Date : July 12, 2022

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 22F27-SDC02
Customer identification : 220516
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 : Pamela Lavoie, M.Sc., Chimiste
Analysis date : July 11, 2022

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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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

Méthode certifiée ISO 17025:2017 Certified method

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PHYSICOCHEMICAL DATA

Physical aspect: Clear liquid
Refractive index: 1.4894 ± 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
Heptanal	0.01	Aliphatic aldehyde
(*E*)-1,3-Nonadiene	0.01	Alkene
α-Pinene	0.94	Monoterpene
Allylbenzene	0.01	Phenylpropanoid
Sabinene	0.03	Monoterpene
β-Pinene	0.02	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.09	Monoterpene
Octanal	0.09	Aliphatic aldehyde
Pseudolimonene	0.01	Monoterpene
α-Phellandrene	0.03	Monoterpene
Δ3-Carene	0.03	Monoterpene
(*E*)-β-Methylstyrene	0.01	Simple phenolic
para-Cymene	0.02	Monoterpene
β-Phellandrene	0.39	Monoterpene
Limonene	0.12	Monoterpene
2-Heptanyl acetate	0.04	Aliphatic ester
2-Heptyl acetate	0.01	Aliphatic ester
Octanol	0.01	Aliphatic alcohol
Terpinolene	0.01	Monoterpene
Linalool	0.04	Monoterpenic alcohol
Nonanal	0.03	Aliphatic aldehyde
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	0.16	Monoterpene
(2*E*)-Nonenal	0.01	Aliphatic aldehyde
Ectocarpene?	0.01	Alkene
(3*E*,5*Z*)-Undeca-1,3,5-triene	1.34	Alkene
(3*E*,5*E*)-Undeca-1,3,5-triene	0.01	Alkene
3-Isobutyl-2-methoxypyrazine	0.05	Pyrazine
(2*E*)-Octenyl acetate?	0.01	Aliphatic ester
Octyl acetate	0.04	Aliphatic ester
Unknown	0.18	Unknown
2-Nonyl acetate	0.03	Aliphatic ester
Decenol isomer	0.02	Aliphatic alcohol
(2*E*)-Decenal	0.05	Aliphatic aldehyde
(2*E*)-Decenol	0.01	Aliphatic alcohol
Decanol	0.02	Aliphatic alcohol
4-Vinylguaiacol	0.02	Simple phenolic
(2*E*,4*E*)-Decadienol?	0.06	Aliphatic alcohol
Bicycloelemene analog	0.02	Sesquiterpene
Bicycloelemene	0.19	Sesquiterpene
α-Cubebene	0.04	Sesquiterpene
Cyclosativene II	0.06	Sesquiterpene
α-Ylangene	0.41	Sesquiterpene
α-Copaene	0.21	Sesquiterpene

cis-β-Elemene	0.02	Sesquiterpene
Geranyl acetate	0.01	Monoterpenic ester
β-Cubebene	0.05	Sesquiterpene
β-Elemene	0.26	Sesquiterpene
α-Gurjunene	0.05	Sesquiterpene
β-Caryophyllene	0.15	Sesquiterpene
α-Santalene	0.02	Sesquiterpene
β-Copaene	0.03	Sesquiterpene
β-Gurjunene	0.03	Sesquiterpene
γ-Elemene	0.21	Sesquiterpene
Aromadendrene	0.22	Sesquiterpene
Cadina-3,5-diene isomer I?	0.03	Sesquiterpene
Unknown	0.04	Sesquiterpene
Cadina-3,5-diene?	0.27	Sesquiterpene
α-Humulene	0.25	Sesquiterpene
allo-Aromadendrene	0.22	Sesquiterpene
cis-Muurola-4(15),5-diene	0.10	Sesquiterpene
(*E*)-β-Farnesene	0.41	Sesquiterpene
trans-Cadina-1(6),4-diene	0.06	Sesquiterpene
γ-Muurolene	0.20	Sesquiterpene
Germacrene D	1.29	Sesquiterpene
ar-Curcumene	0.64	Sesquiterpene
Unknown	0.13	Sesquiterpene
Bicyclogermacrene	9.67	Sesquiterpene
Bicyclosesquiphellandrene?	0.08	Sesquiterpene
α-Zingiberene	1.24	Sesquiterpene
α-Muurolene	0.30	Sesquiterpene
Germacrene A	0.19	Sesquiterpene
γ-Cadinene	3.41	Sesquiterpene
(3*E*,6*E*)-α-Farnesene	0.98	Sesquiterpene
Cubebol	0.11	Sesquiterpenic alcohol
δ-Cadinene	2.42	Sesquiterpene
β-Sesquiphellandrene	1.02	Sesquiterpene
trans-Calamenene	0.01	Sesquiterpene
Unknown	0.03	Sesquiterpene
α-Cadinene	0.21	Sesquiterpene
α-Calacorene	0.04	Sesquiterpene
Germacrene B	2.18	Sesquiterpene
Epiglobulol	0.02	Sesquiterpenic alcohol
Palustrol	0.08	Sesquiterpenic alcohol
Spathulenol	1.31	Sesquiterpenic alcohol
(*E*)-Nerolidol	55.34	Sesquiterpenic alcohol
Caryophyllene oxide	0.01	Sesquiterpenic ether
Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
Globulol	0.13	Sesquiterpenic alcohol
Viridiflorol	0.25	Sesquiterpenic alcohol
Gleenol	0.10	Sesquiterpenic alcohol
Unknown	0.20	Oxygenated sesquiterpene
Guaiol	0.15	Sesquiterpenic alcohol
Eudesm-5-en-11-ol analog	0.21	Sesquiterpenic alcohol
Eudesm-5-en-11-ol	0.10	Sesquiterpenic alcohol
10-epi-Cubenol	1.00	Sesquiterpenic alcohol

Rosifoliol	0.02	Sesquiterpenic alcohol
1-epi-Cubenol	0.08	Sesquiterpenic alcohol
τ-Muurolol	0.18	Sesquiterpenic alcohol
τ-Cadinol	5.46	Sesquiterpenic alcohol
Cubenol	0.47	Sesquiterpenic alcohol
Isospathulenol	0.23	Sesquiterpenic alcohol
α-Muurolol	0.16	Sesquiterpenic alcohol
α-Cadinol	0.28	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Bulnesol	0.21	Sesquiterpenic alcohol
(3*Z*)-Caryophylla-3,8(13)-dien-5β-ol	0.03	Sesquiterpenic alcohol
Shyobunol	0.08	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Aromadendrane-4,10-diol	0.02	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
(*Z*)-Falcarinol	0.08	Polyyne
Octadecanol	0.01	Aliphatic alcohol
Unknown	0.04	Oxygenated sesquiterpene
Consolidated total	**97.79%**	

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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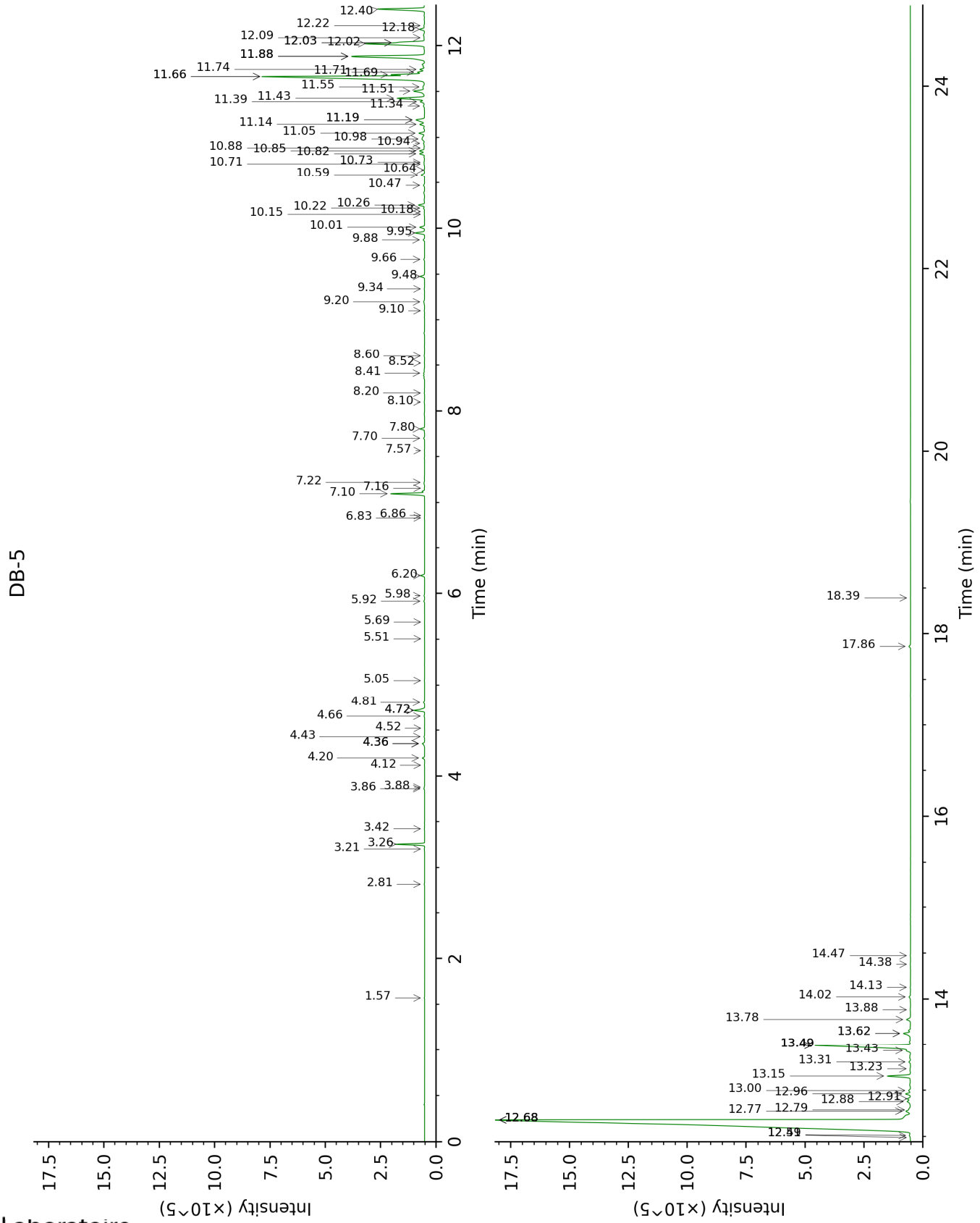
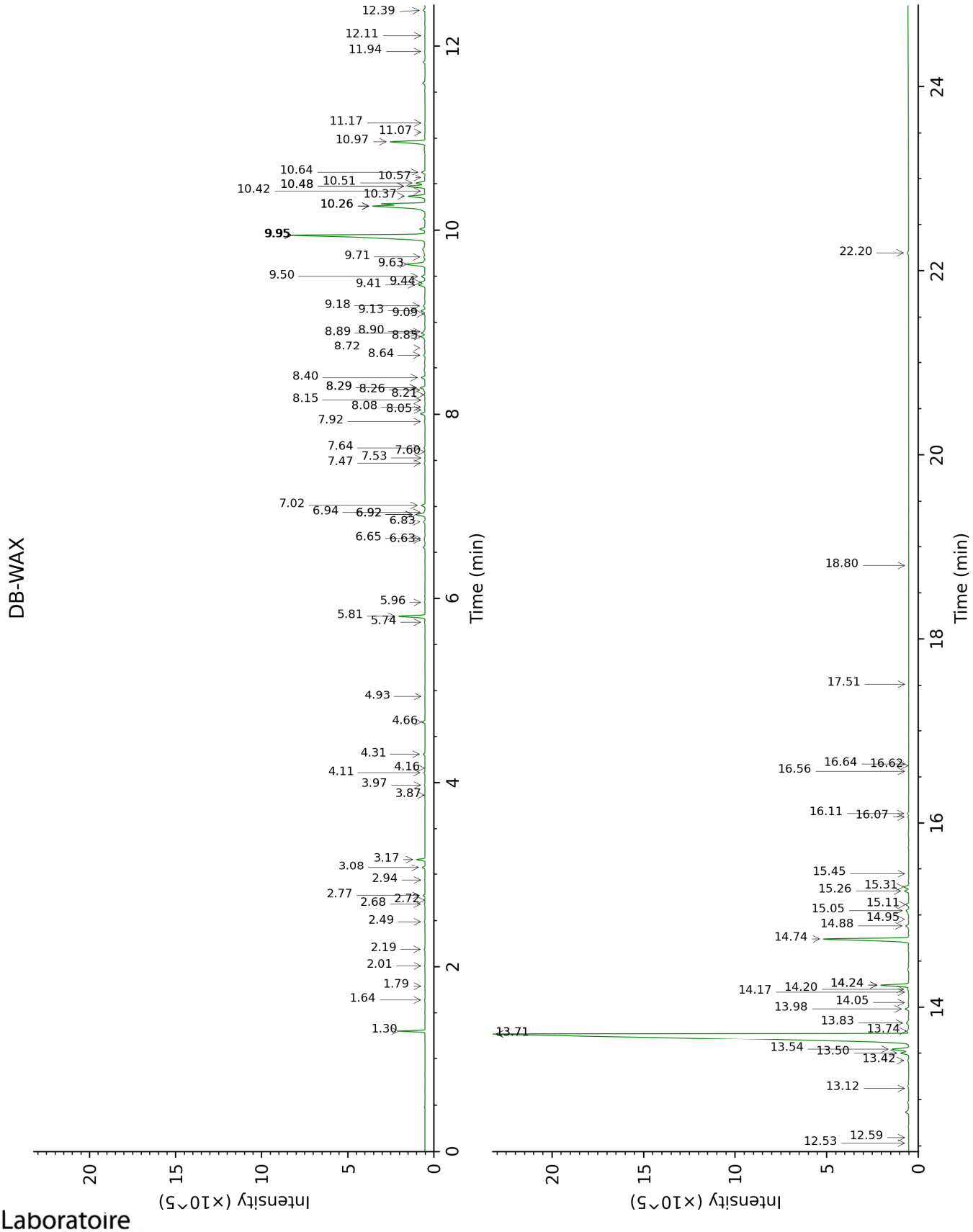

DB-5
Time (min)
Intensity (×10^5)
12.40
12.22
12.18
12.09
12.03
12.02
11.88
11.74
11.71
11.69
11.66
11.55
11.51
11.43
11.39
11.34
11.19
11.14
11.05
10.98
10.94
10.88
10.85
10.82
10.73
10.71
10.64
10.59
10.47
10.26
10.22
10.18
10.15
10.01
9.95
9.88
9.66
9.48
9.34
9.20
9.10
8.60
8.52
8.41
8.20
8.10
7.80
7.70
7.57
7.22
7.16
7.10
6.86
6.83
6.20
5.98
5.92
5.69
5.51
5.05
4.81
4.72
4.66
4.52
4.43
4.36
4.20
4.12
3.88
3.86
3.42
3.26
3.21
2.81
1.57
18.39
17.86
14.47
14.38
14.13
14.02
13.88
13.78
13.62
13.49
13.43
13.31
13.23
13.15
13.00
12.96
12.91
12.88
12.79
12.77
12.68



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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Hexanal	1.57	799	0.01	1.79	1043	0.01
Heptanal	2.81	901	0.01	2.94	1146	0.02
(*E*)-1,3-Nonadiene	3.20	927	0.01	1.64	1028	0.02
α-Pinene	3.26	930	0.94	1.30	990	0.94
Allylbenzene	3.42	941	0.01	3.87	1218	0.01
Sabinene	3.86†	970	0.04	2.19	1083	0.03
β-Pinene	3.88†	971	[0.04]	2.01	1065	0.02
6-Methyl-5-hepten-2-one	4.12	987	0.01	4.93	1297	0.01
Myrcene	4.20	992	0.09	2.77	1132	0.08
Octanal	4.36*	1002	0.12	4.31	1251	0.09
Pseudolimonene	4.36*	1002	[0.12]	2.72	1128	0.01
α-Phellandrene	4.36*	1002	[0.12]	2.68	1125	0.03
Δ3-Carene	4.43	1007	0.03	2.49	1110	0.02
(*E*)-β-Methylstyrene	4.52	1013	0.01			
para-Cymene	4.66	1022	0.02	3.97	1226	0.03
β-Phellandrene	4.72*	1025	0.50	3.17	1164	0.39
Limonene	4.72*	1025	[0.50]	3.08	1156	0.12
2-Heptanyl acetate	4.81	1031	0.04			
2-Heptyl acetate	5.05	1046	0.01	4.11	1236	0.05
Octanol	5.51	1075	0.01	8.05	1525	0.01
Terpinolene	5.69	1086	0.01	4.16	1240	tr
Linalool	5.92	1101	0.04	7.92	1515	0.04
Nonanal	5.98	1105	0.03	5.74	1353	0.03
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	6.20	1119	0.16	4.66	1276	0.16
(2*E*)-Nonenal	6.83	1160	0.01	7.53	1485	0.01
Ectocarpene?	6.86	1162	0.01			
(3*E*,5*Z*)-Undeca-1,3,5-triene	7.10	1177	1.34	5.81	1358	1.36
(3*E*,5*E*)-Undeca-1,3,5-triene	7.16	1181	0.01	5.96	1369	0.03
3-Isobutyl-2-methoxypyrazine	7.22	1185	0.05	7.60	1490	0.02
(2*E*)-Octenyl acetate?	7.57	1208	0.01			
Octyl acetate	7.70	1217	0.04	6.94†	1441	[0.62]
Unknown [m/z 79, 71 (69), 59 (66), 43 (59), 81 (53), 41 (52), 93 (50)...]	7.80	1224	0.18			
2-Nonyl acetate	8.10	1244	0.03	6.92*†	1439	0.62
Decenol isomer	8.20	1250	0.02			
(2*E*)-Decenal	8.41	1265	0.05	8.90†	1592	[0.25]
(2*E*)-Decenol	8.52	1273	0.01	11.17	1779	0.01
Decanol	8.60	1278	0.02	10.57	1728	0.03
4-Vinylguaiacol	9.10	1308	0.02	14.95	2131	0.03
(2*E*,4*E*)-Decadienol?	9.20	1315	0.06			
Bicycloelemene analog	9.34	1325	0.02	6.65†	1419	[0.07]
Bicycloelemene	9.48	1334	0.19	6.92*†	1439	[0.62]
α-Cubebene	9.66	1348	0.04	6.63†	1418	0.07
Cyclosativene II	9.88	1363	0.06	6.83	1433	0.09
α-Ylangene	9.95	1368	0.41	6.92*†	1439	[0.62]

α-Copaene	10.01	1372	0.21	7.02	1447	0.21
cis-β-Elemene	10.15	1382	0.02	8.16	1533	0.02
Geranyl acetate	10.18	1384	0.01	10.42	1716	0.04
β-Cubebene	10.22	1387	0.05	7.64	1493	0.06
β-Elemene	10.26	1390	0.26	8.29*†	1544	[0.35]
α-Gurjunene	10.47	1405	0.05	7.47	1481	0.05
β-Caryophyllene	10.59	1414	0.15	8.29*†	1544	[0.35]
α-Santalene	10.64	1418	0.02	8.08	1527	0.03
β-Copaene	10.71	1422	0.03	8.26†	1542	0.35
β-Gurjunene	10.73	1424	0.03	8.21	1538	0.04
γ-Elemene	10.82	1431	0.21	8.89†	1590	0.25
Aromadendrene	10.85	1433	0.22	8.40	1552	0.22
Cadina-3,5-diene isomer I?	10.88	1436	0.03			
Unknown [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]	10.94	1440	0.04	8.64	1571	0.07
Cadina-3,5-diene?	10.98	1443	0.27	8.72	1578	0.03
α-Humulene	11.05	1448	0.25	9.13	1610	0.24
allo-Aromadendrene	11.14	1455	0.22	8.85	1587	0.26
cis-Muurola-4(15),5-diene	11.19*	1458	0.53	9.18	1614	0.10
(*E*)-β-Farnesene	11.19*	1458	[0.53]	9.41	1632	0.41
trans-Cadina-1(6),4-diene	11.34	1470	0.06	9.09	1607	0.04
γ-Muurolene	11.39	1473	0.20	9.44	1635	0.23
Germacrene D	11.43	1476	1.29	9.63	1651	1.32
ar-Curcumene	11.51	1482	0.64	10.51	1723	0.51
Unknown [m/z 79, 107 (99), 91 (88), 93 (86), 81 (78), 105 (73), 41 (73)... 204? (12)]	11.55	1485	0.13	9.50	1640	0.21
Bicyclogermacrene	11.66*	1494	10.22	9.95*	1676	11.21
Bicyclosesquiphellandrene?	11.66*	1494	[10.22]	9.71	1657	0.08
α-Zingiberene	11.68	1495	1.24	9.95*	1676	[11.21]
α-Muurolene	11.71	1497	0.30	9.95*	1676	[11.21]
Germacrene A	11.74	1500	0.19	10.26*†	1702	6.02
γ-Cadinene	11.88*	1511	4.50	10.26*†	1702	[6.02]
(3*E*,6*E*)-α-Farnesene	11.88*	1511	[4.50]	10.37	1711	0.98
Cubebol	11.88*	1511	[4.50]	12.39	1887	0.11
δ-Cadinene	12.02†	1522	3.71	10.26*†	1702	[6.02]
β-Sesquiphellandrene	12.03*†	1522	[3.71]	10.48*	1720	1.05
trans-Calamenene	12.03*†	1522	[3.71]	11.07	1771	0.01
Unknown [m/z 119, 105 (53), 161 (33), 93 (28), 91 (25), 40 (20)...204]	12.09	1527	0.03	10.48*	1720	[1.05]
α-Cadinene	12.18	1534	0.21	10.64	1734	0.19
α-Calacorene	12.22	1537	0.04	11.94	1847	0.03
Germacrene B	12.40	1551	2.18	10.97	1762	2.16
Epiglobulol	12.49	1558	0.02	13.12	1954	0.01
Palustrol	12.51	1560	0.08	12.11	1862	0.02
Spathulenol	12.68*	1573	57.36	14.24*	2061	1.51
(*E*)-Nerolidol	12.68*	1573	[57.36]	13.71*	2010	55.41
Caryophyllene oxide	12.68*	1573	[57.36]	12.59	1905	0.01
Caryophyllene oxide isomer	12.68*	1573	[57.36]	12.53	1900	0.02

Globulol	12.68*	1573	[57.36]	13.74	2013	0.13
Viridiflorol	12.77	1580	0.25	13.83	2021	0.17
Gleenol	12.79	1582	0.10	13.42	1982	0.07
Unknown [m/z 120, 59 (55), 121 (24), 93 (24), 81 (23), 107 (20)...]	12.88	1589	0.20	14.24*	2061	[1.51]
Guaiol	12.91	1591	0.15	13.98	2036	0.19
Eudesm-5-en-11-ol analog	12.96	1595	0.21	14.05	2043	0.02
Eudesm-5-en-11-ol	13.00	1598	0.10	14.20	2056	0.06
10-epi-Cubenol	13.16	1611	1.00	13.54†	1994	[1.47]
Rosifoliol	13.23	1617	0.02	14.17	2054	0.02
1-epi-Cubenol	13.31	1624	0.08	13.71*	2010	[55.41]
τ-Muurolol	13.43	1634	0.18	14.88	2124	0.19
τ-Cadinol	13.49*	1638	5.74	14.74	2109	5.46
Cubenol	13.49*	1638	[5.74]	13.50†	1990	1.47
Isospathulenol	13.49*	1638	[5.74]	15.26	2162	0.23
α-Muurolol	13.49*	1638	[5.74]	15.05	2140	0.16
α-Cadinol	13.62*	1650	0.40	15.31	2166	0.28
Unknown [m/z 202, 187 (89), 121 (45), 105 (42), 93 (40), 95 (38)...]	13.62*	1650	[0.40]	15.45	2181	0.02
Bulnesol	13.78	1662	0.21	15.11	2147	0.15
(3*Z*)-Caryophylla-3,8(13)-dien-5β-ol	13.88	1671	0.03	16.64	2305	0.01
Shyobunol	14.02	1683	0.08	16.11	2249	0.06
Unknown [m/z 69, 41 (59), 118 (33), 43 (32), 55 (31)... 234? (t)]	14.13	1691	0.02	16.56	2297	0.02
Aromadendrane-4,10-diol	14.38	1713	0.02	16.62	2303	0.01
Unknown [m/z 159, 220 (92), 93 (88), 177 (63), 91 (57), 107 (55)]	14.47	1721	0.02	17.51	2399	0.01
(*Z*)-Falcarinol	17.86	2032	0.08	22.20	2967	0.08
Octadecanol	18.39	2085	0.01	18.80	2545	0.01
Unknown [m/z 159, 93 (89), 205 (88), 91 (81), 107 (75), 105 (74), 119 (70)... 220 (16)]				16.07	2245	0.04
Total identified		**97.94%**			**96.36%**	
Total reported		**98.56%**			**96.74%**	

*: 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