Date : 2023-08-10

Certificate of Analysis - GC Profiling

Sample Identification

Internal code : 23H03-PTH02
Customer Identification : Buchu - South Africa - BP2100
Type : Essential Oil
Source : *Agathosma betulina*
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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

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 : Amélie Simard, Analyste
Date : 2023-08-10

Physicochemical data

Refractive index : 1.4753 ± 0.0003 (20 °C)
Method : PC-MAT-016 - Measure of the refractive index of a liquid.
Analyst : Cindy Caron B. Sc.
Date : 2023-08-03

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
α-Thujene	0.12	Monoterpene
α-Pinene	0.88	Monoterpene
3-Methylcyclohexanone	0.01	Aliphatic ketone
Camphene	0.02	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
6-Methyl-2-heptanone	0.01	Aliphatic ketone
β-Pinene	0.40	Monoterpene
Sabinene	0.08	Monoterpene
Myrcene	1.94	Monoterpene
Menthatriene isomer I	0.03	Monoterpene
Pseudolimonene	0.02	Monoterpene
α-Phellandrene	0.03	Monoterpene
α-Terpinene	0.39	Monoterpene
para-Cymene	0.04	Monoterpene
1,8-Cineole	2.25	Monoterpenic ether
Limonene	18.21	Monoterpene
(*Z*)-β-Ocimene	0.08	Monoterpene
(*E*)-β-Ocimene	0.78	Monoterpene
γ-Terpinene	0.51	Monoterpene
cis-Sabinene hydrate	0.19	Monoterpenic alcohol
Terpinolene	0.13	Monoterpene
para-Cymenene	0.05	Monoterpene
trans-Sabinene hydrate	0.14	Monoterpenic alcohol
Linalool	0.45	Monoterpenic alcohol
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	0.04	Monoterpene
trans-para-Mentha-2,8-dien-1-ol	0.03	Monoterpenic alcohol
cis-para-Mentha-2,8-dien-1-ol	0.04	Monoterpenic alcohol
Isopulegol	0.11	Monoterpenic alcohol
Menthone	8.95	Monoterpenic ketone
Isomenthone	20.04	Monoterpenic ketone
Menthofuran	0.19	Monoterpenic ether
Menthol	0.07	Monoterpenic alcohol
Terpinen-4-ol	0.34	Monoterpenic alcohol
cis-Isopulegone	1.55	Monoterpenic ketone
Isopulegone analogue I	1.90	Monoterpenic ketone
Isomenthol	0.04	Monoterpenic alcohol
α-Terpineol	0.16	Monoterpenic alcohol
cis-Dihydrocarvone	0.15	Monoterpenic ketone
trans-Dihydrocarvone	0.03	Monoterpenic ketone
trans-Isopiperitenol	0.07	Monoterpenic alcohol

Verbenone	0.02	Monoterpenic ketone
Unknown	0.01	Unknown
Unknown	0.03	Unknown
Pulegone	8.49	Monoterpenic ketone
3,4-Dimethoxytoluene	0.03	Phenolic ester
Unknown	0.47	Unknown
Pseudodiosphenol	10.81	Monoterpenic alcohol
Isopulegyl acetate	0.06	Monoterpenic ester
Unknown	0.38	Unknown
Bornyl acetate	0.03	Monoterpenic ester
trans-Sabinyl acetate	0.02	Monoterpenic ester
Diosphenol	12.84	Monoterpenic alcohol
2-Acetyl-*para*-cresol?	0.01	Simple phenolic
neo-Dihydrocarvyl acetate	0.03	Monoterpenic ester
Unknown	0.04	Unknown
Unknown	0.12	Unknown
Myrtenyl acetate	0.13	Monoterpenic ester
Dihydrocarvyl acetate	0.10	Monoterpenic ester
trans-Carvyl acetate	0.05	Monoterpenic ester
exo-2-Hydroxycineole acetate	0.02	Monoterpenic ester
cis-*para*-Mentha-8-thiol-3-one	0.77	Monoterpenic thiol
trans-*para*-Mentha-8-thiol-3-one	2.30	Monoterpenic thiol
trans-Myrtanyl acetate	0.05	Monoterpenic ester
Methyleugenol	0.06	Phenylpropanoid
para-Menth-1-en-9-yl acetate?	0.02	Monoterpenic ester
Germacrene D	0.03	Sesquiterpene
8-(Methylthio)-*para*-menthan-3-one	0.03	Monoterpenic thiol
Viridiflorene	0.06	Sesquiterpene
Bicyclogermacrene	0.02	Sesquiterpene
Unknown	0.15	Unknown
(*E*)-Nerolidol	0.01	Sesquiterpenic alcohol
S-Acetyl-*cis*-*para*-Mentha-8-thiol-3-one	0.30	Monoterpenic thioester
S-Acetyl-*trans*-*para*-Mentha-8-thiol-3-one	0.10	Monoterpenic thioester
Isospathulenol	0.01	Sesquiterpenic alcohol
Benzyl benzoate	0.02	Phenolic ester
Unknown	0.04	Unknown
Unknown	0.07	Unknown
Unknown	0.08	Unknown
Unknown	0.04	Unknown
Unknown	0.05	Unknown
Consolidated total	**98.40**	

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

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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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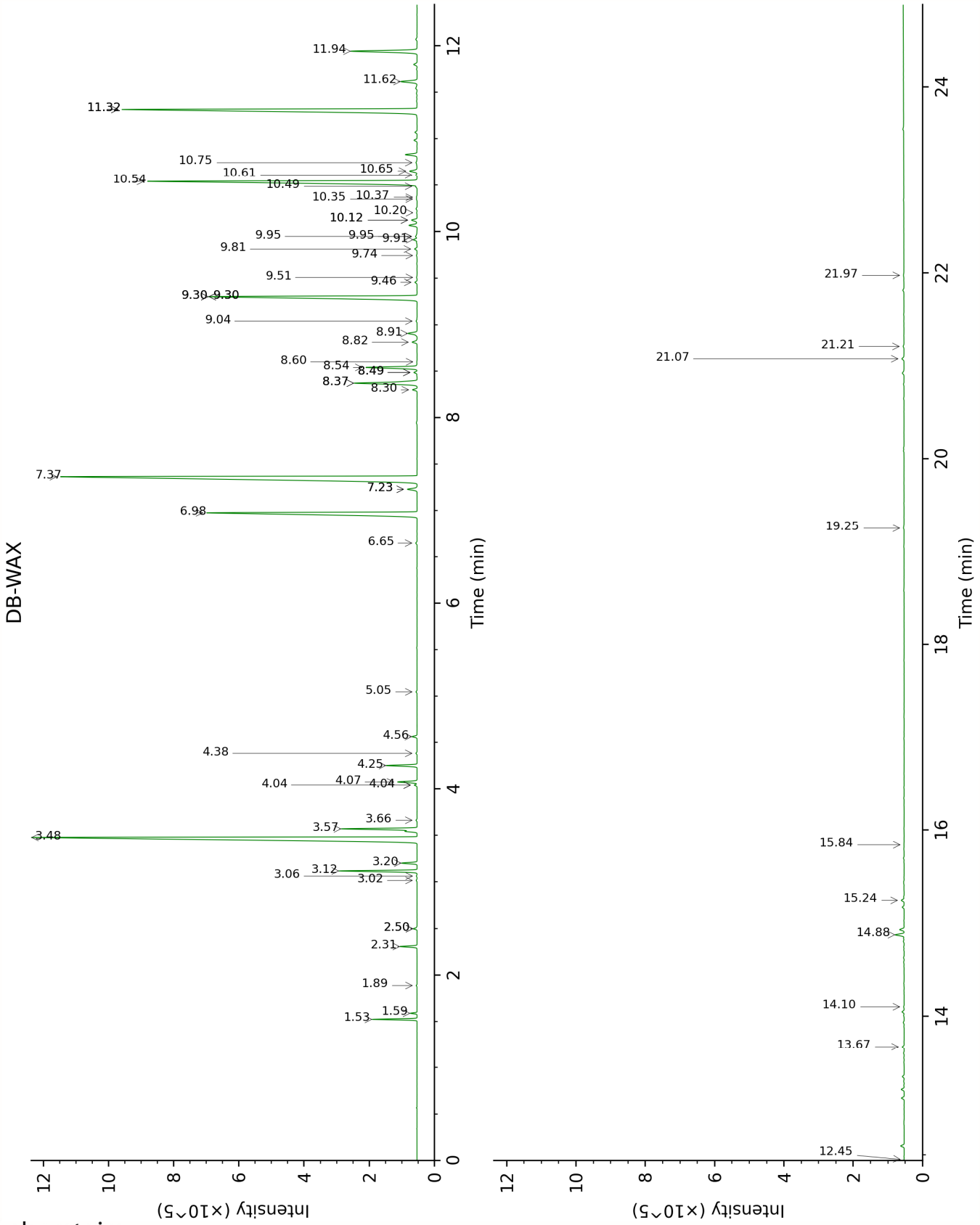
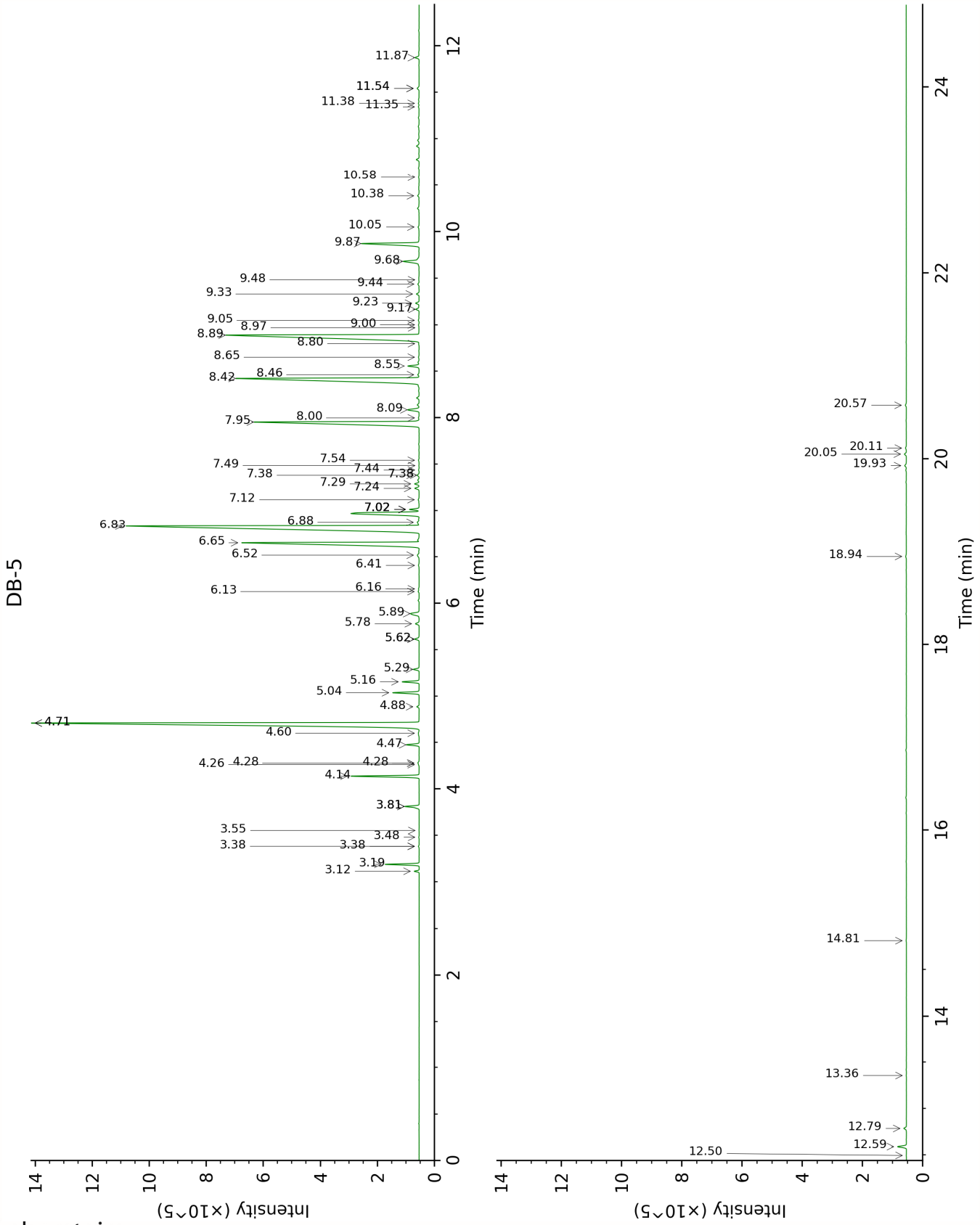

DB-WAX
Time (min)
Intensity (×10^5)
11.94
11.62
11.32
10.75
10.61
10.65
10.54
10.49
10.35
10.37
10.20
10.12
9.95
9.95
9.91
9.81
9.74
9.51
9.46
9.30
9.30
9.04
8.91
8.82
8.60
8.54
8.49
8.37
8.30
7.37
7.23
6.98
6.65
5.05
4.56
4.38
4.25
4.04
4.07
4.04
3.66
3.57
3.48
3.20
3.12
3.06
3.02
2.50
2.31
1.89
1.59
1.53
21.97
21.21
21.07
19.25
15.84
15.24
14.88
14.10
13.67
12.45


DB-5
11.87
11.54
11.38
11.35
10.58
10.38
10.05
9.87
9.68
9.48
9.44
9.33
9.23
9.17
9.05
8.97
9.00
8.89
8.80
8.65
8.55
8.42
8.46
8.09
8.00
7.95
7.49
7.54
7.44
7.38
7.38
7.29
7.24
7.12
7.02
6.83
6.88
6.65
6.52
6.41
6.13
6.16
5.89
5.78
5.62
5.29
5.16
5.04
4.88
4.71
4.60
4.47
4.26
4.28
4.28
4.14
3.81
3.55
3.48
3.38
3.38
3.19
3.12
Time (min)
Intensity (×10^5)
20.57
20.05
20.11
19.93
18.94
14.81
13.36
12.79
12.59
12.50
Time (min)
Intensity (×10^5)

FULL ANALYSIS DATA

	Column DB-WAX			Column DB-5		
α-Thujene	1.59	996.3	0.13	3.12	926.1	0.12
α-Pinene	1.53	989.6	0.89	3.19	931.0	0.88
3-Methylcyclohexanone				3.38*	943.7	[0.03]
Camphene	1.89	1024.7	0.02	3.38*	943.7	[0.03]
Thuja-2,4(10)-diene	2.50*	1082.9	[0.10]	3.48	950.1	0.01
6-Methyl-2-heptanone	4.04*	1203.0	[0.07]	3.55	954.9	0.01
β-Pinene	2.31	1064.6	0.40	3.81*	971.9	[0.49]
Sabinene	2.50*	1082.9	[0.10]	3.81*	971.9	[0.49]
Myrcene	3.12	1132.3	1.96	4.14	993.2	1.94
Menthatriene isomer I	3.66	1174.4	0.03	4.26*†	1001.3	[0.02]
Pseudolimonene	3.06	1128.1	0.02	4.28*†	1002.4	[0.05]
α-Phellandrene	3.02	1124.5	0.03	4.28*†	1002.4	[0.05]
α-Terpinene	3.20	1138.8	0.39	4.47	1014.8	0.39
para-Cymene	4.38	1227.9	0.03	4.60	1022.5	0.04
1,8-Cineole	3.57†	1167.2	1.98	4.71*	1029.3	[20.38]
Limonene	3.48	1160.1	18.21	4.71*	1029.3	[20.38]
(*Z*)-β-Ocimene	4.04*	1203.0	[0.07]	4.88	1040.3	0.08
(*E*)-β-Ocimene	4.25	1218.3	0.78	5.04	1050.1	0.78
γ-Terpinene	4.07	1205.5	0.52	5.16	1057.5	0.51
cis-Sabinene hydrate	7.23*	1429.5	[0.33]	5.29	1065.8	0.19
Terpinolene	4.56	1241.0	0.13	5.62*	1086.0	[0.16]
para-Cymenene	6.65	1386.3	0.05	5.62*	1086.0	[0.16]
trans-Sabinene hydrate	8.30	1509.3	0.13	5.78	1096.4	0.14
Linalool	8.37*	1514.7	[2.35]	5.89	1103.2	0.45
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	5.05	1276.7	0.03	6.13	1118.2	0.04
trans-para-Mentha-2,8-dien-1-ol	9.30*	1586.6	[8.54]	6.16	1120.1	0.03
cis-para-Mentha-2,8-dien-1-ol	9.74	1621.9	0.03	6.41	1136.1	0.04
Isopulegol	8.49*	1523.6	[0.09]	6.52	1143.1	0.11
Menthone	6.98	1410.8	8.98	6.65	1151.6	8.95
Isomenthone	7.37	1439.5	20.04	6.83*†	1163.1	[20.13]
Menthofuran	7.23*	1429.5	[0.33]	6.88*†	1166.1	[0.10]
Menthol	9.46	1598.9	0.07	7.02*†	1174.9	[0.29]
Terpinen-4-ol	8.91	1556.4	0.34	7.02*†	1174.9	[0.29]
cis-Isopulegone	8.54	1527.8	1.55	7.02*†	1174.9	[0.29]
Isopulegone analogue I	8.37*	1514.7	[2.35]	7.02*†	1174.9	[0.29]
Isomenthol	9.30*	1586.6	[8.54]	7.12	1181.6	0.04

α-Terpineol	10.12*	1652.3	[0.19]	7.24	1189.3	0.16
cis-Dihydrocarvone	8.82	1549.2	0.17	7.29	1192.4	0.15
trans-Dihydrocarvone	9.04	1566.5	0.03	7.38*	1198.3	[0.07]
trans-Isopiperitenol	10.75	1703.0	0.07	7.38*	1198.3	[0.07]
Verbenone	9.95*	1638.3	[0.07]	7.44	1201.8	0.02
Unknown MEPU IX [m/z 150, 79 (89), 80 (64), 135 (57), 77 (29), 108 (27)...]				7.49	1204.9	0.01
Unknown MEPU X [m/z 97, 69 (90), 41 (77), 43 (77), 125 (50), 124 (47)...]	10.20	1658.7	0.02	7.54	1208.8	0.03
Pulegone	9.30*	1586.6	[8.54]	7.95	1236.1	8.49
3,4-Dimethoxytoluene	11.32*	1750.7	[12.90]	8.00	1239.1	0.03
Unknown BUGR I [m/z 112, 43 (70), 70 (63), 59 (53), 97 (46), 84 (25)...]	10.65	1695.3	0.27	8.08	1244.9	0.47
Pseudodiosphenol	10.54	1685.7	10.93	8.42	1267.4	10.81
Isopulegyl acetate	8.49*	1523.6	[0.09]	8.46	1270.1	0.06
Unknown AGBE I [m/z 84, 41 (27), 69 (24), 57 (23), 71 (22)...]				8.56	1276.3	0.38
Bornyl acetate	8.60	1532.4	0.01	8.65	1282.6	0.03
trans-Sabinyl acetate	9.51	1603.1	0.02	8.80	1292.8	0.02
Diosphenol	11.32*	1750.7	[12.90]	8.89	1298.9	12.84
2-Acetyl-*para*-cresol?	12.45	1848.1	0.01	8.97	1304.2	0.01
neo-Dihydrocarvyl acetate	9.30*	1586.6	[8.54]	9.00	1306.4	0.03
Unknown MISC CLVIII [m/z 43, 136 (55), 121 (55), 107 (48), 93 (48), 81 (30), 79 (29)...]				9.05	1309.8	0.04
Unknown MEPU XIII [m/z 125, 97 (79), 43 (78), 41 (65), 67 (65), 83 (60), 69 (57)...]				9.17	1318.1	0.12
Myrtenyl acetate	9.91	1635.5	0.12	9.24	1322.7	0.13
Dihydrocarvyl acetate	9.81	1627.5	0.08	9.33	1329.6	0.10
trans-Carvyl acetate	10.49	1681.4	0.04	9.44	1337.0	0.05
exo-2-Hydroxycineole acetate	10.37	1672.0	0.02	9.48	1340.3	0.02
cis-para-Mentha-8-	11.62	1775.8	0.56	9.68	1354.2	0.77

thiol-3-one						
trans-para-Mentha-8-thiol-3-one	11.94	1803.9	2.28	9.87	1367.6	2.30
trans-Myrtanyl acetate	10.61	1691.6	0.04	10.05	1380.0	0.05
Methyleugenol	13.67	1957.3	0.06	10.38	1403.5	0.06
para-Menth-1-en-9-yl acetate?				10.58	1418.4	0.02
Germacrene D	10.12*	1652.3	[0.19]	11.34	1475.0	0.03
8-(Methylthio)-*para*-menthan-3-one				11.38	1477.7	0.03
Viridiflorene	9.95*	1638.3	[0.07]	11.54*	1489.6	[0.09]
Bicyclogermacrene	10.35	1670.4	0.02	11.54*	1489.6	[0.09]
Unknown AGBE II [m/z 43, 107 (90), 135 (73), 69 (52), 41 (47), 122 (44)...]				11.87	1514.8	0.15
(*E*)-Nerolidol	14.10	1997.1	0.02	12.50	1563.6	0.01
S-Acetyl-*cis-para*-Mentha-8-thiol-3-one	14.88	2069.9	0.29	12.59	1571.0	0.30
S-Acetyl-*trans-para*-Mentha-8-thiol-3-one	15.24	2105.7	0.09	12.79	1586.3	0.10
Isospathulenol	15.84	2164.2	0.01	13.36	1632.4	0.01
Benzyl benzoate	19.25	2524.1	0.03	14.81	1754.8	0.02
Unknown AGBE VI [m/z 191, 192 (15), 302 (3), 91 (3), 41 (3)...]				18.94	2145.6	0.04
Unknown AGBE IV [m/z 69, 41 (65), 93 (54), 109 (53), 153 (44), 81 (42)...]	21.07	2735.5	0.08	19.93	2249.1	0.07
Unknown AGBE III [m/z 69, 41 (65), 109 (52), 93 (47), 153 (40), 81 (37)...]	21.21	2752.1	0.03	20.05	2262.4	0.08
Unknown AGBE V [m/z 69, 93 (81), 41 (57), 81 (46), 109 (37), 80 (32)...]				20.12	2269.4	0.04
Unknown AGBE VII [m/z 69, 41 (44), 109 (30), 81 (28), 93 (27), 153 (19)...]	21.97	2844.8	0.02	20.58	2319.6	0.05
Total reported		96.98%			98.17%	

*: 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

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