Date : February 01, 2022

Certificate of Analysis – GC Profiling

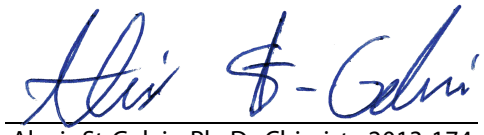
Sample identification

Internal code : 22A19-SDC01
Customer identification : Sample
Type : Essential oil
Source : *Oplopanax horridus*
Customer : Southeast Devilsclub

Analysis

Method: PC-MAT-014 ISO - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.
Analyst : Sylvain Mercier, M. Sc., Chimiste 2014-005
Analysis date : January 21, 2022

Checked and approved by :



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

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Méthode certifiée ISO 17025:2017 Certified method

Laboratoire PhytoChemia

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PHYSICOCHEMICAL DATA

Physical aspect: Yellow liquid
Refractive index: 1.4914 ± 0.0003 (20 °C; method PC-MAT-016)

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
Hexanal	0.01	Aliphatic aldehyde
α-Pinene	0.36	Monoterpene
Allylbenzene	0.01	Phenylpropanoid
β-Pinene	0.01	Monoterpene
Sabinene	0.02	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.03	Monoterpene
α-Phellandrene	0.01	Monoterpene
Octanal	0.03	Aliphatic aldehyde
Δ3-Carene	0.01	Monoterpene
para-Cymene	0.01	Monoterpene
Limonene	0.04	Monoterpene
β-Phellandrene	0.15	Monoterpene
2-Heptyl acetate	0.01	Aliphatic ester
Octanol	0.01	Aliphatic alcohol
Linalool	0.06	Monoterpenic alcohol
Nonanal	0.02	Aliphatic aldehyde
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	0.08	Monoterpene
(2*E*)-Nonenal	0.01	Aliphatic aldehyde
(3*E*,5*Z*)-Undeca-1,3,5-triene	0.60	Alkene
(3*E*,5*E*)-Undeca-1,3,5-triene	0.04	Alkene
3-Isobutyl-2-methoxypyrazine	0.06	Pyrazine
(2*E*)-Octenyl acetate?	0.01	Aliphatic ester
Octyl acetate	0.05	Aliphatic ester
Unknown	0.12	Unknown
2-Nonyl acetate	0.01	Aliphatic ester
(2*Z*)-Decenal	0.01	Aliphatic aldehyde
(4*Z*)-Decenol	0.02	Aliphatic alcohol
(2*E*)-Decenal	0.09	Aliphatic aldehyde
(2*E*)-Decenol	0.01	Aliphatic alcohol
Decanol	0.03	Aliphatic alcohol
4-Vinylguaiacol	0.02	Simple phenolic
(2*E*,4*E*)-Decadienol?	0.04	Aliphatic alcohol
Bicycloelemene analog	0.02	Sesquiterpene
Bicycloelemene	0.13	Sesquiterpene
α-Cubebene	0.03	Sesquiterpene
Cyclosativene II	0.06	Sesquiterpene
α-Ylangene	0.42	Sesquiterpene
α-Copaene	0.17	Sesquiterpene
cis-β-Elemene	0.02	Sesquiterpene
Geranyl acetate	0.05	Monoterpenic ester
β-Cubebene	0.02	Sesquiterpene
Dodecenyl acetate isomer?	0.06	Aliphatic ester
β-Elemene	0.21	Sesquiterpene
α-Gurjunene	0.04	Sesquiterpene

β-Caryophyllene	0.14	Sesquiterpene
α-Santalene	0.02	Sesquiterpene
β-Copaene	0.02	Sesquiterpene
β-Gurjunene	0.04	Sesquiterpene
γ-Elemene	0.25	Sesquiterpene
Aromadendrene	0.18	Sesquiterpene
Cadina-3,5-diene isomer I?	0.05	Sesquiterpene
Unknown	0.08	Sesquiterpene
Cadina-3,5-diene?	0.03	Sesquiterpene
α-Humulene	0.22	Sesquiterpene
allo-Aromadendrene	0.23	Sesquiterpene
cis-Muurola-4(15),5-diene	0.14	Sesquiterpene
(*E*)-β-Farnesene	0.34	Sesquiterpene
trans-Cadina-1(6),4-diene	0.05	Sesquiterpene
γ-Muurolene	0.17	Sesquiterpene
Germacrene D	1.42	Sesquiterpene
ar-Curcumene	0.67	Sesquiterpene
Unknown	0.07	Sesquiterpene
Bicyclogermacrene	7.36	Sesquiterpene
Bicyclosesquiphellandrene?	0.07	Sesquiterpene
α-Zingiberene	0.68	Sesquiterpene
α-Muurolene	0.24	Sesquiterpene
Germacrene A	0.12	Sesquiterpene
Cubebol	0.13	Sesquiterpenic alcohol
γ-Cadinene	2.93	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	0.71	Sesquiterpene
trans-Calamenene	0.06	Sesquiterpene
δ-Cadinene	2.28	Sesquiterpene
β-Sesquiphellandrene	0.93	Sesquiterpene
Unknown	0.11	Sesquiterpene
α-Cadinene	0.20	Sesquiterpene
α-Calacorene	0.04	Sesquiterpene
Germacrene B	2.31	Sesquiterpene
(*E*)-Nerolidol	55.27	Sesquiterpenic alcohol
Spathulenol	2.29	Sesquiterpenic alcohol
Caryophyllene oxide	0.03	Sesquiterpenic ether
Caryophyllene oxide isomer	0.05	Sesquiterpenic ether
Globulol	0.28	Sesquiterpenic alcohol
Viridiflorol	0.26	Sesquiterpenic alcohol
Unknown	0.27	Oxygenated sesquiterpene
Eudesm-5-en-11-ol analog	0.07	Sesquiterpenic alcohol
Guaiol	0.28	Sesquiterpenic alcohol
Eudesm-5-en-11-ol	0.14	Sesquiterpenic alcohol
10-epi-Cubenol	1.20	Sesquiterpenic alcohol
Rosifoliol	0.14	Sesquiterpenic alcohol
1-epi-Cubenol	0.10	Sesquiterpenic alcohol
Cubenol	0.55	Sesquiterpenic alcohol
τ-Muurolol	0.27	Sesquiterpenic alcohol
τ-Cadinol	7.50	Sesquiterpenic alcohol
α-Muurolol	0.22	Sesquiterpenic alcohol
α-Cadinol	0.74	Sesquiterpenic alcohol
Bulnesol	0.39	Sesquiterpenic alcohol

(3*Z*)-Caryophylla-3,8(13)-dien-5β-ol	0.02	Sesquiterpenic alcohol
Shyobunol	0.14	Sesquiterpenic alcohol
Unknown	0.10	Oxygenated sesquiterpene
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Cembrene?	0.01	Diterpene
para-Camphorene	0.02	Diterpene
(*Z*)-Falcarinol	0.11	Polyyne
Consolidated total	**96.04%**	

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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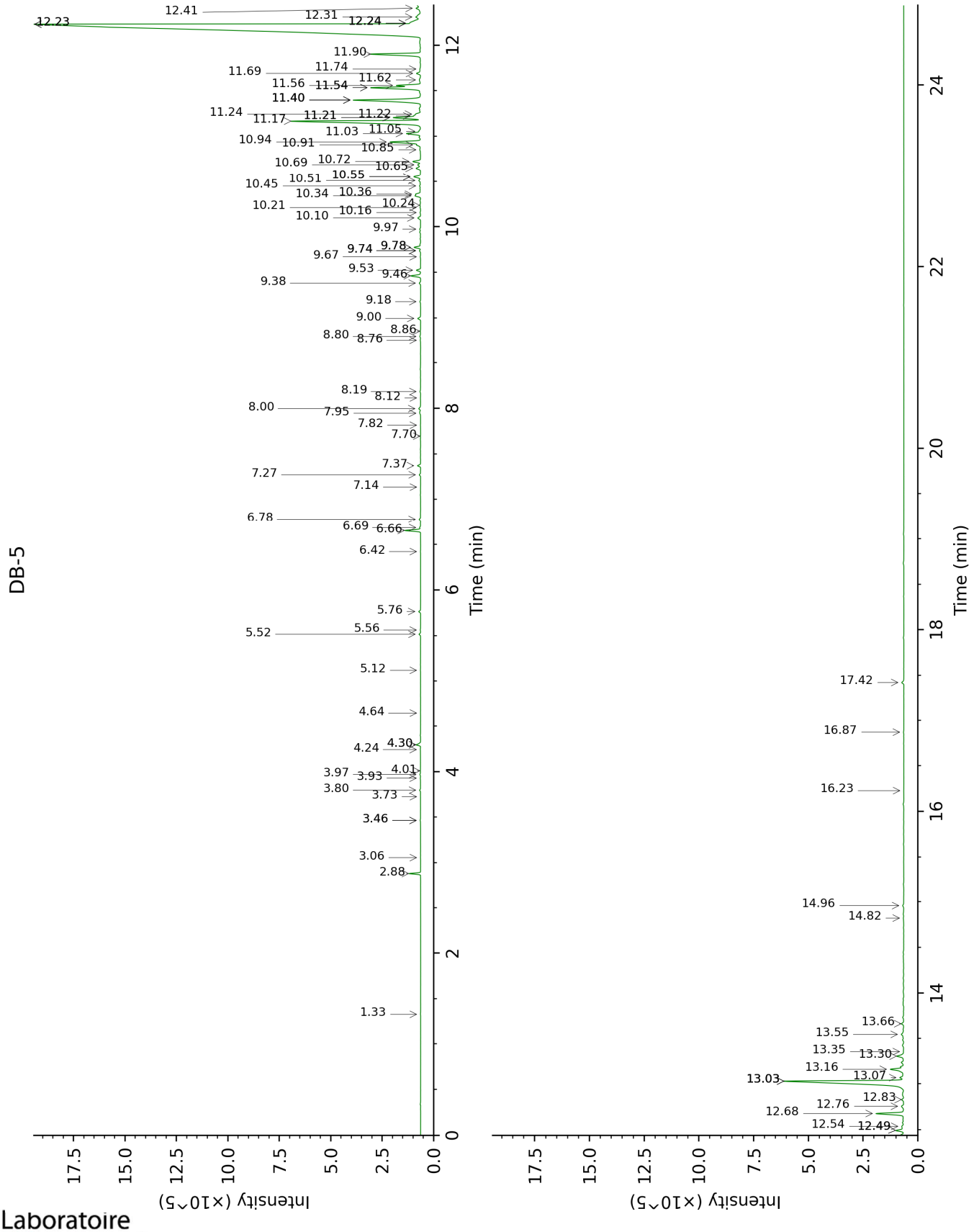
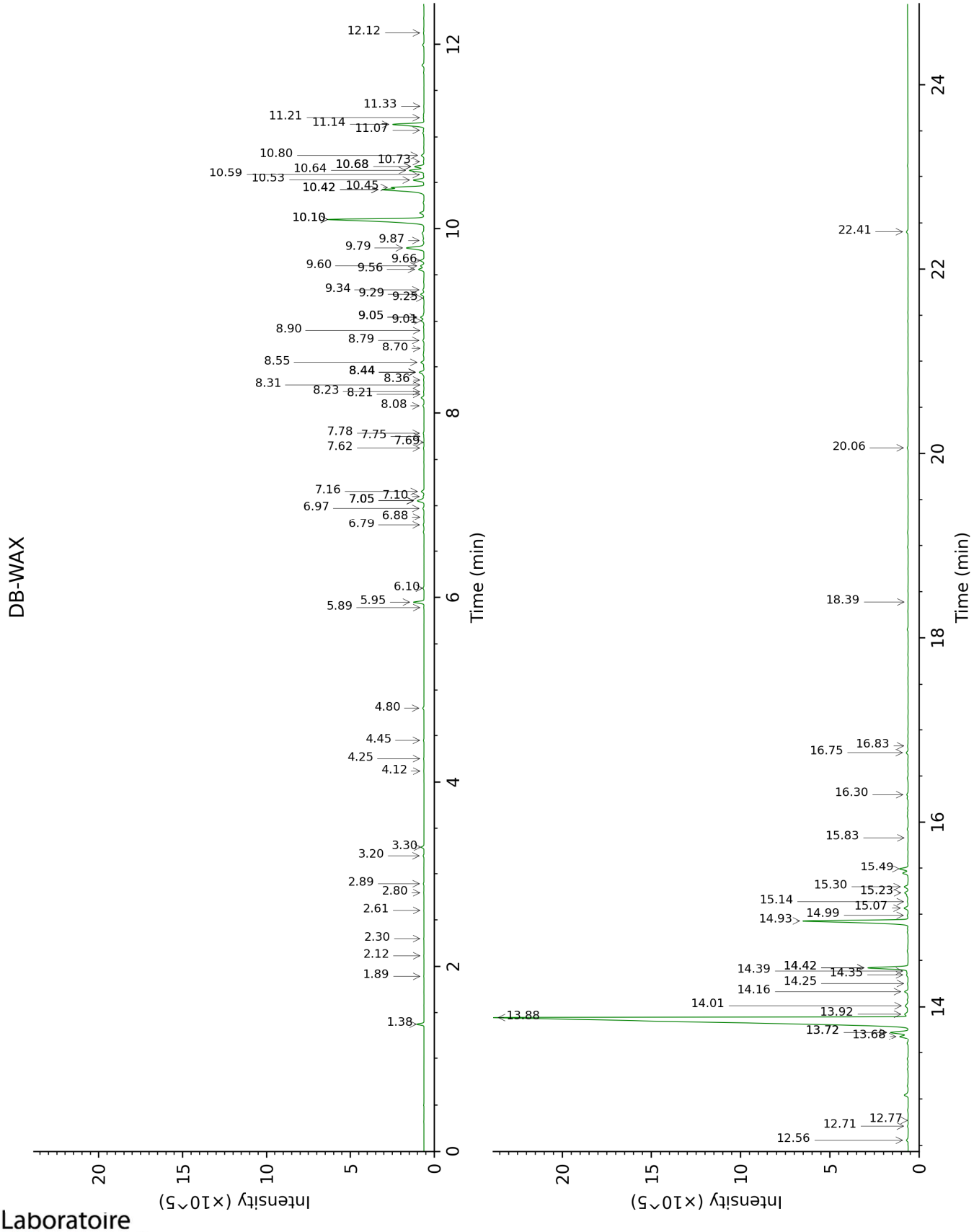

DB-5
12.41
12.31
12.24
12.23
11.90
11.69
11.74
11.62
11.56
11.54
11.40
11.24
11.17
11.21
11.22
11.03
11.05
10.94
10.91
10.85
10.69
10.72
10.65
10.45
10.51
10.55
10.34
10.36
10.21
10.24
10.10
10.16
9.97
9.67
9.74
9.78
9.53
9.46
9.38
9.18
9.00
8.80
8.86
8.76
8.19
8.12
8.00
7.95
7.82
7.70
7.37
7.27
7.14
6.78
6.69
6.66
6.42
5.76
5.52
5.56
5.12
4.64
4.24
4.30
3.97
3.93
4.01
3.80
3.73
3.46
3.06
2.88
1.33
Time (min)
Intensity (×10^5)
17.42
16.87
16.23
14.96
14.82
13.66
13.55
13.35
13.30
13.16
13.07
13.03
12.83
12.76
12.68
12.54
12.49
Time (min)
Intensity (×10^5)


DB-WAX
Time (min)
Intensity (×10^5)
12.12
11.33
11.21
11.14
11.07
10.80
10.73
10.68
10.64
10.59
10.53
10.45
10.42
10.10
9.87
9.79
9.66
9.60
9.56
9.34
9.29
9.25
9.05
9.01
8.90
8.79
8.70
8.55
8.44
8.36
8.31
8.23
8.21
8.08
7.78
7.75
7.69
7.62
7.16
7.10
7.05
6.97
6.88
6.79
6.10
5.95
5.89
4.80
4.45
4.25
4.12
3.30
3.20
2.89
2.80
2.61
2.30
2.12
1.89
1.38
22.41
20.06
18.39
16.83
16.75
16.30
15.83
15.49
15.30
15.23
15.14
15.07
14.99
14.93
14.42
14.39
14.35
14.25
14.16
14.01
13.92
13.88
13.72
13.68
12.77
12.71
12.56

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Hexanal	1.33	801	0.01	1.89	1044	0.02
α-Pinene	2.88	930	0.36	1.38	991	0.36
Allylbenzene	3.06	942	0.01			
β-Pinene	3.46*	970	0.02	2.12	1066	0.01
Sabinene	3.46*	970	[0.02]	2.30	1084	0.02
6-Methyl-5-hepten-2-one	3.73	988	0.01			
Myrcene	3.80	993	0.03	2.89	1133	0.03
α-Phellandrene	3.93	1002	0.01	2.80	1126	0.02
Octanal	3.97	1004	0.03	4.45	1253	0.03
Δ3-Carene	4.01	1007	0.01	2.61	1111	0.01
para-Cymene	4.24	1022	0.01	4.12	1228	0.02
Limonene	4.30*	1025	0.20	3.20	1158	0.04
β-Phellandrene	4.30*	1025	[0.20]	3.30	1165	0.15
2-Heptyl acetate	4.64	1047	0.01	4.25	1238	0.02
Octanol	5.12	1077	0.01	8.20	1526	0.01
Linalool	5.52	1102	0.06	8.08	1516	0.06
Nonanal	5.56	1105	0.02	5.89	1354	0.01
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	5.76	1118	0.08	4.80	1279	0.08
(2*E*)-Nonenal	6.42	1161	0.01	7.69	1486	0.01
(3*E*,5*Z*)-Undeca-1,3,5-triene	6.66	1176	0.60	5.95	1358	0.61
(3*E*,5*E*)-Undeca-1,3,5-triene	6.69	1178	0.04	6.10	1369	0.06
3-Isobutyl-2-methoxypyrazine	6.78	1184	0.06	7.78	1493	0.05
(2*E*)-Octenyl acetate?	7.14	1207	0.01			
Octyl acetate	7.27	1216	0.05	7.10	1442	0.05
Unknown [m/z 79, 71 (69), 59 (66), 43 (59), 81 (53), 41 (52), 93 (50)...]	7.37	1222	0.12			
2-Nonyl acetate	7.70	1244	0.01	7.06*	1439	0.52
(2*Z*)-Decenal	7.82	1252	0.01	8.70	1564	0.01
(4*Z*)-Decenol	7.95	1261	0.02	11.07	1758	0.03
(2*E*)-Decenal	8.00	1264	0.09	9.05*†	1591	[0.42]
(2*E*)-Decenol	8.12	1272	0.01	11.33	1780	0.02
Decanol	8.19	1277	0.03	10.73	1729	0.04
4-Vinylguaiacol	8.76	1316	0.02	15.14	2132	0.08
(2*E*,4*E*)-Decadienol?	8.80	1319	0.04			
Bicycloelemene analog	8.86	1323	0.02	6.88	1426	0.03
Bicycloelemene	9.00	1333	0.13	7.06*	1439	[0.52]
α-Cubebene	9.18	1346	0.03	6.79	1419	0.05
Cyclosativene II	9.38	1360	0.06	6.97	1433	0.08
α-Ylangene	9.46	1366	0.42	7.06*	1439	[0.52]
α-Copaene	9.52	1370	0.17	7.16	1446	0.17
cis-β-Elemene	9.67	1381	0.02	8.31	1533	0.02
Geranyl acetate	9.74*	1386	0.05	10.59	1716	0.05
β-Cubebene	9.74*	1386	[0.05]	7.75	1490	0.02
Dodecenyl acetate isomer?	9.78*	1388	0.27			
β-Elemene	9.78*	1388	[0.27]	8.44*	1544	0.37

α-Gurjunene	9.98	1402	0.04	7.62	1481	0.04
β-Caryophyllene	10.10	1411	0.14	8.44*	1544	[0.37]
α-Santalene	10.16	1416	0.02	8.23	1528	0.03
β-Copaene	10.21	1420	0.02	8.44*	1544	[0.37]
β-Gurjunene	10.24	1422	0.04	8.36	1537	0.03
γ-Elemene	10.34	1430	0.25	9.05*†	1591	[0.42]
Aromadendrene	10.36	1431	0.18	8.55	1552	0.22
Cadina-3,5-diene isomer I?	10.45	1438	0.05			
Unknown [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]	10.51	1442	0.08	8.80	1571	0.07
Cadina-3,5-diene?	10.55*	1445	0.33	8.90	1580	0.03
α-Humulene	10.55*	1445	[0.33]	9.29	1610	0.22
allo-Aromadendrene	10.65	1453	0.23	9.01†	1588	0.42
cis-Muurola-4(15),5-diene	10.69	1456	0.14	9.34	1614	0.07
(*E*)-β-Farnesene	10.72	1458	0.34	9.56	1632	0.36
trans-Cadina-1(6),4-diene	10.85	1468	0.05	9.25	1607	0.03
γ-Muurolene	10.91	1472	0.17	9.60	1635	0.23
Germacrene D	10.94	1474	1.42	9.79	1651	1.46
ar-Curcumene	11.03	1481	0.67	10.68*†	1724	[1.63]
Unknown [m/z 79, 107 (99), 91 (88), 93 (86), 81 (78), 105 (73), 41 (73)... 204? (12)]	11.06	1483	0.07	9.66	1640	0.24
Bicyclogermacrene	11.17	1491	7.36	10.10*	1676	8.29
Bicyclosesquiphellandrene?	11.21*	1494	1.27	9.87	1658	0.07
α-Zingiberene	11.21*	1494	[1.27]	10.10*	1676	[8.29]
α-Muurolene	11.22	1496	0.24	10.10*	1676	[8.29]
Germacrene A	11.24	1497	0.12	10.42*†	1702	5.05
Cubebol	11.40*	1509	3.77	12.56	1888	0.13
γ-Cadinene	11.40*	1509	[3.77]	10.42*†	1702	[5.05]
(3*E*,6*E*)-α-Farnesene	11.40*	1509	[3.77]	10.53	1711	0.71
trans-Calamenene	11.54*	1520	2.33	11.21	1769	0.06
δ-Cadinene	11.54*	1520	[2.33]	10.45†	1704	[5.05]
β-Sesquiphellandrene	11.56	1521	0.93	10.64†	1721	1.63
Unknown [m/z 119, 105 (53), 161 (33), 93 (28), 91 (25), 40 (20)...204]	11.62	1526	0.11	10.68*†	1724	[1.63]
α-Cadinene	11.69	1532	0.20	10.80	1735	0.17
α-Calacorene	11.74	1536	0.04	12.12	1849	0.03
Germacrene B	11.90	1548	2.31	11.14	1763	2.26
(*E*)-Nerolidol	12.23*†	1574	58.59	13.88	2010	55.27
Spathulenol	12.23*†	1574	[58.59]	14.42*	2062	2.56
Caryophyllene oxide	12.24*†	1575	[58.59]	12.77	1907	0.03
Caryophyllene oxide isomer	12.24*†	1575	[58.59]	12.71	1901	0.05
Globulol	12.24*†	1575	[58.59]	13.92	2014	0.28
Viridiflorol	12.31	1581	0.26	14.01	2023	0.32
Unknown [m/z 120, 59 (55), 121 (24), 93 (24), 81 (23), 107 (20)...]	12.41	1588	0.27	14.42*	2062	[2.56]
Eudesm-5-en-11-ol analog	12.49*	1595	0.35	14.25	2046	0.07
Guaiol	12.49*	1595	[0.35]	14.16	2037	0.28

Eudesm-5-en-11-ol	12.54	1598	0.14	14.39	2059	0.08
10-epi-Cubenol	12.68	1610	1.20	13.72*	1995	1.19
Rosifoliol	12.76	1616	0.14	14.35	2055	0.12
1-epi-Cubenol	12.83	1622	0.10	13.72*	1995	[1.19]
Cubenol	13.03*	1639	8.23	13.68	1991	0.55
τ-Muurolol	13.03*	1639	[8.23]	15.07	2126	0.27
τ-Cadinol	13.03*	1639	[8.23]	14.93	2112	7.50
α-Muurolol	13.07	1642	0.22	15.23	2142	0.25
α-Cadinol	13.16	1650	0.74	15.49	2168	0.55
Bulnesol	13.30	1662	0.39	15.30	2149	0.27
(3*Z*)-Caryophylla-3,8(13)-dien-5β-ol	13.35	1666	0.02	16.83	2306	0.05
Shyobunol	13.55	1682	0.14	16.30	2251	0.10
Unknown [m/z 69, 41 (59), 118 (33), 43 (32), 55 (31)... 234? (t)]	13.66	1692	0.10	16.76	2298	0.12
Unknown [m/z 69, 41 (96), 43 (90), 109 (51), 55 (42), 81 (33)...]	14.82	1792	0.03	18.39	2478	0.02
Unknown [m/z 69, 43 (95), 41 (84), 109 (78), 95 (54), 93 (49)... 177 (36), 220 (2)...]	14.96	1804	0.05	20.06	2674	0.05
Cembrene?	16.23	1920	0.01	14.99	2118	0.06
para-Camphorene	16.87	1981	0.02	15.83	2202	0.01
(*Z*)-Falcarinol	17.42	2035	0.11	22.41	2969	0.11
Total identified		**96.40%**			**94.64%**	
Total reported		**97.22%**			**95.14%**	

*: 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

Note: no correction factor was applied
R.T.: Retention time (minutes)
R.I.: Retention index