[m/z 41, 69 (98), 55 (55), 81 (46), 109 (46)... 290 (8)]					
Unknown COCI LXIV [m/z 69, 41 (96), 55 (53), 109 (48), 95 (43), 67 (35)...]			17.70	2027.1	0.01
Unknown CYWI II [m/z 69, 81 (79), 81 (70), 137 (53), 139 (35), 95 (30)...]	21.96	2875.9	0.02	23.77	2706.5
Unknown CYWI III [m/z 69, 81 (84), 137 (53), 83 (30), 95 (27), 41 (19)...]	22.89	2998.4	0.07	24.22	2765.1
Unknown CYWI IV [m/z 69, 81 (64), 95 (29), 137 (19), 41 (19)...]	23.81	3123.8	0.08	24.66	2822.9
Total reported		98.24%		98.88%	

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

[xx]: Duplicate percentage due to coelutions, only the first one is 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