

Date : 2024-08-27

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24H13-NPA02

Customer Identification : Item: NP0380 - Cymbopogon flexuosus - Lot: NPS00169

Type : Essential Oil

Source : Cymbopogon flexuosus

Customer : Nature Packaged

Checked and approved by:

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

Notes: 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.

This report is an update from the first version issued on 2024-08-26 to format it for online publication.

GAS CHROMATOGRAPHIC ANALYSIS

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

✖ISO

Results : See analysis summary (next page)

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

Date : 2024-08-26

PHYSICOCHEMICAL DATA

Refractive index : 1.4861 ± 0.0003 (20 °C)

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

Analyst : Cassandra Baker

Date : 2024-08-13

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
Isobutyral	tr	Aliphatic aldehyde
2-Methyl-3-buten-2-ol	0.03	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Toluene	tr	Simple phenolic
Unknown	0.01	Unknown
Furfuryl alcohol	0.02	Furan
4-Heptanone	0.02	Aliphatic ketone
Unknown	0.01	Unknown
Tricyclene	0.16	Monoterpene
α -Pinene	0.22	Monoterpene
Camphene	1.19	Monoterpene
β -Pinene	0.03	Monoterpene
6-Methyl-5-hepten-2-one	1.82	Aliphatic ketone
Myrcene	0.11	Monoterpene
6-Methyl-5-hepten-2-ol	0.07	Aliphatic alcohol
α -Phellandrene	0.01	Monoterpene
Octanal	0.04	Aliphatic aldehyde
Δ^3 -Carene	0.02	Monoterpene
α -Terpinene	0.01	Monoterpene
<i>para</i> -Cymene	0.04	Monoterpene
1,8-Cineole	0.07	Monoterpenic ether
Limonene	0.71	Monoterpene
(<i>Z</i>)- β -Ocimene	0.33	Monoterpene
(<i>E</i>)- β -Ocimene	0.22	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.03	Aliphatic aldehyde
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
4-Nonanone	1.11	Aliphatic ketone
Octanol	0.02	Aliphatic alcohol
<i>trans</i> -Linalool oxide (fur.)	0.03	Monoterpenic alcohol
Terpinolene	0.07	Monoterpene
α -Pinene oxide	0.01	Monoterpenic ether
4-Nonanol	0.03	Aliphatic alcohol
Perillene	0.02	Monoterpenic ether
Rosefuran	0.13	Monoterpenic ether
Linalool	1.56	Monoterpenic alcohol
<i>cis</i> -Chrysanthemal?	0.03	Monoterpenic aldehyde
<i>trans-para</i> -Mentha-2,8-dien-1-ol	0.05	Monoterpenic alcohol

Unknown	0.17	Unknown
Unknown	0.03	Unknown
exo-Isocitral	0.04	Monoterpenic aldehyde
trans-Chrysanthemal	0.26	Monoterpenic aldehyde
Citronellal	0.24	Monoterpenic aldehyde
Borneol	0.16	Monoterpenic alcohol
Isoneral	0.30	Monoterpenic aldehyde
α -Phellandren-8-ol	0.10	Monoterpenic alcohol
Rosefuran oxide	0.12	Monoterpenic ether
Terpinen-4-ol	0.14	Monoterpenic alcohol
Unknown	0.26	Oxygenated monoterpene
Isogeraniol	0.62	Monoterpenic aldehyde
Unknown	0.02	Unknown
α -Terpineol	0.17	Monoterpenic alcohol
Myrtenal	0.07	Monoterpenic aldehyde
Myrtenol	0.02	Monoterpenic alcohol
trans-Isopiperitenol	0.06	Monoterpenic alcohol
Unknown	0.10	Oxygenated monoterpene
Decanal	0.11	Aliphatic aldehyde
cis-Isopiperitenol	0.07	Monoterpenic alcohol
2,3-Epoxyneral?	0.03	Monoterpenic aldehyde
Nerol	0.24	Monoterpenic alcohol
Citronellol	0.13	Monoterpenic alcohol
Neral	28.39	Monoterpenic aldehyde
(Z)-Isogeraniol	0.03	Monoterpenic alcohol
Piperitone	0.07	Monoterpenic ketone
Geraniol	7.21	Monoterpenic alcohol
Geranial	37.99	Monoterpenic aldehyde
Unknown	0.25	Oxygenated monoterpene
Bornyl acetate	0.04	Monoterpenic ester
2-Undecanone	0.01	Aliphatic ketone
Geranyl formate	0.02	Monoterpenic ester
Methyl nerate?	0.02	Monoterpenic ester
Methyl geranate	0.06	Monoterpenic ester
α -Cubebene	0.03	Sesquiterpene
Citronellyl acetate	0.06	Monoterpenic ester
Cyclosativene I	0.08	Sesquiterpene
Cyclosativene II	0.08	Sesquiterpene
Neryl acetate	0.03	Monoterpenic ester
α -Ylangene	0.06	Sesquiterpene
Geranic acid	0.11	Aliphatic acid
α -Copaene	0.03	Sesquiterpene
Unknown	0.06	Unknown
β -Bourbonene	0.05	Sesquiterpene
1,5-diepi- β -Bourbonene	0.01	Sesquiterpene

Geranyl acetate	4.16	Monoterpenic ester
β-Elemene	0.13	Sesquiterpene
β-Cubebene	tr	Sesquiterpene
β-Longipinene	0.02	Sesquiterpene
β-Ylangene	0.04	Sesquiterpene
β-Caryophyllene	1.49	Sesquiterpene
β-Copaene	0.03	Sesquiterpene
<i>trans</i> -α-Bergamotene	0.01	Sesquiterpene
6,9-Guaiadiene	0.01	Sesquiterpene
α-Humulene	0.14	Sesquiterpene
(<i>E</i>)-Isoeugenol	0.37	Phenylpropanoid
<i>cis</i> -Muurolo-4(15),5-diene	0.05	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.04	Sesquiterpene
Germacrene D	0.22	Sesquiterpene
γ-Amorphene	0.03	Sesquiterpene
epi-Cubebol	0.09	Sesquiterpenic alcohol
α-Muurolole	0.03	Sesquiterpene
δ-Amorphene	0.03	Sesquiterpene
γ-Cadinene	1.01	Sesquiterpene
Cubebol	0.18	Sesquiterpenic alcohol
Kessane	0.07	Sesquiterpenic ether
δ-Cadinene	0.22	Sesquiterpene
10-epi-Cubebol?	0.03	Sesquiterpenic alcohol
<i>trans</i> -Cadina-1,4-diene	0.02	Sesquiterpene
(<i>E</i>)-γ-Bisabolene	0.11	Sesquiterpene
Unknown	0.04	Unknown
Neryl butyrate	0.02	Monoterpenic ester
(<i>E</i>)-α-Bisabolene	0.05	Sesquiterpene
Germacrene B	0.04	Sesquiterpene
Geranyl butyrate	0.09	Monoterpenic ester
Caryophyllene oxide	0.38	Sesquiterpenic ether
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Humulene epoxide II	0.01	Sesquiterpenic ether
1,10-diepi-Cubenol	0.02	Sesquiterpenic alcohol
1-epi-Cubenol	0.03	Sesquiterpenic alcohol
γ-Eudesmol	0.01	Sesquiterpenic alcohol
Cubenol	0.02	Sesquiterpenic alcohol
τ-Muurolol	0.03	Sesquiterpenic alcohol
Unknown	0.01	Oxygenated sesquiterpene
(2 <i>Z</i> ,6 <i>Z</i>)-Farnesol	0.01	Sesquiterpenic alcohol
Farnesal isomer	0.01	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>E</i>)-Farnesal	0.01	Sesquiterpenic aldehyde
Neophytadiene	0.01	Diterpene
<i>meta</i> -Camphorene	0.02	Diterpene
<i>para</i> -Camphorene	0.01	Diterpene

Unknown	0.05	Unknown
Unknown	0.24	Unknown
Unknown	0.33	Unknown
Dicitral	0.16	Diterpenic aldehyde
Unknown	0.17	Unknown
Phytol	0.01	Diterpenic alcohol
Unknown	[0.83]	Unknown
Benzyl (<i>E</i>)-isoeugenol	[0.83]	Phenolic ester
Phytol isomer I	0.02	Diterpenic alcohol
Unknown	0.09	Unknown
Unknown	0.09	Unknown
Consolidated total	97.88	

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

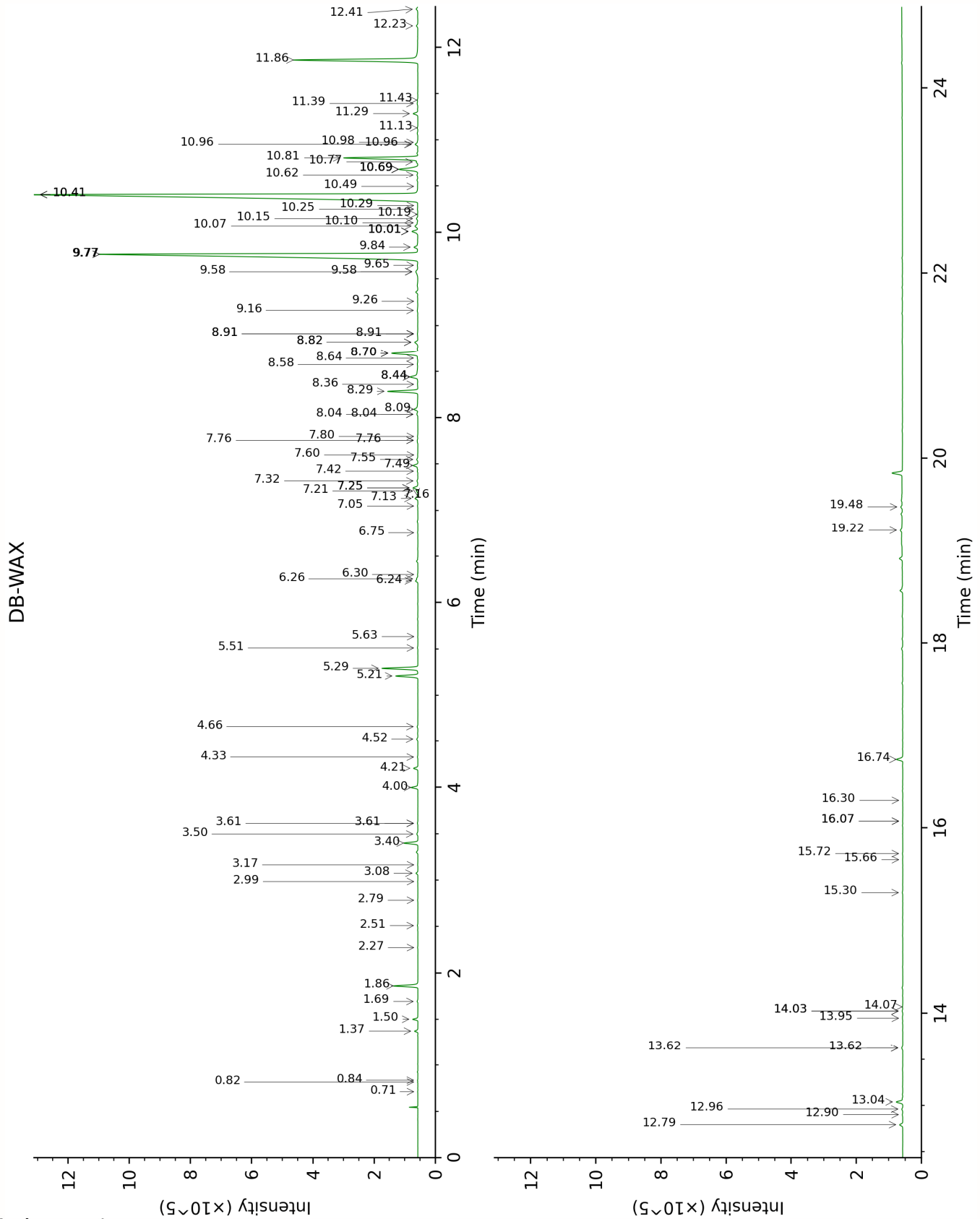
Note: no correction factor was applied

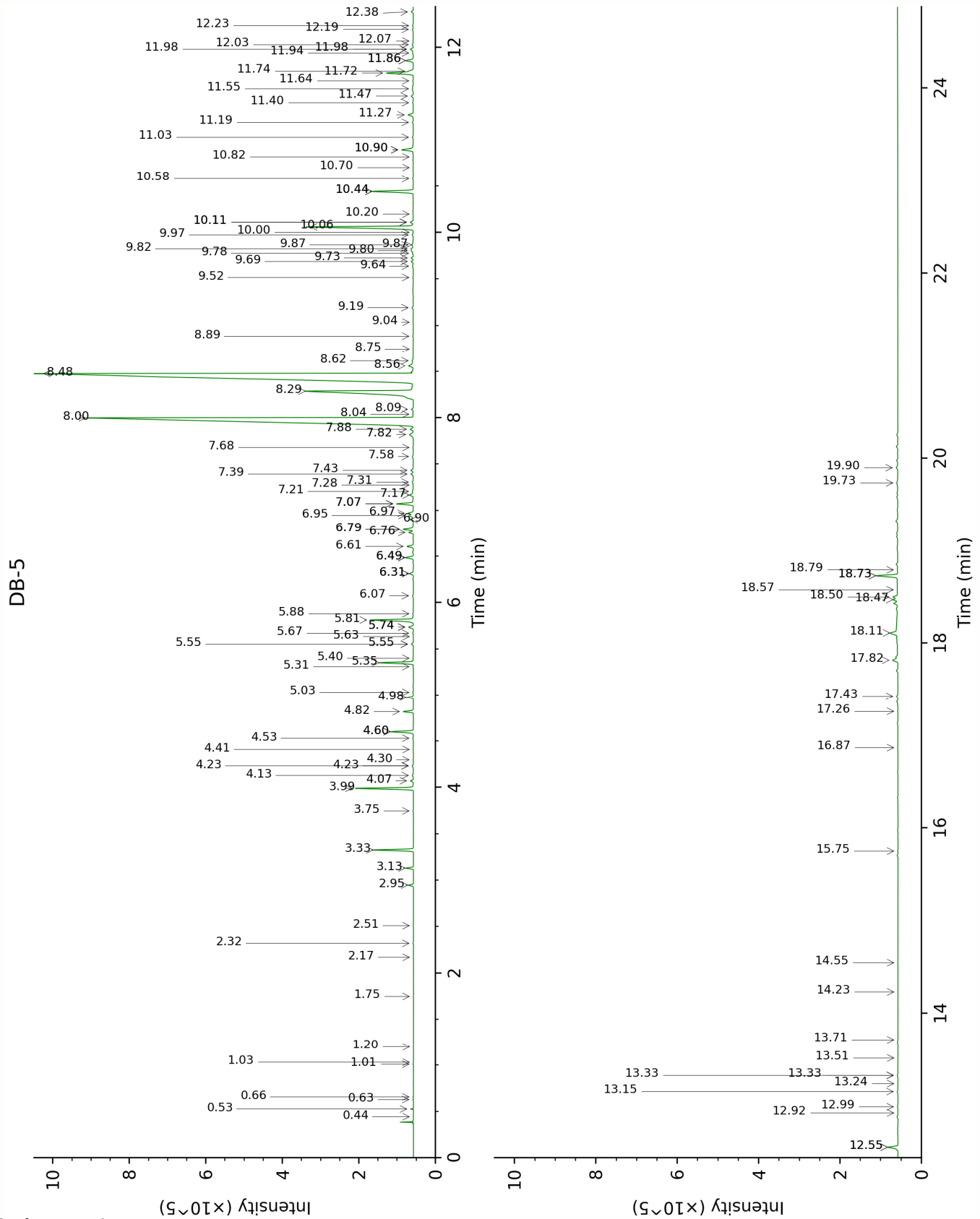
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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

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FULL ANALYSIS DATA

Isobutyral	Column DB-WAX			Column DB-5		
				0.44	535.9	tr
2-Methyl-3-buten-2-ol	1.69	1011.4	0.04	0.53	605.3	0.03
Isovaleral	0.84	884.8	0.01	0.63	640.5	0.01
2-Methylbutyral	0.82	878.0	0.01	0.66	650.6	0.01
Isoamyl alcohol	3.61*	1174.5	[0.03]	1.01	731.9	0.01
2-Methylbutanol	3.61*	1174.5	[0.03]	1.03	734.9	tr
Toluene				1.20	758.5	tr
Unknown PEGR III [m/z 81, 69 (80), 41 (65), 83 (52), 109 (48), 55 (47)...]	0.71	842.8	tr	1.75	822.3	0.01
Furfuryl alcohol	9.26	1588.8	0.02	2.17	857.2	0.02
4-Heptanone	2.51	1089.2	0.03	2.32	869.7	0.02
Unknown CULE I [m/z 69, 41 (57), 81 (57), 80 (18), 79 (18), 67 (17)...]				2.51	885.4	0.01
Tricyclene	1.37	972.5	0.14	2.95	918.0	0.16
α -Pinene	1.50	992.1	0.22	3.13	930.1	0.22
Camphene	1.86	1027.4	1.20	3.33	943.0	1.19
β -Pinene	2.28	1066.7	0.01	3.75	970.7	0.03
6-Methyl-5-hepten-2-one	5.29	1295.8	1.84	3.99	986.8	1.82
Myrcene	3.08	1133.5	0.09	4.07	992.2	0.11
6-Methyl-5-hepten-2-ol	7.21	1433.8	0.07	4.13	996.0	0.07
α -Phellandrene	2.99	1126.6	0.01	4.23*	1002.8	[0.07]
Octanal	4.66	1250.2	0.04	4.23*	1002.8	[0.07]
Δ^3 -Carene	2.78	1111.2	0.02	4.30	1006.9	0.02
α -Terpinene	3.17	1140.3	0.02	4.41	1013.8	0.01
<i>para</i> -Cymene	4.33	1226.8	0.03	4.53	1021.5	0.04
1,8-Cineole	3.50	1165.7	0.07	4.60*	1025.8	[0.76]
Limonene	3.40	1158.3	0.71	4.60*	1025.8	[0.76]
(Z)- β -Ocimene	4.00	1203.4	0.34	4.82	1039.4	0.33
(E)- β -Ocimene	4.21	1218.2	0.22	4.98	1049.2	0.22
2,6-Dimethyl-5-heptenal (melonal)	5.51	1311.4	0.03	5.03	1052.8	0.03
<i>cis</i> -Linalool oxide (fur.)	6.75	1400.1	0.02	5.31	1070.1	0.02
4-Nonanone	5.21	1289.8	1.16	5.35	1072.8	1.11

Octanol	8.44*	1525.7	[0.64]	5.40	1075.8	0.02
<i>trans</i> -Linalool oxide (fur.)	7.16	1430.0	0.03	5.55*	1085.3	[0.08]
Terpinolene	4.52	1240.6	0.07	5.55*	1085.3	[0.08]
α -Pinene oxide	5.63	1320.1	0.01	5.63	1090.4	0.01
4-Nonanol				5.67	1092.7	0.03
Perillene	6.30	1367.8	0.02	5.74*	1096.8	[0.20]
Rosefuran	6.24	1362.9	0.13	5.74*	1096.8	[0.20]
Linalool	8.29	1513.8	1.53	5.81	1101.6	1.56
<i>cis</i> -Chrysanthemal?	6.26	1364.5	0.08	5.88	1105.9	0.03
<i>trans-para</i> -Mentha-2,8-dien-1-ol	9.16	1581.3	0.06	6.07	1118.2	0.05
Unknown CYFL III [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	7.13	1427.9	0.17	6.31*	1133.5	[0.18]
Unknown CYFL IV [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	7.80	1477.1	0.03	6.31*	1133.5	[0.18]
<i>exo</i> -Isocitral	7.76*	1474.0	[0.06]	6.49*	1144.5	[0.31]
<i>trans</i> -Chrysanthemal	7.49	1454.1	0.26	6.49*	1144.5	[0.31]
Citronellal	7.24*	1436.3	[0.29]	6.61	1152.2	0.24
Borneol	10.01*	1649.0	[0.38]	6.76	1161.8	0.16
Isoneral	8.09	1498.9	0.30	6.79*	1164.0	[0.40]
α -Phellandren-8-ol	10.41*	1680.8	[38.73]	6.79*	1164.0	[0.40]
Rosefuran oxide	8.82*	1555.0	[0.21]	6.90	1171.1	0.12
Terpinen-4-ol	8.82*	1555.0	[0.21]	6.95*†	1173.8	[0.19]
Unknown CYFL V [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	9.84	1635.5	0.26	6.97*†	1175.4	[0.20]
Isogeranial	8.44*	1525.7	[0.64]	7.07*	1181.9	[0.64]
Unknown CYFL XIV [m/z 69, 41 (65), 109 (36), 67 (16), 84 (11), 43 (10), 55 (9)...]				7.07*	1181.9	[0.64]
α -Terpineol	10.01*	1649.0	[0.38]	7.17	1187.9	0.17

Myrtenal	8.91*	1562.0	[0.06]	7.21	1190.4	0.07
Myrtenol	11.13	1741.5	0.03	7.28	1194.8	0.02
<i>trans</i> - Isopiperitenol	10.69*	1703.9	[1.35]	7.31	1196.8	0.06
Unknown CYFL VI [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]	10.41*	1680.8	[38.73]	7.39	1202.3	0.10
Decanal	7.55	1458.8	0.07	7.43	1205.0	0.11
<i>cis</i> - Isopiperitenol	10.62	1698.7	0.07	7.58	1214.9	0.07
2,3-Epoxyneral?				7.68	1221.5	0.03
Nerol	11.29	1754.4	0.26	7.82	1230.8	0.24
Citronellol	10.96*	1726.6	[0.15]	7.88	1234.6	0.13
Neral	9.77*	1629.3	[28.80]	8.00	1242.8	28.39
(<i>Z</i>)-Isogeraniol	11.43	1766.7	0.03	8.04	1245.4	0.03
Piperitone	10.15	1660.0	0.09	8.09	1248.9	0.07
Geraniol	11.86	1803.7	7.61	8.29	1262.0	7.21
Geranial	10.41*	1680.8	[38.73]	8.48	1274.7	37.99
Unknown CYFL VII [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]				8.56	1280.2	0.25
Bornyl acetate	8.58	1536.1	0.05	8.62	1283.9	0.04
2-Undecanone	8.91*	1562.0	[0.06]	8.75	1292.7	0.01
Geranyl formate	10.19	1663.8	0.02	8.89	1302.0	0.02
Methyl nerate?				9.04	1312.5	0.02
Methyl geranate	10.01*	1649.0	[0.38]	9.19	1323.6	0.06
α -Cubebene	7.05	1421.9	0.02	9.52	1346.4	0.03
Citronellyl acetate	9.77*	1629.3	[28.80]	9.64	1354.9	0.06
Cyclosativene I				9.69	1358.5	0.08
Cyclosativene II	7.24*	1436.3	[0.29]	9.73	1361.2	0.08
Neryl acetate	10.49	1687.9	0.03	9.78	1364.6	0.03
α -Ylangene	7.32	1441.8	0.06	9.80*†	1366.7	[0.09]
Geranic acid				9.82*†	1368.0	[0.09]
α -Copaene	7.42	1449.5	0.03	9.87*	1371.0	[0.10]
Unknown ZIOF XI [m/z 81, 59 (94), 41 (74), 85 (40), 43 (55)...]	13.62*	1961.5	[0.08]	9.87*	1371.0	[0.10]
β -Bourbonene	7.76*	1474.0	[0.06]	9.97	1378.5	0.05

1,5-diepi- β -Bourbonene	7.60	1462.4	0.02	10.00	1380.5	0.01
Geranyl acetate	10.81	1714.3	4.21	10.06	1384.6	4.16
β -Elemene	8.70*	1545.5	[1.62]	10.11*	1388.1	[0.13]
β -Cubebene	8.04*	1494.7	[0.08]	10.11*	1388.1	[0.13]
β -Longipinene	8.04*	1494.7	[0.08]	10.20	1394.2	0.02
β -Ylangene	8.36	1519.6	0.04	10.44*	1412.0	[1.53]
β -Caryophyllene	8.70*	1545.5	[1.62]	10.44*	1412.0	[1.53]
β -Copaene	8.64	1541.4	0.04	10.58	1422.3	0.03
<i>trans</i> - α -Bergamotene	8.70*	1545.5	[1.62]	10.70	1431.5	0.01
6,9-Guaiadiene	8.91*	1562.0	[0.06]	10.82	1440.1	0.01
α -Humulene	9.58*	1614.2	[0.23]	10.90*	1445.8	[0.51]
(<i>E</i>)-Isoeugenol	16.74	2268.5	0.37	10.90*	1445.8	[0.51]
<i>cis</i> -Muurola-4(15),5-diene	9.65	1619.8	0.05	11.03	1455.8	0.05
<i>trans</i> -Cadina-1(6),4-diene	9.58*	1614.2	[0.23]	11.19	1467.7	0.04
Germacrene D	10.07	1653.6	0.22	11.27	1473.7	0.22
γ -Amorphene	10.10	1656.5	0.03	11.40	1483.5	0.03
epi-Cubebol	12.23	1836.0	0.09	11.48	1488.8	0.09
α -Muurolene	10.29	1671.3	0.02	11.55	1494.6	0.03
δ -Amorphene	10.25	1668.3	0.03	11.64	1501.0	0.03
γ -Cadinene	10.69*	1703.9	[1.35]	11.72*†	1507.5	[1.07]
Cubebol	12.79	1885.4	0.18	11.74*†	1509.0	[0.12]
Kessane	10.77	1710.6	0.07	11.86*	1518.1	[0.30]
δ -Cadinene	10.69*	1703.9	[1.35]	11.86*	1518.1	[0.30]
10-epi-Cubebol?	14.07	2003.3	0.02	11.94	1524.4	0.03
<i>trans</i> -Cadina-1,4-diene	10.98	1728.3	0.02	11.98*	1527.6	[0.13]
(<i>E</i>)- γ -Bisabolene	10.69*	1703.9	[1.35]	11.98*	1527.6	[0.13]
Unknown CYFL XV [m/z 85, 59 (82), 71 (58), 41 (36), 43 (34)...]				12.03	1531.4	0.04
Neryl butyrate				12.07	1534.6	0.02
(<i>E</i>)- α -Bisabolene	10.96*	1726.6	[0.15]	12.19	1544.4	0.05
Germacrene B	11.40	1763.6	0.06	12.23	1547.5	0.04
Geranyl butyrate	12.41	1852.1	0.11	12.38	1559.4	0.09
Caryophyllene oxide	13.04	1907.9	0.38	12.55*	1572.3	[0.43]
Caryophyllene oxide isomer	12.96	1900.8	0.06	12.55*	1572.3	[0.43]
Humulene epoxide II	13.62*	1961.5	[0.08]	12.92	1601.3	0.01

1,10-diepi-Cubenol	14.03*	1999.0	[0.04]	12.99	1606.8	0.02
1-epi-Cubenol	14.03*	1999.0	[0.04]	13.15	1620.2	0.03
γ-Eudesmol				13.24	1627.4	0.01
Cubenol	13.95	1991.6	0.02	13.33*	1634.7	[0.04]
τ-Muurolol	15.30	2122.5	0.03	13.33*	1634.7	[0.04]
Unknown JUVI XVI [m/z 43, 81 (84), 41 (64), 67 (62), 95 (58), 79 (58)... 204 (48), 220 (2)]	15.72	2164.4	0.02	13.51	1650.2	0.01
(2Z,6Z)-Farnesol	16.30	2222.8	0.01	13.72	1666.8	0.01
Farnesal isomer				14.23	1709.9	0.01
(2E,6E)-Farnesal	16.07*	2199.6	[0.02]	14.55	1737.2	0.01
Neophytadiene	12.90	1895.3	0.03	15.75	1843.2	0.01
meta-Camphorene	15.66	2157.8	0.02	16.87	1946.3	0.02
para-Camphorene	16.07*	2199.6	[0.02]	17.26	1983.5	0.01
Unknown LICU V [m/z 41, 69 (95), 109 (41), 95 (39), 55 (36), 121 (36)...]				17.42	1999.3	0.05
Unknown LICU VII [m/z 69, 41 (94), 81 (42), 109 (39), 107 (33), 43 (31)...]				17.82	2038.1	0.24
Unknown CYFL IX [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53), 109 (50)... 235 (10)...]				18.11	2067.1	0.33
Dicitral				18.47	2102.9	0.16
Unknown DRMO VI [m/z 69, 41 (37), 81 (23), 95 (19), 109 (18)...]	19.22	2541.7	0.10	18.50	2105.9	0.17
Phytol	19.48	2571.3	0.08	18.58	2113.9	0.01
Unknown LICU II [m/z 69, 41 (38), 151 (36), 123				18.73*	2129.6	[0.83]

(34), 82 (24), 43 (23), 109 (21)...				
Benzyl (E)- isoeugenol		18.73*	2129.6	[0.83]
Phytol isomer I		18.79	2136.2	0.02
Unknown CYFL XI [m/z 93, 69 (79), 43 (70), 137 (53), 41 (41), 119 (37)... 289 (33)...		19.74	2235.2	0.09
Unknown CYFL XII [m/z 123, 94 (100), 43 (86), 69 (75), 95 (47), 41 (47), 93 (45)...		19.90	2252.8	0.09
Total reported	96.76%		97.86%	

*: 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