Date : 2024-04-17

Certificate of Analysis - GC Profiling

Sample Identification

Internal code : 24D02-PTH04
Customer Identification : Organic Lemongrass - India - L90113R
Type : Essential Oil
Source : *Cymbopogon flexuosus*
Customer : Plant Therapy

Checked an 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

This report is an update from the first version issued on 2024-04-16 to correct a compound assignment.

Méthode certifiée ISO 17025:2017 Certified method

Laboratoire PhytoChemia

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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 : 2024-04-17

Physicochemical data

Refractive index : 1.4847 ± 0.0003 (20 °C)
Method : PC-MAT-016 - Measure of the refractive index of a liquid.
Analyst : Cindy Caron B. Sc.
Date : 2024-04-04

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
Isobutyral	tr	Aliphatic aldehyde
Methacrolein	tr	Aliphatic aldehyde
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
Hexanal	0.01	Aliphatic aldehyde
(3*Z*)-Hexenol	0.02	Aliphatic alcohol
4-Heptanone	0.01	Aliphatic ketone
Nonane	0.01	Alkane
Tricyclene	0.13	Monoterpene
α-Pinene	0.19	Monoterpene
Camphene	1.06	Monoterpene
β-Pinene	0.01	Monoterpene
Sabinene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	1.13	Aliphatic ketone
Myrcene	0.07	Monoterpene
6-Methyl-5-hepten-2-ol	0.07	Aliphatic alcohol
Octanal	0.08	Aliphatic aldehyde
para-Cymene	0.01	Monoterpene
1,8-Cineole	0.03	Monoterpenic ether
Limonene	0.25	Monoterpene
(*Z*)-β-Ocimene	0.29	Monoterpene
(*E*)-β-Ocimene	0.19	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.03	Aliphatic aldehyde
γ-Terpinene	0.01	Monoterpene
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
4-Nonanone	0.92	Aliphatic ketone
Octanol	0.02	Aliphatic alcohol
Terpinolene	0.04	Monoterpene
trans-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
4-Nonanol	0.03	Aliphatic alcohol
Rosefuran	0.21	Monoterpenic ether
Linalool	1.09	Monoterpenic alcohol
(*Z*)-6-Methyl-3,5-heptadien-2-one	0.04	Aliphatic ketone
trans-para-Mentha-2,8-dien-1-ol	0.03	Monoterpenic alcohol
Unknown	0.13	Unknown
Unknown	0.03	Unknown
trans-Chrysanthemal	0.27	Monoterpenic aldehyde
exo-Isocitral	0.07	Monoterpenic aldehyde
Citronellal	0.23	Monoterpenic aldehyde

Borneol	0.18	Monoterpenic alcohol
Isoneral	0.56	Monoterpenic aldehyde
α-Phellandren-8-ol	0.02	Monoterpenic alcohol
Rosefuran oxide	[0.23]	Monoterpenic ether
Terpinen-4-ol	[0.23]	Monoterpenic alcohol
Unknown	0.08	Oxygenated monoterpene
Isogeranial	0.98	Monoterpenic aldehyde
α-Terpineol	0.14	Monoterpenic alcohol
Unknown	0.06	Unknown
trans-Isopiperitenol	0.03	Monoterpenic alcohol
Unknown	0.04	Oxygenated monoterpene
Decanal	0.16	Aliphatic aldehyde
2,3-Epoxyneral?	0.04	Monoterpenic aldehyde
Nerol	0.18	Monoterpenic alcohol
Citronellol	0.10	Monoterpenic alcohol
Neral	30.92	Monoterpenic aldehyde
Piperitone	0.07	Monoterpenic ketone
Geraniol	6.28	Monoterpenic alcohol
Geranial	40.19	Monoterpenic aldehyde
Unknown	0.11	Oxygenated monoterpene
Bornyl acetate	0.02	Monoterpenic ester
Geranyl formate	0.05	Monoterpenic ester
Unknown	0.06	Unknown
α-Cubebene	0.02	Sesquiterpene
Citronellyl acetate	0.06	Monoterpenic ester
Cyclosativene I	0.08	Sesquiterpene
Cyclosativene II	0.08	Sesquiterpene
Neryl acetate	0.02	Monoterpenic ester
α-Ylangene	0.06	Sesquiterpene
Geranic acid	0.10	Aliphatic acid
α-Copaene	0.04	Sesquiterpene
β-Bourbonene	0.04	Sesquiterpene
β-Cubebene	0.07	Sesquiterpene
Geranyl acetate	3.47	Monoterpenic ester
β-Elemene	0.12	Sesquiterpene
Longifolene	0.01	Sesquiterpene
β-Caryophyllene	1.54	Sesquiterpene
β-Copaene	0.03	Sesquiterpene
trans-α-Bergamotene	0.02	Sesquiterpene
6,9-Guaiadiene	0.02	Sesquiterpene
α-Humulene	0.17	Sesquiterpene
(*E*)-Isoeugenol	0.48	Phenylpropanoid
cis-Muurola-4(15),5-diene	0.04	Sesquiterpene
trans-Cadina-1(6),4-diene	0.03	Sesquiterpene
Germacrene D	0.21	Sesquiterpene

γ-Amorphene	0.02	Sesquiterpene
epi-Cubebol	0.11	Sesquiterpenic alcohol
α-Muurolene	0.02	Sesquiterpene
Methyl (*E*)-isoeugenol	0.03	Phenylpropanoid
δ-Amorphene	0.06	Sesquiterpene
γ-Cadinene	1.03	Sesquiterpene
Cubebol	0.27	Sesquiterpenic alcohol
δ-Cadinene	0.26	Sesquiterpene
10-epi-Cubebol?	0.05	Sesquiterpenic alcohol
(*E*)-γ-Bisabolene	0.14	Sesquiterpene
α-Cadinene	0.12	Sesquiterpene
α-Elemol	0.07	Sesquiterpenic alcohol
Germacrene B	0.05	Sesquiterpene
Geranyl butyrate	0.08	Monoterpenic ester
Caryophyllene oxide	0.38	Sesquiterpenic ether
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Humulene epoxide II	0.05	Sesquiterpenic ether
Selin-6-en-4α-ol isomer	0.03	Sesquiterpenic alcohol
1-epi-Cubenol	0.03	Sesquiterpenic alcohol
Cubenol	0.03	Sesquiterpenic alcohol
Farnesal isomer	0.01	Sesquiterpenic aldehyde
(2*E*,6*E*)-Farnesal	0.01	Sesquiterpenic aldehyde
Neophytadiene	0.03	Diterpene
Unknown	0.01	Unknown
Unknown	0.03	Unknown
Unknown	0.04	Unknown
Unknown	0.01	Unknown
Dicitral	0.05	Diterpenic aldehyde
Linoleic acid	0.02	Aliphatic acid
Oleic acid	0.07	Aliphatic acid
Unknown	0.01	Unknown
Consolidated total	**97.16**	

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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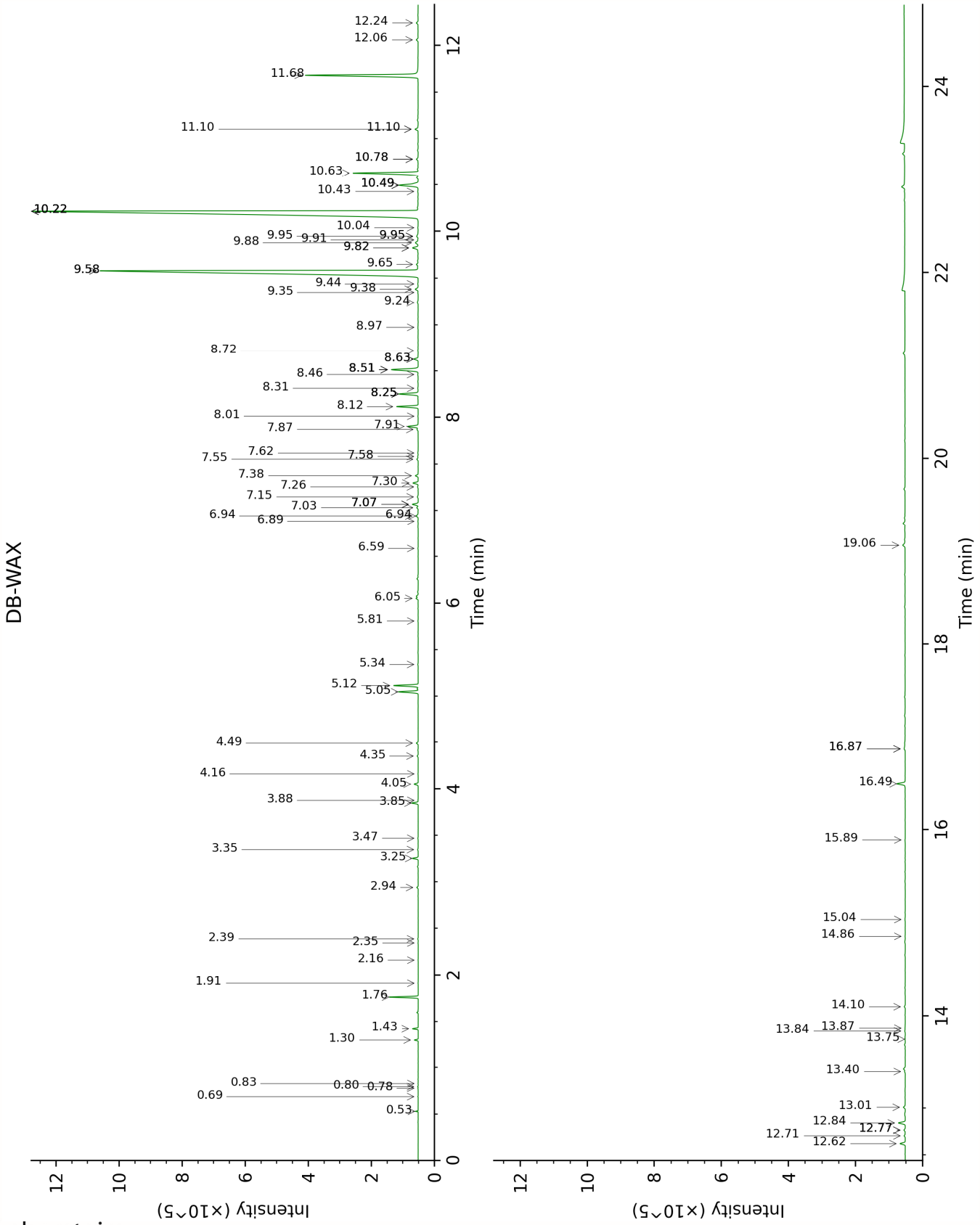
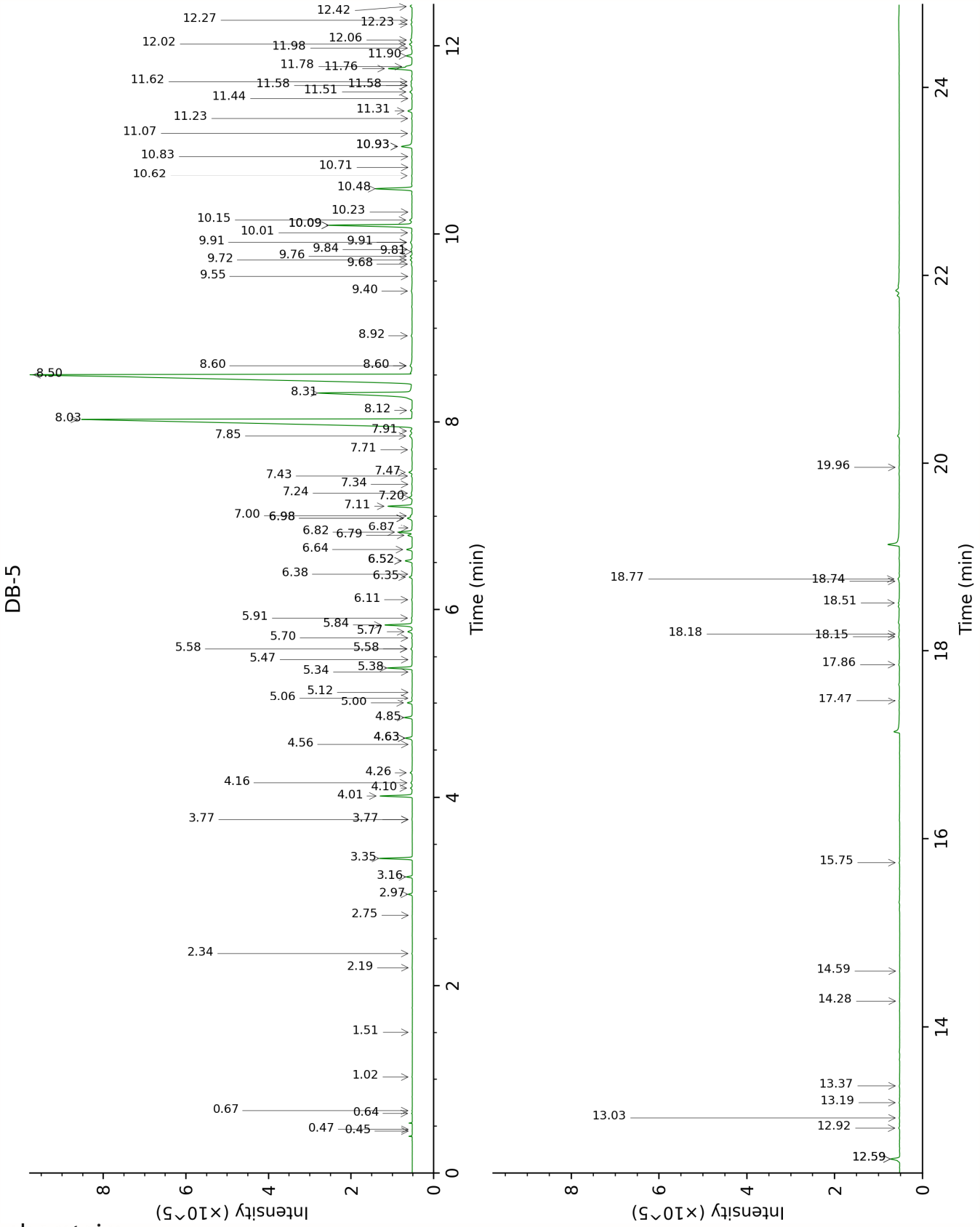

DB-WAX
Time (min)
Intensity (×10^5)
12.24
12.06
11.68
11.10
11.10
10.78
10.63
10.49
10.43
10.22
10.04
9.88
9.95
9.91
9.95
9.82
9.65
9.58
9.44
9.35
9.38
9.24
8.97
8.72
8.63
8.46
8.51
8.31
8.25
8.12
8.01
7.87
7.91
7.55
7.62
7.58
7.38
7.26
7.30
7.15
7.03
7.07
6.94
6.89
6.94
6.59
6.05
5.81
5.34
5.12
5.05
4.49
4.35
4.16
4.05
3.88
3.85
3.47
3.35
3.25
2.94
2.39
2.35
2.16
1.91
1.76
1.43
1.30
0.83
0.80
0.78
0.69
0.53
19.06
16.87
16.49
15.89
15.04
14.86
14.10
13.84
13.87
13.75
13.40
13.01
12.84
12.77
12.71
12.62


DB-5
Intensity (×10^5)
Time (min)
12.42
12.27
12.23
12.06
12.02
11.98
11.90
11.78
11.76
11.62
11.58
11.58
11.51
11.44
11.31
11.23
11.07
10.93
10.83
10.71
10.62
10.48
10.23
10.15
10.09
10.01
9.91
9.91
9.84
9.81
9.76
9.72
9.68
9.55
9.40
8.92
8.60
8.60
8.50
8.31
8.12
8.03
7.91
7.85
7.71
7.47
7.43
7.34
7.24
7.20
7.11
7.00
6.98
6.87
6.82
6.79
6.64
6.52
6.38
6.35
6.11
5.91
5.84
5.77
5.70
5.58
5.58
5.47
5.38
5.34
5.12
5.06
5.00
4.85
4.63
4.56
4.26
4.16
4.10
4.01
3.77
3.77
3.35
3.16
2.97
2.75
2.34
2.19
1.51
1.02
0.67
0.64
0.47
0.45
19.96
18.77
18.74
18.51
18.18
18.15
17.86
17.47
15.75
14.59
14.28
13.37
13.19
13.03
12.92
12.59

FULL ANALYSIS DATA

	Column DB-WAX			Column DB-5		
Isobutyral	0.53	776.6	0.05	0.45	533.3	tr
Methacrolein	0.69	848.7	0.01	0.47	548.4	tr
Isovaleral	0.80	884.0	0.01	0.64	639.4	0.01
2-Methylbutyral	0.78	878.5	0.01	0.67	649.4	0.01
Isoamyl alcohol	3.47	1174.5	0.02	1.02	732.0	0.01
Hexanal	1.91	1044.6	0.01	1.51	798.4	0.01
(3*Z*)-Hexenol	5.81	1343.5	0.01	2.19	857.7	0.02
4-Heptanone	2.39	1089.2	0.02	2.34	870.1	0.01
Nonane	0.83	895.0	tr	2.75	903.4	0.01
Tricyclene	1.30	974.7	0.13	2.97	918.6	0.13
α-Pinene	1.42	992.8	0.19	3.16	930.7	0.19
Camphene	1.76	1030.7	1.05	3.35	943.7	1.06
β-Pinene	2.16	1067.8	0.01	3.76*	970.9	[0.02]
Sabinene	2.35	1085.2	0.01	3.76*	970.9	[0.02]
6-Methyl-5-hepten-2-one	5.12	1293.7	1.13	4.02	987.3	1.13
Myrcene	2.94	1134.5	0.06	4.10	992.9	0.07
6-Methyl-5-hepten-2-ol	7.03	1432.9	0.08	4.16	996.6	0.07
Octanal	4.49	1249.2	0.08	4.26	1003.6	0.08
para-Cymene	4.16	1225.6	0.01	4.56	1022.5	0.01
1,8-Cineole	3.35	1165.3	0.03	4.63*	1026.7	[0.28]
Limonene	3.25	1158.2	0.25	4.63*	1026.7	[0.28]
(*Z*)-β-Ocimene	3.85	1203.1	0.28	4.85	1040.4	0.29
(*E*)-β-Ocimene	4.05	1217.8	0.18	5.00	1050.2	0.19
2,6-Dimethyl-5-heptenal (melonal)	5.34	1309.9	0.02	5.06	1053.7	0.03
γ-Terpinene	3.88	1205.3	0.01	5.12	1057.6	0.01
cis-Linalool oxide (fur.)	6.59	1399.9	0.01	5.34	1071.1	0.02
4-Nonanone	5.05	1288.9	0.94	5.38	1073.8	0.92
Octanol	8.25*	1525.5	[0.96]	5.47	1079.3	0.02
Terpinolene	4.35	1239.3	0.04	5.58*	1086.5	[0.06]
trans-Linalool oxide (fur.)	6.94*	1426.2	[0.14]	5.58*	1086.5	[0.06]
4-Nonanol				5.70	1093.7	0.03
Rosefuran	6.05†	1361.1	0.11	5.77	1097.9	0.21
Linalool	8.12	1514.8	1.01	5.84	1102.4	1.09
(*Z*)-6-Methyl-3,5-heptadien-2-one	8.25*	1525.5	[0.96]	5.91	1107.0	0.04
trans-para-Mentha-2,8-	8.98	1582.5	0.02	6.11	1119.4	0.03

dien-1-ol						
Unknown CYFL III [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	6.94*	1426.2	[0.14]	6.35	1134.7	0.13
Unknown CYFL IV [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	7.62	1477.1	0.03	6.38	1136.7	0.03
trans-Chrysanthemal	7.30	1452.8	0.27	6.52*	1145.8	[0.31]
exo-Isocitral	7.55	1472.0	0.07	6.52*	1145.8	[0.31]
Citronellal	7.07*	1435.6	[0.30]	6.64	1153.4	0.23
Borneol	9.82*	1651.6	[0.34]	6.79	1163.0	0.18
Isoneral	7.90	1498.5	0.53	6.82	1165.2	0.56
α-Phellandren-8-ol	10.22*	1684.2	[39.96]	6.87	1168.1	0.02
Rosefuran oxide	8.63*	1555.1	[0.23]	6.98*	1175.1	[0.23]
Terpinen-4-ol	8.63*	1555.1	[0.23]	6.98*	1175.1	[0.23]
Unknown CYFL V [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	9.65	1636.9	0.09	7.00	1176.7	0.08
Isogeranial	8.25*	1525.5	[0.96]	7.11	1183.3	0.98
α-Terpineol	9.82*	1651.6	[0.34]	7.20	1189.2	0.14
Unknown DRMO III [m/z 43, 81 (47), 67 (45), 69 944), 41 (42), 59 (40), 55 (39)...]	9.24	1603.3	0.05	7.24	1192.0	0.06
trans-Isopiperitenol	10.43	1701.8	0.03	7.34	1198.1	0.03
Unknown CYFL VI [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]	10.22*	1684.2	[39.96]	7.43	1203.7	0.04
Decanal	7.38	1458.7	0.14	7.47	1206.3	0.16
2,3-Epoxyneral?				7.71	1222.3	0.04
Nerol	11.10*	1760.3	[0.17]	7.85	1232.1	0.18
Citronellol	10.78*	1732.1	[0.10]	7.90	1235.6	0.10

Neral	9.58*	1631.2	[30.69]	8.03	1243.8	30.92
Piperitone	9.95*	1661.8	[0.11]	8.12	1250.2	0.07
Geraniol	11.68	1801.1	6.52	8.31	1262.6	6.28
Geranial	10.22*	1684.2	[39.96]	8.50	1275.6	40.19
Unknown CYFL VII [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	13.01	1922.8	0.11	8.60*	1281.9	[0.19]
Bornyl acetate	8.31	1530.3	0.02	8.60*	1281.9	[0.19]
Geranyl formate	9.95*	1661.8	[0.11]	8.92	1303.7	0.05
Unknown CYFL VIII [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	12.77*	1899.8	[0.08]	9.40	1337.0	0.06
α-Cubebene	6.89	1421.9	0.02	9.55	1347.8	0.02
Citronellyl acetate	9.58*	1631.2	[30.69]	9.68	1357.0	0.06
Cyclosativene I	7.07*	1435.6	[0.30]	9.72	1360.1	0.08
Cyclosativene II	7.07*	1435.6	[0.30]	9.76	1362.9	0.08
Neryl acetate	10.22*	1684.2	[39.96]	9.81	1366.2	0.02
α-Ylangene	7.15	1441.6	0.05	9.84	1367.9	0.06
Geranic acid	16.87*	2309.0	[0.15]	9.91*	1373.2	[0.14]
α-Copaene	7.26	1449.7	0.04	9.91*	1373.2	[0.14]
β-Bourbonene	7.58	1474.3	0.03	10.01	1380.4	0.04
β-Cubebene	7.87	1496.1	0.07	10.09*	1386.0	[3.53]
Geranyl acetate	10.63	1719.0	3.47	10.09*	1386.0	[3.53]
β-Elemene	8.51*	1546.1	[1.58]	10.15	1389.9	0.12
Longifolene	8.01	1506.8	0.01	10.23	1395.8	0.01
β-Caryophyllene	8.51*	1546.1	[1.58]	10.48	1413.7	1.54
β-Copaene	8.46	1542.0	0.02	10.62	1424.2	0.03
trans-α-Bergamotene	8.51*	1546.1	[1.58]	10.71	1431.0	0.02
6,9-Guaiadiene	8.72	1562.5	0.02	10.83	1439.5	0.02
α-Humulene	9.38	1614.9	0.17	10.93*	1447.5	[0.58]
(*E*)-Isoeugenol	16.49	2269.4	0.48	10.93*	1447.5	[0.58]
cis-Muurola-4(15),5-diene	9.44	1619.6	0.02	11.07	1457.8	0.04
trans-Cadina-1(6),4-diene	9.35	1612.0	0.02	11.23	1469.7	0.03
Germacrene D	9.88	1656.2	0.19	11.31	1475.6	0.21
γ-Amorphene	9.91	1658.7	0.02	11.44	1485.5	0.02
epi-Cubebol	12.06	1835.6	0.10	11.51	1490.7	0.11
α-Muurolene	10.04	1669.5	0.02	11.58*	1495.8	[0.09]
Methyl (*E*)-	15.04	2118.8	0.03	11.58*	1495.8	[0.09]

isoeugenol						
δ-Amorphene	9.95*	1661.8	[0.11]	11.62	1498.8	0.06
γ-Cadinene	10.50*	1707.4	[1.31]	11.76*†	1509.3	[1.09]
Cubebol	12.62	1886.6	0.27	11.78*†	1510.9	[0.21]
δ-Cadinene	10.50*	1707.4	[1.31]	11.90	1519.9	0.26
10-epi-Cubebol?	13.84	2001.3	0.04	11.98	1526.4	0.05
(*E*)-γ-Bisabolene	10.50*	1707.4	[1.31]	12.02	1529.6	0.14
α-Cadinene	10.78*	1732.1	[0.10]	12.06	1533.1	0.12
α-Elemol	14.10	2026.5	0.05	12.23	1546.3	0.07
Germacrene B	11.10*	1760.3	[0.17]	12.27	1549.6	0.05
Geranyl butyrate	12.24	1852.2	0.10	12.42	1561.3	0.08
Caryophyllene oxide	12.84	1906.9	0.38	12.59*	1574.4	[0.44]
Caryophyllene oxide isomer	12.77*	1899.8	[0.08]	12.59*	1574.4	[0.44]
Humulene epoxide II	13.40	1959.3	0.04	12.92	1600.1	0.05
Selin-6-en-4α-ol isomer	14.86	2100.8	0.02	13.03	1608.8	0.03
1-epi-Cubenol	13.87	2004.1	0.02	13.19	1622.2	0.03
Cubenol	13.75	1993.0	0.01	13.37	1636.9	0.03
Farnesal isomer				14.28	1712.2	0.01
(2*E*,6*E*)-Farnesal	15.89	2206.0	0.02	14.59	1739.8	0.01
Neophytadiene	12.70	1894.3	0.06	15.75	1841.4	0.03
Unknown LICU V [m/z 41, 69 (95), 109 (41), 95 (39), 55 (36), 121 (36)...]				17.47	2002.0	0.01
Unknown LICU VII [m/z 69, 41 (94), 81 (42), 109 (39), 107 (33), 43 (31)...]				17.86	2040.5	0.03
Unknown CYFL IX [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53), 109 (50)... 235 (10)...]				18.15	2070.0	0.04
Unknown LIMU XXI [m/z 57, 85 (55), 163 (47), 41 (44), 120 (35), 202 (30), 145	19.06	2554.0	0.19	18.18	2072.8	0.01

(25)... 219 (17), 304 (t)]						
Dicitral	16.87*	2309.0	[0.15]	18.51	2105.5	0.05
Linoleic acid				18.74	2129.3	0.02
Oleic acid				18.76	2131.8	0.07
Unknown CYFL XII [m/z 123, 94 (100), 43 (86), 69 (75), 95 (47), 41 (47), 93 (45)...]				19.96	2257.5	0.01
Total reported		95.79%			97.17%	

*: 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