Date : June 07, 2019

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 19E28-PTH05-1-SCC
Customer identification : Ylang Ylang Complete - Madagascar - Y1010994R
Type : Essential oil
Source : *Cananga odorata* var. *genuina (Ylang-ylang)*
Customer : Plant Therapy

Analysis

Method: PC-PA-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 : Benoit Roger, Ph. D.
Analysis date : June 04, 2019

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Yellow liquid
Refractive index: 1.5072 ± 0.0003 (20 °C)

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	%	Classe
Toluene	tr	Simple phenolic
Prenol	tr	Aliphatic alcohol
Butyl acetate	tr	Aliphatic ester
Isoamyl acetate	tr	Aliphatic ester
2-Methylbutyl acetate	tr	Aliphatic ester
3-Methyl-3-butenyl acetate	0.05	Aliphatic ester
Prenyl acetate	0.11	Aliphatic ester
α-Pinene	0.07	Monoterpene
Benzaldehyde	tr	Simple phenolic
β-Pinene	0.02	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.02	Monoterpene
(3*Z*)-Hexenyl acetate	0.01	Aliphatic ester
para-Methylanisole	2.14	Simple phenolic
Hexyl acetate	0.01	Aliphatic ester
Limonene	0.01	Monoterpene
1,8-Cineole	0.02	Monoterpenic ether
Benzyl alcohol	0.02	Simple phenolic
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Terpinolene	0.01	Monoterpene
trans-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Methyl benzoate	1.20	Phenolic ester
para-Cresol	0.14	Simple phenolic
Linalool	2.70	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
ortho-Dimethoxybenzene	0.02	Simple phenolic
Benzyl acetate	4.12	Phenolic ester
Ethyl benzoate	0.01	Phenolic ester
para-Cresyl acetate	0.01	Phenolic ester
Methyl salicylate	0.01	Phenolic ester
α-Terpineol	0.01	Monoterpenic alcohol
Nerol	0.01	Monoterpenic alcohol
Phenylethyl acetate	0.01	Phenolic ester
Geraniol	0.52	Monoterpenic alcohol
(*E*)-Anethole	0.05	Phenylpropanoid
1-Nitro-2-phenylethane	0.02	Simple phenolic
δ-Elemene	0.08	Sesquiterpene
Bicycloelemene	tr	Sesquiterpene
Benzyl butyrate	0.01	Phenolic ester
α-Cubebene	0.17	Sesquiterpene
Eugenol	0.01	Phenylpropanoid
Neryl acetate	0.03	Monoterpenic ester
α-Ylangene	0.12	Sesquiterpene
α-Copaene	1.26	Sesquiterpene
β-Bourbonene	0.01	Sesquiterpene
Geranyl acetate	3.31	Monoterpenic ester
β-Cubebene	0.37	Sesquiterpene

β-Elemene	0.06	Sesquiterpene
Methyleugenol	0.02	Phenylpropanoid
β-Caryophyllene	7.26	Sesquiterpene
Caryophylla-4(12),8(13)-diene	0.03	Sesquiterpene
β-Copaene	0.26	Sesquiterpene
Aromadendrene	0.06	Sesquiterpene
(*E*)-Cinnamyl acetate	2.48	Phenylpropanoid ester
Isogermacrene D	0.07	Sesquiterpene
9-epi-Isocaryophyllene	0.05	Sesquiterpene
(*E*)-Isoeugenol	0.67	Phenylpropanoid
trans-Muurola-3,5-diene	0.12	Sesquiterpene
α-Humulene	1.88	Sesquiterpene
cis-Cadina-1(6),4-diene	0.07	Sesquiterpene
cis-Muurola-4(15),5-diene	0.14	Sesquiterpene
trans-Cadina-1(6),4-diene	0.14	Sesquiterpene
Germacrene D	22.25	Sesquiterpene
γ-Muurolene	1.33	Sesquiterpene
trans-Muurola-4(15),5-diene	0.16	Sesquiterpene
γ-Amorphene	0.21	Sesquiterpene
Prenyl benzoate	0.09	Phenolic ester
epi-Cubebol	0.05	Sesquiterpenic alcohol
Bicyclogermacrene	0.86	Sesquiterpene
(3*Z*,6*E*)-α-Farnesene	0.06	Sesquiterpene
α-Muurolene	0.69	Sesquiterpene
δ-Amorphene	0.28	Sesquiterpene
Unknown	tr	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	18.81	Sesquiterpene
Cubebol	0.04	Sesquiterpenic alcohol
γ-Cadinene	0.70	Sesquiterpene
(*Z*)-γ-Bisabolene	0.04	Sesquiterpene
trans-Calamenene	0.03	Sesquiterpene
δ-Cadinene	2.35*	Sesquiterpene
Zonarene	[2.35]*	Sesquiterpene
trans-Cadina-1,4-diene	0.15	Sesquiterpene
α-Cadinene	0.22	Sesquiterpene
α-Calacorene	0.03	Sesquiterpene
cis-Dracunculifoliol	0.04	Sesquiterpenic alcohol
α-Elemol	0.08	Sesquiterpenic alcohol
Germacrene B	0.01	Sesquiterpene
β-Calacorene	0.09	Sesquiterpene
(*E*)-Nerolidol	0.05	Sesquiterpenic alcohol
(3*Z*)-Hexenyl benzoate	0.03	Phenolic ester
Spathulenol	0.10	Sesquiterpenic alcohol
Caryophyllene oxide	0.07	Sesquiterpenic ether
10-epi-Junenol	0.08	Sesquiterpenic alcohol
Unknown	0.03	Sesquiterpenic alcohol
Unknown	0.06	Oxygenated sesquiterpene
Viridiflorol	0.05	Sesquiterpenic alcohol
Guaiol	0.15	Sesquiterpenic alcohol
Copaborneol	0.03	Sesquiterpenic alcohol
Humulene epoxide II	0.04	Sesquiterpenic ether
10-epi-Cubenol	0.28	Sesquiterpenic alcohol

(*E*)-Isoeugenyl acetate	0.05	Phenylpropanoid ester
Junenol	0.20	Sesquiterpenic alcohol
1-epi-Cubenol	0.09	Sesquiterpenic alcohol
τ-Cadinol	0.40	Sesquiterpenic alcohol
τ-Muurolol	0.66	Sesquiterpenic alcohol
Cubenol	0.14	Sesquiterpenic alcohol
α-Muurolol	0.21	Sesquiterpenic alcohol
α-Cadinol	1.26	Sesquiterpenic alcohol
trans-Calamenen-10-ol	0.14	Sesquiterpenic alcohol
Unknown	0.11	Oxygenated sesquiterpene
(2*E*,6*Z*)-Farnesol	0.01	Sesquiterpenic alcohol
(2*E*,6*E*)-Farnesol	1.54	Sesquiterpenic alcohol
(2*E*,6*E*)-Farnesal	0.01	Sesquiterpenic aldehyde
Benzyl benzoate	5.72	Phenolic ester
(2*E*,6*E*)-Farnesyl acetate	4.02	Sesquiterpenic ester
Benzyl salicylate	3.44	Phenolic ester
Geranyl benzoate	0.01	Phenolic ester
Unknown	0.17	Sesquiterpenic alcohol
Consolidated total	**97.79%**	

*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
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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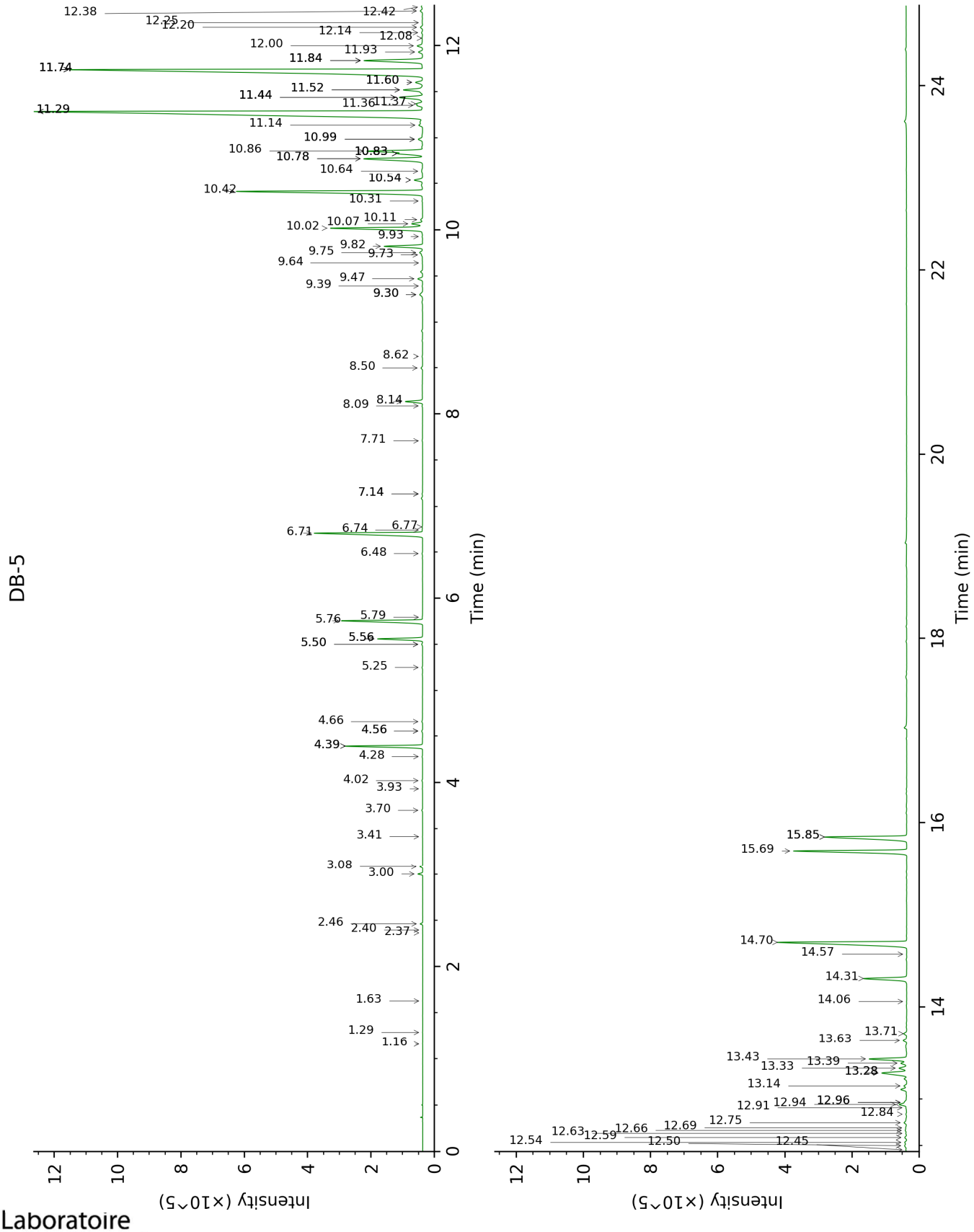
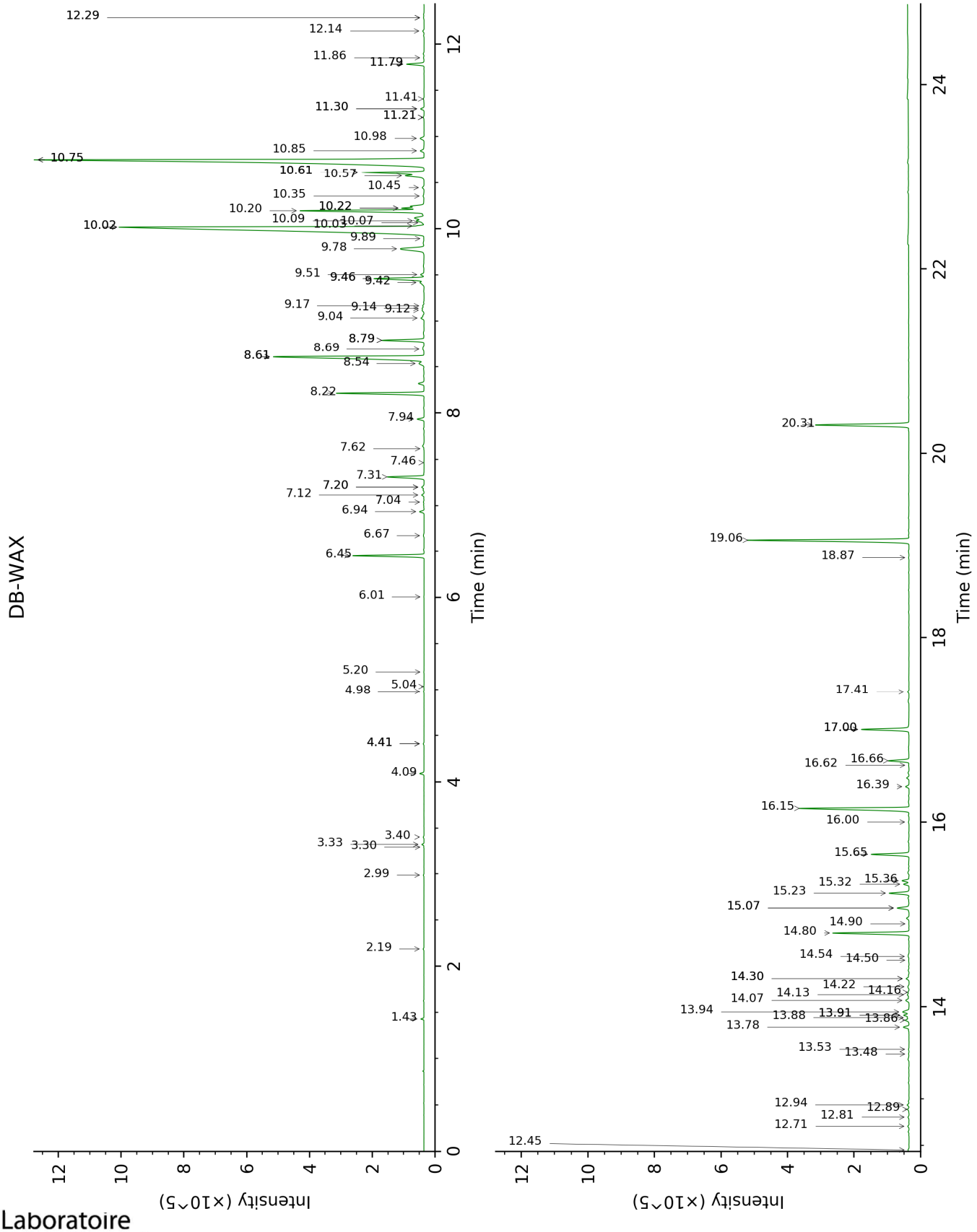

DB-5
Time (min)
Intensity (×10^5)
12.38
12.42
12.25
12.20
12.14
12.08
12.00
11.93
11.84
11.74
11.60
11.52
11.44
11.36
11.37
11.29
11.14
10.99
10.86
10.83
10.78
10.64
10.54
10.42
10.31
10.11
10.07
10.02
9.93
9.82
9.75
9.73
9.64
9.47
9.39
9.30
8.62
8.50
8.14
8.09
7.71
7.14
6.77
6.74
6.71
6.48
5.79
5.76
5.56
5.50
5.25
4.66
4.56
4.39
4.28
4.02
3.93
3.70
3.41
3.08
3.00
2.46
2.40
2.37
1.63
1.29
1.16
15.85
15.69
14.70
14.57
14.31
14.06
13.71
13.63
13.43
13.39
13.33
13.28
13.14
12.96
12.94
12.91
12.84
12.75
12.69
12.66
12.63
12.59
12.54
12.50
12.45


DB-WAX
12.29
12.14
11.86
11.79
11.41
11.30
11.21
10.98
10.85
10.75
10.61
10.57
10.45
10.35
10.22
10.20
10.09
10.07
10.02
9.89
9.78
9.51
9.46
9.42
9.17
9.14
9.12
9.04
8.79
8.69
8.61
8.54
8.22
7.94
7.62
7.46
7.31
7.20
7.12
7.04
6.94
6.67
6.45
6.01
5.20
5.04
4.98
4.41
4.09
3.40
3.33
3.30
2.99
2.19
1.43
Time (min)
Intensity (×10^5)
20.31
19.06
18.87
17.41
17.00
16.66
16.62
16.39
16.15
16.00
15.65
15.36
15.32
15.23
15.07
14.90
14.80
14.54
14.50
14.30
14.22
14.16
14.13
14.07
13.94
13.91
13.88
13.86
13.78
13.53
13.48
12.94
12.89
12.81
12.71
12.45
Time (min)
Intensity (×10^5)

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Toluene	1.16	759	tr			
Prenol	1.29	777	tr	5.04	1290	0.01
Butyl acetate	1.63	816	tr			
Isoamyl acetate	2.37	876	tr			
2-Methylbutyl acetate	2.40	878	tr			
3-Methyl-3-butenyl acetate	2.46	884	0.05	3.33	1160	0.05
Prenyl acetate	3.00	923	0.11	4.09	1220	0.12
α-Pinene	3.08	928	0.07	1.43	992	0.06
Benzaldehyde	3.41	950	tr	7.46	1458	0.01
β-Pinene	3.70	968	0.02	2.19	1066	0.02
6-Methyl-5-hepten-2-one	3.93	984	0.01	5.20	1302	0.01
Myrcene	4.02	989	0.02	2.99	1134	0.01
(3*Z*)-Hexenyl acetate	4.28	1006	0.01	4.98	1286	0.01
para-Methylanisole	4.39*	1013	2.21	6.45	1383	2.14
Hexyl acetate	4.39*	1013	[2.21]	4.41*	1243	0.02
Limonene	4.56*	1024	0.03	3.30	1158	0.01
1,8-Cineole	4.56*	1024	[0.03]	3.40	1167	0.02
Benzyl alcohol	4.66	1030	0.02	11.86	1814	0.03
cis-Linalool oxide (fur.)	5.25	1067	0.02	6.67	1399	0.03
Terpinolene	5.50*	1083	0.03	4.41*	1243	[0.02]
trans-Linalool oxide (fur.)	5.50*	1083	[0.03]	7.04	1427	0.02
Methyl benzoate	5.56*	1087	1.34	8.80*	1561	1.34
para-Cresol	5.56*	1087	[1.34]	14.07	2016	0.14
Linalool	5.76	1099	2.70	8.22	1516	2.69
Nonanal	5.80	1101	0.02	6.01	1351	0.01
ortho-Dimethoxybenzene	6.48	1146	0.02			
Benzyl acetate	6.70	1160	4.12	10.20	1673	4.29
Ethyl benzoate	6.74	1162	0.01	9.46*	1613	1.79
para-Cresyl acetate	6.77	1164	0.01			
Methyl salicylate	7.14*	1188	0.02	10.61*	1708	2.24
α-Terpineol	7.14*	1188	[0.02]	9.89	1649	0.01
Nerol	7.71	1226	0.01	11.21*	1758	0.03
Phenylethyl acetate	8.09	1252	0.01	11.21*	1758	[0.03]
Geraniol	8.14	1255	0.52	11.79*	1808	0.55
(*E*)-Anethole	8.50	1280	0.05	11.30*	1766	0.12
1-Nitro-2-phenylethane	8.62	1289	0.02	14.30*	2038	0.13
δ-Elemene	9.30*	1331	0.14	7.12	1432	0.08
Bicycloelemene	9.30*	1331	[0.14]	7.20*†	1439	0.12
Benzyl butyrate	9.39	1338	0.01	11.79*	1808	[0.55]

α-Cubebene	9.47	1343	0.17	6.94	1419	0.15
Eugenol	9.64	1355	0.01	14.90	2095	0.01
Neryl acetate	9.73	1361	0.03	10.35	1686	0.05
α-Ylangene	9.75	1363	0.12	7.20*†	1439	[0.12]
α-Copaene	9.82	1368	1.26	7.31	1447	1.22
β-Bourbonene	9.93	1375	0.01	7.62	1470	0.01
Geranyl acetate	10.02	1381	3.31	10.75*	1720	22.12
β-Cubebene	10.07	1385	0.37	7.94	1494	0.23
β-Elemene	10.11	1388	0.06	8.61*	1546	7.27
Methyleugenol	10.31	1402	0.02	13.48	1961	0.02
β-Caryophyllene	10.42	1410	7.26	8.61*	1546	[7.27]
Caryophylla-4(12),8(13)-diene	10.54*	1419	0.29	8.80*	1561	[1.34]
β-Copaene	10.54*	1419	[0.29]	8.54	1541	0.26
Aromadendrene	10.64	1426	0.06	8.69	1553	0.09
(*E*)-Cinnamyl acetate	10.78*	1437	2.46	14.80	2086	2.48
Isogermacrene D	10.78*	1437	[2.46]	9.12	1586	0.07
9-epi-Isocaryophyllene	10.83*	1441	0.75	9.17	1590	0.05
(*E*)-Isoeugenol	10.83*	1441	[0.75]	16.66	2274	0.67
trans-Muurola-3,5-diene	10.83*	1441	[0.75]	9.04	1579	0.12
α-Humulene	10.86	1443	1.88	9.46*	1613	[1.79]
cis-Cadina-1(6),4-diene	10.99*	1452	0.18	9.14	1588	0.07
cis-Muurola-4(15),5-diene	10.99*	1452	[0.18]	9.50	1617	0.14
trans-Cadina-1(6),4-diene	11.14	1463	0.14	9.42	1610	0.20
Germacrene D	11.29*†	1474	24.18	10.02*	1659	22.46
γ-Muurolene	11.29*†	1474	[24.18]	9.78	1640	1.33
trans-Muurola-4(15),5-diene	11.36	1479	0.16	10.03	1660	0.10
γ-Amorphene	11.37	1480	0.21	10.02*	1659	[22.46]
Prenyl benzoate	11.44*	1486	1.00	13.91*	2000	0.18
epi-Cubebol	11.44*	1486	[1.00]	12.14	1840	0.05
Bicyclogermacrene	11.44*	1486	[1.00]	10.22*†	1675	1.06
(3*Z*,6*E*)-α-Farnesene	11.52*	1492	0.75	10.44	1694	0.06
α-Muurolene	11.52*	1492	[0.75]	10.22*†	1675	[1.06]
δ-Amorphene	11.60*	1498	0.28	10.09	1664	0.28
Unknown [m/z 119, 41 (95), 123 (53), 80 (49), 161 (44), 105 (42)... 204 (2)]	11.60*	1498	[0.28]			
(3*E*,6*E*)-α-Farnesene	11.74*	1508	19.64	10.75*	1720	[22.12]
Cubebol	11.74*	1508	[19.64]	12.71	1890	0.04
γ-Cadinene	11.74*	1508	[19.64]	10.58	1704	0.70
(*Z*)-γ-Bisabolene	11.74*	1508	[19.64]	10.07	1663	0.04
trans-Calamenene	11.84*	1516	2.37	11.41	1775	0.03
δ-Cadinene	11.84*	1516	[2.37]	10.61*	1708	[2.24]

Zonarene	11.84*	1516	[2.37]	10.61*	1708	[2.24]
trans-Cadina-1,4-diene	11.93	1523	0.15	10.85	1728	0.16
α-Cadinene	12.00	1528	0.22	10.98	1739	0.16
α-Calacorene	12.08	1535	0.03	12.29*	1852	0.03
cis-Dracunculifoliol	12.14	1540	0.04	12.29*	1852	[0.03]
α-Elemol	12.20	1544	0.08	14.22	2030	0.06
Germacrene B	12.25	1548	0.01	11.30*	1766	[0.12]
β-Calacorene	12.38	1558	0.09	12.81	1898	0.04
(*E*)-Nerolidol	12.42	1562	0.05	13.88	1998	0.05
(3*Z*)-Hexenyl benzoate	12.45	1564	0.03	14.50	2057	0.02
Spathulenol	12.50	1567	0.10	14.54	2061	0.05
Caryophyllene oxide	12.54	1570	0.07	12.94	1910	0.06
10-epi-Junenol	12.59	1574	0.08	12.89	1906	0.06
Unknown cadinol or muurolol analog [m/z 161, 119 (77), 120 (76), 105 (73), 93 (57)... 204 (36)]	12.63	1578	0.03	12.45	1867	0.04
Unknown [m/z 161, 105 (84), 43 (80), 119 (72), 93 (62), 121 (54)... 204 (38), 222 (2)]	12.66	1580	0.06	14.13	2022	0.06
Viridiflorol	12.69	1582	0.05	14.16	2024	0.04
Guaiol	12.75	1587	0.15	14.30*	2038	[0.13]
Copaborneol	12.84	1594	0.03	15.07*	2112	0.43
Humulene epoxide II	12.91	1599	0.04	13.53	1966	0.02
10-epi-Cubenol	12.94	1602	0.28	13.94	2004	0.27
(*E*)-Isoeugenyl acetate	12.96*	1604	0.08	17.41	2354	0.05
Junenol	12.96*	1604	[0.08]	13.78	1988	0.20
1-epi-Cubenol	13.14	1618	0.09	13.91*	2000	[0.18]
τ-Cadinol	13.28*†	1630	1.40	15.07*	2112	[0.43]
τ-Muurolol	13.28*†	1630	[1.40]	15.23	2128	0.66
Cubenol	13.33†	1634	[1.40]	13.86	1995	0.14
α-Muurolol	13.39	1638	0.21	15.36	2142	0.23
α-Cadinol	13.43	1642	1.26	15.66	2171	1.26
trans-Calamenen-10-ol	13.63	1658	0.14	17.00*	2310	1.58
Unknown [m/z 123, 95 (31), 81 (29), 105 (27)... 222 (5)]	13.71	1665	0.11	16.39	2246	0.12
(2*E*,6*Z*)-Farnesol	14.06	1694	0.01	16.62	2270	0.02
(2*E*,6*E*)-Farnesol	14.31	1715	1.54	17.00*	2310	[1.58]
(2*E*,6*E*)-Farnesal	14.57	1737	0.01	16.00	2206	0.03
Benzyl benzoate	14.70	1749	5.72	19.06	2536	5.73
(2*E*,6*E*)-Farnesyl acetate	15.69	1836	4.02	16.15	2221	4.04

Benzyl salicylate	15.85*	1850	3.46	20.31	2682	3.44
Geranyl benzoate	15.85*	1850	[3.46]	18.87	2514	0.01
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109)40)... 204 (35), 222 (2)]				15.32	2138	0.17
Total identified		**98.03%**			**96.44%**	
Total reported		**98.23%**			**96.84%**	

*: 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