Date : 2025-02-10

Certificate of Analysis - GC Profiling

Sample Identification

Internal code : 25A27-PTH02
Customer Identification : Blue Tansy - Morocco - B50113R
Type : Essential Oil
Source : *Tanacetum annuum*
Customer : Plant Therapy

Checked an approved by:

Sylvain Mercier, M. Sc., Chimiste 2014-005

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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

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 : Sylvain Mercier, M. Sc., Chimiste 2014-005
Date : 2025-01-29

Physicochemical data

Refractive index : 1.5078 ± 0.0003 (20 °C)
Method : PC-MAT-016 - Measure of the refractive index of a liquid.
Analyst : Cindy Caron B. Sc.
Date : 2025-01-28

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
1,3-Cyclohexadiene	tr	Alkene
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
2-Methylbutanol	tr	Aliphatic alcohol
Toluene	tr	Simple phenolic
Unknown	0.01	Unknown
Ethyl 2-methylbutyrate	0.03	Aliphatic ester
Ethyl isovalerate	0.01	Aliphatic ester
Hexanol	0.01	Aliphatic alcohol
Nonane	0.01	Alkane
Hashishene	0.01	Monoterpene
Tricyclene	0.06	Monoterpene
α-Thujene	0.44	Monoterpene
Ethyl tiglate?	0.01	Aliphatic ester
α-Pinene	2.85	Monoterpene
Camphene	0.97	Monoterpene
α-Fenchene	0.01	Monoterpene
Propyl 2-methylbutyrate	0.04	Aliphatic ester
Propyl isovalerate	0.01	Aliphatic ester
Thuja-2,4(10)-diene	0.01	Monoterpene
Benzaldehyde	0.02	Simple phenolic
Sabinene	18.48	Monoterpene
β-Pinene	6.33	Monoterpene
6-Methyl-5-hepten-2-one	0.03	Aliphatic ketone
2-Pentylfuran	0.01	Furan
Myrcene	4.34	Monoterpene
α-Phellandrene	5.35	Monoterpene
Octanal	0.02	Aliphatic aldehyde
Δ3-Carene	0.03	Monoterpene
α-Terpinene	0.99	Monoterpene
Isoamyl isobutyrate	0.02	Aliphatic ester
meta-Cymene	0.03	Monoterpene
para-Cymene	5.13	Monoterpene
β-Phellandrene	0.42	Monoterpene
Limonene	2.13	Monoterpene
1,8-Cineole	0.55	Monoterpenic ether
(*Z*)-β-Ocimene	0.03	Monoterpene
Butyl 2-methylbutyrate	0.02	Aliphatic ester
(*E*)-β-Ocimene	0.02	Monoterpene

Butyl isovalerate	0.03	Aliphatic ester
γ-Terpinene	1.67	Monoterpene
Prenyl isobutyrate	0.01	Aliphatic ester
cis-Sabinene hydrate	0.09	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.06	Aliphatic alcohol
Terpinolene	0.57	Monoterpene
para-Cymenene	0.04	Monoterpene
6,7-Epoxymyrcene	0.21	Monoterpenic ether
trans-Sabinene hydrate	0.07	Monoterpenic alcohol
Linalool	0.14	Monoterpenic alcohol
Perillene	0.01	Monoterpenic ether
2-Methylbutyl 2-methylbutyrate	0.09	Aliphatic ester
para-Mentha-1,3,8-triene	0.01	Monoterpene
Nonanal	0.02	Aliphatic aldehyde
Amyl isovalerate	0.01	Aliphatic ester
Unknown	0.16	Unknown
cis-para-Menth-2-en-1-ol	0.10	Monoterpenic alcohol
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	0.03	Monoterpene
Limona ketone	0.26	Normonoterpenic ketone
Camphor	10.02	Monoterpenic ketone
α,4-Dimethyl-3-cyclohexene-1-methanol	0.15	Normonoterpenic alcohol
Citronellal	0.04	Monoterpenic aldehyde
α,4-Dimethyl-3-cyclohexene-1-methanol epimer	tr	Normonoterpenic alcohol
Sabinaketone	0.02	Normonoterpenic ketone
Pinocarvone	0.02	Monoterpenic ketone
Unknown	0.07	Oxygenated monoterpene
Borneol	1.69	Monoterpenic alcohol
Unknown	0.10	Oxygenated monoterpene
Terpinen-4-ol	1.96	Monoterpenic alcohol
Unknown	0.08	Unknown
para-Cymen-8-ol	0.05	Monoterpenic alcohol
α-Terpineol	0.23	Monoterpenic alcohol
Myrtenal	0.02	Monoterpenic aldehyde
Myrtenol	0.03	Monoterpenic alcohol
Unknown	0.08	Unknown
cis-α-Phellandrene epoxide (iPr vs Me)	0.13	Monoterpenic ether
trans-Piperitol	0.04	Monoterpenic alcohol
Decanal	0.03	Aliphatic aldehyde
Unknown	0.03	Oxygenated monoterpene
trans-Carveol	0.04	Monoterpenic alcohol
trans-α-Phellandrene epoxide (iPr vs Me)	0.10	Monoterpenic ether
(3*Z*)-Hexenyl 2-methylbutyrate	0.05	Aliphatic ester
Hexyl 2-methylbutyrate	0.02	Aliphatic ester

Pulegone	0.03	Monoterpenic ketone
Carvotanacetone	0.11	Monoterpenic ketone
Piperitone	0.04	Monoterpenic ketone
Phellandral	0.07	Monoterpenic aldehyde
α-Terpinen-7-al	0.04	Monoterpenic aldehyde
Bornyl acetate	0.02	Monoterpenic ester
Cuminol	0.04	Monoterpenic alcohol
Thymol	0.74	Monoterpenic alcohol
4-Methylhexyl 2-methylbutyrate	0.07	Aliphatic ester
Carvacrol	0.07	Monoterpenic alcohol
para-Menth-5-en-1,2-diol isomer III	0.06	Monoterpenic alcohol
1,4-*para*-Menthadien-7-ol	0.04	Monoterpenic alcohol
α-Cubebene	0.01	Sesquiterpene
α-Terpinyl acetate	0.02	Monoterpenic ester
α-Copaene	0.11	Sesquiterpene
(*E*)-β-Damascenone	0.05	Apocarotenoid
7-epi-Sesquithujene?	0.03	Sesquiterpene
β-Elemene	0.28	Sesquiterpene
Benzyl isovalerate	0.01	Phenolic ester
α-Cedrene	0.02	Sesquiterpene
β-Caryophyllene	1.76	Sesquiterpene
β-Copaene	0.03	Sesquiterpene
Octyl 2-methylbutyrate	0.14	Aliphatic ester
trans-α-Bergamotene	0.10	Sesquiterpene
Sesquisabinene A	1.00	Sesquiterpene
α-Humulene	0.20	Sesquiterpene
(*E*)-β-Farnesene	0.10	Sesquiterpene
4,5-diepi-Aristolochene	0.09	Sesquiterpene
Dehydrosesquicineole	0.05	Sesquiterpenic ether
γ-Muurolene	0.15	Sesquiterpene
Germacrene D	1.16	Sesquiterpene
Piperonyl methyl ketone	0.12	Synthetic
γ-Curcumene	0.22	Sesquiterpene
β-Selinene	0.21	Sesquiterpene
Phenylethyl isovalerate	0.02	Phenolic ester
ar-Curcumene	0.08	Sesquiterpene
Phenylethyl 2-methylbutyrate	0.02	Phenolic ester
α-Selinene	0.25	Sesquiterpene
Bicyclogermacrene	0.13	Sesquiterpene
α-Muurolene	0.10	Sesquiterpene
δ-Guaiene	0.07	Sesquiterpene
γ-Cadinene	0.10	Sesquiterpene
3,6-Dihydrochamazulene	5.13	Azulene
β-Curcumene	0.10	Sesquiterpene
Dihydrochamazulene isomer I	0.96	Azulene

δ-Cadinene	0.07	Sesquiterpene
Dihydrochamazulene isomer II	0.13	Azulene
β-Sesquiphellandrene	0.68	Sesquiterpene
Phenylethyl angelate?	0.02	Phenolic ester
α-Elemol	0.07	Sesquiterpenic alcohol
(*E*)-Nerolidol	0.02	Sesquiterpenic alcohol
Spathulenol	0.08	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Caryophyllene oxide	0.27	Sesquiterpenic ether
10-epi-Junenol	0.05	Sesquiterpenic alcohol
Humulene epoxide II	0.03	Sesquiterpenic ether
5,6-Dihydrochamazulene	0.38	Azulene
Junenol	0.02	Sesquiterpenic alcohol
7,12-Dehydro-5,6,7,8-tetrahydrochamazulene	0.51	Azulene
γ-Eudesmol	0.05	Sesquiterpenic alcohol
Eremoligenol	0.06	Sesquiterpenic alcohol
τ-Cadinol	0.05	Sesquiterpenic alcohol
β-Eudesmol	0.59	Sesquiterpenic alcohol
Dihydrochamazulene isomer IV	0.27	Azulene
α-Eudesmol	0.16	Sesquiterpenic alcohol
(3*E*,5*E*)-7-Hydroxyfarnesene	0.03	Sesquiterpenic alcohol
Unknown	0.28	Azulene
Chamazulene	8.16	Azulene
α-Phellandrene dimer II	0.05	Diterpene
Dehydrochamazulene	0.02	Azulene
Phytone	0.07	Terpenic ketone
meta-Camphorene	0.11	Diterpene
9-(15,16-Dihydro-15-methyleneneryl)-α-terpinene?	0.21	Homoditerpene
9-(15,16-Dihydro-15-methylenegeranyl)-*para*-cymene	0.21	Homoditerpene
9-(15,16-Dihydro-15-methylenegeranyl)-α-terpinene	0.70	Homoditerpene
Unknown	0.16	Unknown
Unknown	0.51	Unknown
Unknown	0.04	Unknown
Unknown	0.03	Unknown
Consolidated total	**95.34**	

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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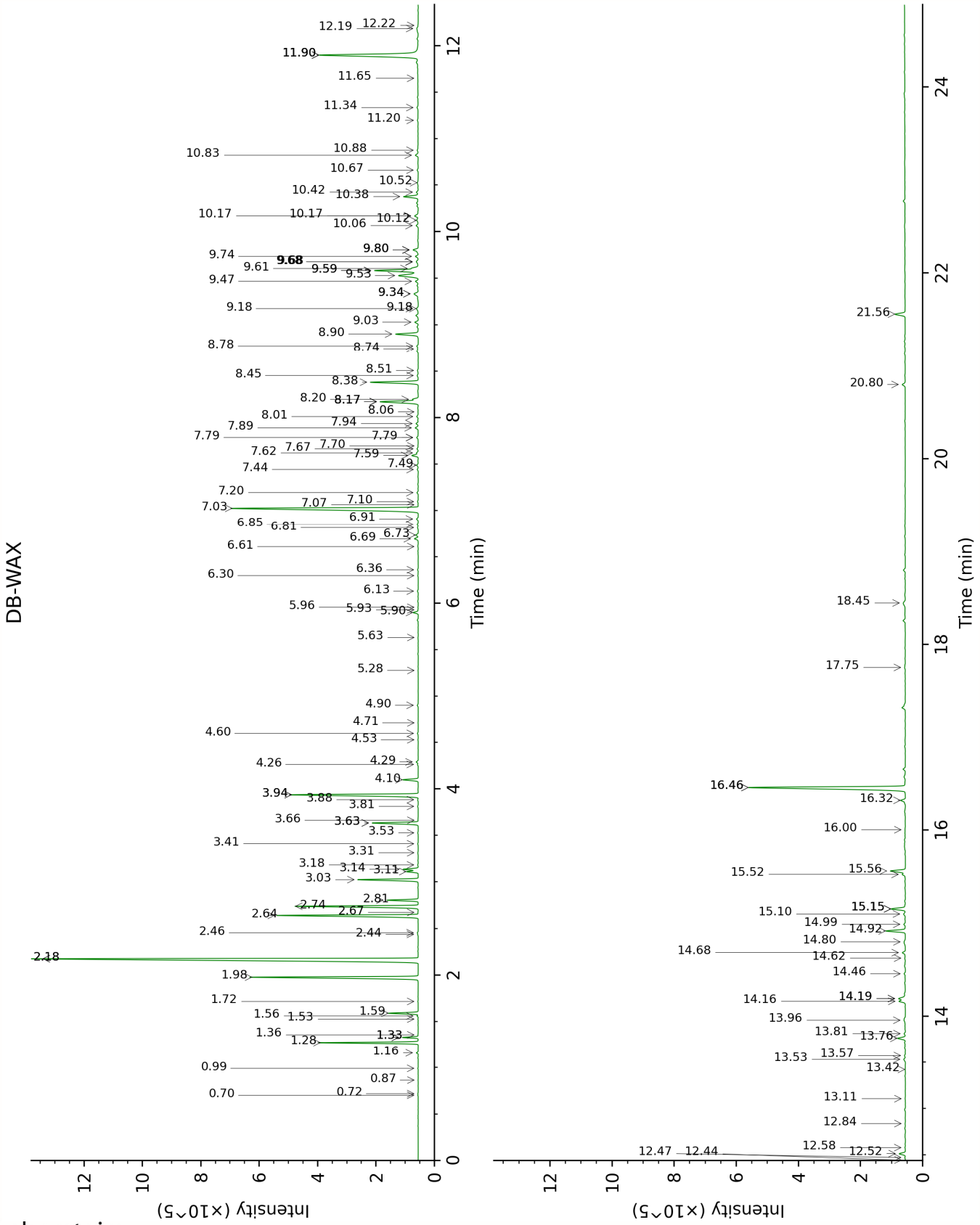
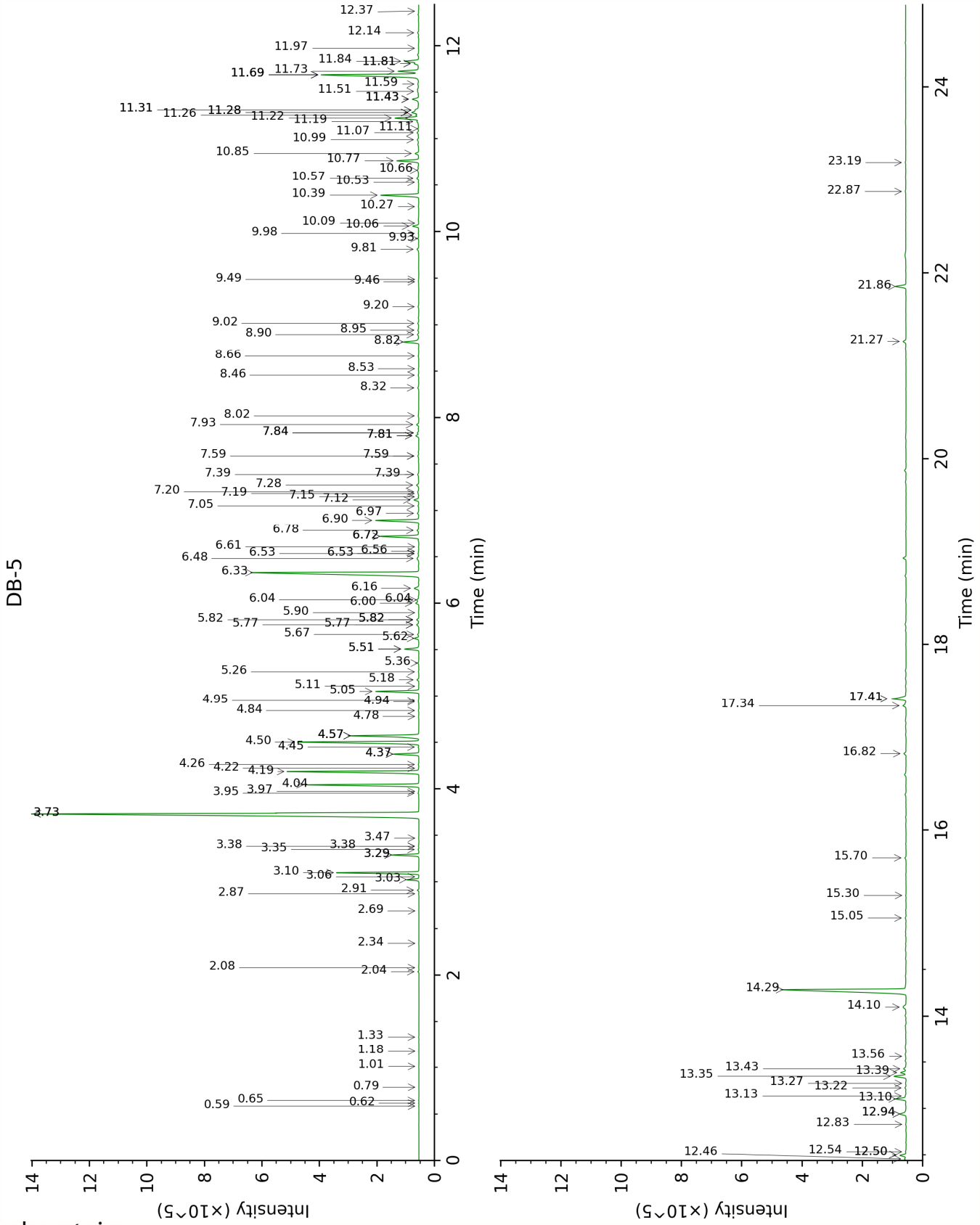

DB-WAX
Time (min)
Intensity (×10^5)
12.19
12.22
11.90
11.65
11.34
11.20
10.83
10.88
10.67
10.52
10.42
10.38
10.17
10.17
10.06
10.12
9.74
9.80
9.61
9.68
9.59
9.53
9.47
9.34
9.18
9.18
9.03
8.90
8.78
8.74
8.45
8.51
8.38
8.20
8.17
8.06
8.01
7.94
7.89
7.79
7.79
7.62
7.67
7.70
7.59
7.44
7.49
7.20
7.03
7.07
7.10
6.85
6.81
6.91
6.69
6.73
6.61
6.30
6.36
6.13
5.96
5.93
5.90
5.63
5.28
4.90
4.71
4.60
4.53
4.26
4.29
4.10
3.94
3.88
3.81
3.66
3.63
3.53
3.41
3.31
3.18
3.14
3.11
3.03
2.81
2.74
2.67
2.64
2.46
2.44
2.18
1.98
1.72
1.56
1.53
1.59
1.36
1.33
1.28
1.16
0.99
0.87
0.70
0.72
21.56
20.80
18.45
17.75
16.46
16.32
16.00
15.52
15.56
15.10
15.15
14.99
14.92
14.80
14.68
14.62
14.46
14.16
14.19
13.96
13.81
13.76
13.53
13.57
13.42
13.11
12.84
12.58
12.52
12.47
12.44


DB-5
Time (min)
Intensity (×10^5)
12.37
12.14
11.97
11.84
11.81
11.69
11.73
11.59
11.51
11.43
11.31
11.26
11.28
11.22
11.19
11.07
11.11
10.99
10.85
10.77
10.66
10.57
10.53
10.39
10.27
10.09
10.06
9.98
9.93
9.81
9.49
9.46
9.20
9.02
8.90
8.95
8.82
8.66
8.53
8.46
8.32
8.02
7.93
7.84
7.81
7.59
7.59
7.39
7.39
7.28
7.20
7.19
7.15
7.12
7.05
6.97
6.90
6.78
6.72
6.61
6.48
6.53
6.53
6.56
6.33
6.16
6.04
6.00
6.04
5.90
5.82
5.77
5.77
5.82
5.67
5.62
5.51
5.36
5.26
5.18
5.11
5.05
4.95
4.94
4.84
4.78
4.57
4.50
4.45
4.37
4.26
4.22
4.19
4.04
3.95
3.97
3.73
3.47
3.38
3.35
3.38
3.29
3.10
3.06
3.03
2.87
2.91
2.69
2.34
2.08
2.04
1.33
1.18
1.01
0.79
0.59
0.65
0.62
23.19
22.87
21.86
21.27
17.34
17.41
16.82
15.70
15.30
15.05
14.29
14.10
13.56
13.35
13.43
13.39
13.27
13.22
13.13
13.10
12.94
12.83
12.46
12.54
12.50

FULL ANALYSIS DATA

1,3-Cyclohexadiene	Column DB-WAX			Column DB-5		
				0.59	627.7	tr
Isovaleral	0.72	885.0	0.01	0.62	639.2	tr
2-Methylbutyral	0.70	878.1	0.01	0.65	649.2	0.01
2-Ethylfuran	0.87	917.7	tr	0.79	699.4	tr
2-Methylbutanol	3.32	1178.9	0.02	1.01	734.1	tr
Toluene	1.36	1001.2	0.01	1.18	757.5	tr
Unknown HEIT II [m/z 73, 87 (52), 41 (45), 56 (42), 100 (29)...]	0.99	939.5	0.01	1.34	779.8	0.01
Ethyl 2-methylbutyrate	1.56	1022.0	0.03	2.04	848.6	0.03
Ethyl isovalerate	1.72	1037.9	0.01	2.08	852.2	0.01
Hexanol	5.28	1326.3	0.01	2.34	874.0	0.01
Nonane				2.69	903.1	0.01
Hashishene	1.33*	998.2	[0.43]	2.87	915.6	0.01
Tricyclene	1.16	968.5	0.05	2.91	918.1	0.06
α-Thujene	1.33*	998.2	[0.43]	3.03	925.7	0.44
Ethyl tiglate?	3.41	1186.6	0.02	3.06	927.7	0.01
α-Pinene	1.28	988.5	2.88	3.10	930.6	2.85
Camphene	1.59	1025.0	0.97	3.29*	943.3	[0.97]
α-Fenchene	1.53	1018.6	0.01	3.29*	943.3	[0.97]
Propyl 2-methylbutyrate	2.46	1110.3	0.03	3.35	947.1	0.04
Propyl isovalerate	2.67	1127.7	0.01	3.38*	949.5	[0.02]
Thuja-2,4(10)-diene	2.18*	1084.8	[18.87]	3.38*	949.5	[0.02]
Benzaldehyde	7.06	1456.1	0.01	3.47	955.2	0.02
Sabinene	2.18*	1084.8	[18.87]	3.73*	972.6	[24.81]
β-Pinene	1.98	1064.5	6.33	3.73*	972.6	[24.81]
6-Methyl-5-hepten-2-one	4.90	1297.8	0.04	3.95	987.3	0.03
2-Pentylfuran	3.53	1196.0	0.02	3.97	988.7	0.01
Myrcene	2.74	1133.0	4.41	4.04	993.3	4.34
α-Phellandrene	2.64	1125.2	5.39	4.19	1002.8	5.35
Octanal	4.26*†	1250.7	[0.03]	4.22	1005.0	0.02
Δ3-Carene	2.44	1108.9	0.02	4.26	1007.6	0.03
α-Terpinene	2.81	1138.2	0.99	4.37*	1014.6	[0.98]
Isoamyl isobutyrate	3.18	1168.5	0.02	4.37*	1014.6	[0.98]
meta-Cymene	3.94*	1226.7	[5.20]	4.45	1019.3	0.03
para-Cymene	3.94*	1226.7	[5.20]	4.50	1022.7	5.13
β-Phellandrene	3.11	1162.7	0.42	4.57*	1027.0	[3.06]
Limonene	3.03	1155.8	2.13	4.57*	1027.0	[3.06]
1,8-Cineole	3.14	1164.7	0.55	4.57*	1027.0	[3.06]
(*Z*)-β-Ocimene	3.63*†	1204.2	[1.72]	4.78	1040.0	0.03
Butyl 2-methylbutyrate	3.66*†	1206.4	[0.02]	4.84	1044.0	0.02

(*E*)-β-Ocimene	3.88	1222.7	0.02	4.94	1050.0	0.02
Butyl isovalerate	3.81	1217.4	0.03	4.95	1050.8	0.03
γ-Terpinene	3.63*†	1204.2	[1.72]	5.05	1057.3	1.67
Prenyl isobutyrate	4.71	1283.9	0.01	5.11	1060.8	0.01
cis-Sabinene hydrate	6.73	1431.6	0.11	5.18	1065.1	0.09
cis-Linalool oxide (fur.)	6.36	1403.9	0.02	5.26	1070.5	0.02
Octanol	8.01	1527.5	0.07	5.36	1076.4	0.06
Terpinolene	4.10	1238.6	0.57	5.51*	1085.9	[0.61]
para-Cymenene	6.13	1387.4	0.04	5.51*	1085.9	[0.61]
6,7-Epoxymyrcene	5.90	1371.0	0.20	5.62	1093.1	0.21
trans-Sabinene hydrate	7.79*	1510.1	[0.09]	5.67	1095.7	0.07
Linalool	7.89	1518.2	0.14	5.77*	1102.2	[0.13]
Perillene	5.93	1373.0	0.01	5.77*	1102.2	[0.13]
2-Methylbutyl 2-methylbutyrate	4.29*†	1252.8	[0.08]	5.82*	1105.6	[0.11]
para-Mentha-1,3,8-triene	5.96	1375.0	0.01	5.82*	1105.6	[0.11]
Nonanal	5.63	1351.7	0.02	5.82*	1105.6	[0.11]
Amyl isovalerate	4.53	1270.4	0.01	5.90	1110.5	0.01
Unknown TAAN I [m/z 71, 43 (95), 81 (82), 79 (73), 67 (67), 41 (49), 109 (14)...]	6.69	1428.6	0.17	6.00	1117.0	0.16
cis-para-Menth-2-en-1-ol	7.94	1521.7	0.10	6.04*	1119.3	[0.11]
(*E*)-4,8-Dimethyl-1,3,7-nonatriene	4.60	1275.4	0.03	6.04*	1119.3	[0.11]
Limona ketone	7.60	1495.4	0.28	6.16	1127.3	0.26
Camphor	7.03	1453.4	10.05	6.33	1138.0	10.02
α,4-Dimethyl-3-cyclohexene-1-methanol				6.48	1147.7	0.15
Citronellal	6.81	1437.6	0.04	6.53*	1151.1	[0.05]
α,4-Dimethyl-3-cyclohexene-1-methanol epimer				6.53*	1151.1	[0.05]
Sabinaketone	8.51	1565.9	0.04	6.56	1152.6	0.02
Pinocarvone	7.70	1503.1	0.02	6.61	1155.7	0.02
Unknown CALU II [m/z 95, 110 (38), 81 (21), 79 (16)... 152 (7)]	7.49	1487.7	0.07	6.72*	1162.9	[1.76]
Borneol	9.58*	1651.6	[2.02]	6.72*	1162.9	[1.76]
Unknown CALU III [m/z 95, 110 (43), 81 (28), 41 (15)... 152 (8)]	7.44	1484.3	0.05	6.78	1167.1	0.10

Terpinen-4-ol	8.38	1556.1	1.97	6.90	1174.3	1.96
Unknown EUDI I [m/z 69, 68 (65), 110 (51), 67 (39), 41 (27), 83 (26)...]	7.62	1497.5	0.07	6.97	1179.2	0.08
para-Cymen-8-ol	11.34	1798.2	0.06	7.05	1184.3	0.05
α-Terpineol	9.58*	1651.6	[2.02]	7.12	1188.4	0.23
Myrtenal	8.45	1561.7	0.06	7.15	1190.5	0.02
Myrtenol	10.67	1741.2	0.04	7.19	1192.7	0.03
Unknown ABCO I [m/z 79, 107 (72), 41 (58), 55 (47), 77 (41), 67 (41)...]				7.20	1193.9	0.08
cis-α-Phellandrene epoxide (iPr vs Me)	10.83	1754.7	0.14	7.28	1198.5	0.13
trans-Piperitol	10.17*	1699.0	[0.19]	7.39*	1205.9	[0.08]
Decanal	7.10	1458.7	0.03	7.39*	1205.9	[0.08]
Unknown TAAN II [m/z 93, 41 (68), 79 (67), 91 (66), 92 (57), 67 (42), 77 (41)... 150 (12)]				7.59*	1219.2	[0.07]
trans-Carveol	11.20	1786.5	0.04	7.59*	1219.2	[0.07]
trans-α-Phellandrene epoxide (iPr vs Me)	11.90*	1848.3	[6.00]	7.81*	1233.8	[0.16]
(3*Z*)-Hexenyl 2-methylbutyrate	6.85	1440.3	0.05	7.81*	1233.8	[0.16]
Hexyl 2-methylbutyrate	6.30	1399.4	0.02	7.84*	1235.8	[0.08]
Pulegone	8.74	1584.3	0.03	7.84*	1235.8	[0.08]
Carvotanacetone	9.18*	1618.6	[0.12]	7.93	1241.8	0.11
Piperitone	9.68*	1659.1	[0.13]	8.02	1248.1	0.04
Phellandral	9.74	1663.9	0.13	8.32	1268.2	0.07
α-Terpinen-7-al	10.52	1729.1	0.07	8.46	1277.3	0.04
Bornyl acetate	8.06	1531.5	0.02	8.53	1282.0	0.02
Cuminol	13.96	2038.6	0.14	8.66	1291.2	0.04
Thymol	14.92	2132.7	0.83	8.82	1301.7	0.74
4-Methylhexyl 2-methylbutyrate	7.20	1465.8	0.06	8.90	1307.1	0.07
Carvacrol	15.15*	2156.4	[0.67]	8.95	1310.5	0.07
para-Menth-5-en-1,2-diol isomer III	14.99	2139.8	0.08	9.02	1315.7	0.06
1,4-*para*-Menthadien-7-ol	13.57	2001.2	0.04	9.20	1328.2	0.04
α-Cubebene	6.61	1422.4	0.02	9.46	1347.0	0.01
α-Terpinyl acetate	9.47	1642.2	0.13	9.49	1348.8	0.02
α-Copaene	6.91	1444.8	0.08	9.81	1371.5	0.11
(*E*)-β-Damascenone	10.88	1759.3	0.05	9.93	1379.6	0.05
7-epi-Sesquithujene?	7.67	1500.7	0.06	9.98	1383.5	0.03

β-Elemene	8.20	1541.8	0.21	10.06	1389.0	0.28
Benzyl isovalerate	11.65	1826.1	0.02	10.09	1391.2	0.01
α-Cedrene	7.79*	1510.1	[0.09]	10.27	1403.7	0.02
β-Caryophyllene	8.17*	1539.9	[1.79]	10.39	1412.8	1.76
β-Copaene	8.17*	1539.9	[1.79]	10.53	1423.1	0.03
Octyl 2-methylbutyrate	8.78	1586.6	0.07	10.57	1426.2	0.14
trans-α-Bergamotene	8.17*	1539.9	[1.79]	10.66	1433.2	0.10
Sesquisabinene A	8.90	1596.7	1.01	10.77	1440.9	1.00
α-Humulene	9.03	1606.8	0.15	10.84	1446.7	0.20
(*E*)-β-Farnesene	9.34*	1631.4	[0.27]	10.99	1457.7	0.10
4,5-diepi-Aristolochene	9.18*	1618.6	[0.12]	11.07	1463.3	0.09
Dehydrosesquicineole	9.80*	1669.5	[0.28]	11.11	1466.5	0.05
γ-Muurolene	9.34*	1631.4	[0.27]	11.19	1472.2	0.15
Germacrene D	9.53	1647.2	1.24	11.22	1475.0	1.16
Piperonyl methyl ketone	16.46*	2291.3	[8.19]	11.26	1477.3	0.12
γ-Curcumene				11.28*	1479.4	[0.44]
β-Selinene	9.61	1653.3	0.21	11.28*	1479.4	[0.44]
Phenylethyl isovalerate	12.84	1933.2	0.02	11.31*	1481.4	[0.21]
ar-Curcumene	10.42	1720.5	0.08	11.31*	1481.4	[0.21]
Phenylethyl 2-methylbutyrate	12.58	1909.2	0.02	11.43*	1490.1	[0.40]
α-Selinene	9.68*	1659.1	[0.13]	11.43*	1490.1	[0.40]
Bicyclogermacrene	9.80*	1669.5	[0.28]	11.43*	1490.1	[0.40]
α-Muurolene	9.80*	1669.5	[0.28]	11.51	1496.3	0.10
δ-Guaiene	9.68*	1659.1	[0.13]	11.59	1502.2	0.07
γ-Cadinene	10.12	1695.1	0.10	11.69*	1509.9	[5.33]
3,6-Dihydrochamazulene	11.90*	1848.3	[6.00]	11.69*	1509.9	[5.33]
β-Curcumene	10.06	1690.6	0.10	11.69*	1509.9	[5.33]
Dihydrochamazulene isomer I	11.90*	1848.3	[6.00]	11.73	1512.9	0.96
δ-Cadinene	10.17*	1699.0	[0.19]	11.81*	1519.4	[0.21]
Dihydrochamazulene isomer II	12.19	1873.6	0.13	11.81*	1519.4	[0.21]
β-Sesquiphellandrene	10.38	1716.5	0.67	11.84	1521.4	0.68
Phenylethyl angelate?				11.97	1532.3	0.02
α-Elemol	13.81	2024.6	0.06	12.14	1545.3	0.07
(*E*)-Nerolidol	13.53	1997.3	0.09	12.37	1563.6	0.02
Spathulenol	14.19*†	2061.0	[0.37]	12.46	1570.3	0.08
Caryophyllene oxide isomer	12.44	1896.6	0.01	12.50*	1573.5	[0.30]
Caryophyllene oxide	12.52	1903.2	0.27	12.50*	1573.5	[0.30]
10-epi-Junenol	12.47	1899.3	0.03	12.54	1576.4	0.05
Humulene epoxide II	13.11	1958.0	0.02	12.83	1599.6	0.03

5,6-Dihydrochamazulene	14.19*†	2061.0	[0.37]	12.94*	1608.6	[0.40]
Junenol	13.42	1987.2	0.02	12.94*	1608.6	[0.40]
7,12-Dehydro-5,6,7,8-tetrahydrochamazulene	13.76	2019.8	0.36	13.10	1621.9	0.51
γ-Eudesmol	14.68	2109.3	0.16	13.14	1624.5	0.05
Eremoligenol	14.80	2120.9	0.13	13.22	1631.7	0.06
τ-Cadinol	14.62	2103.3	0.04	13.27	1635.7	0.05
β-Eudesmol	15.15*	2156.4	[0.67]	13.35	1642.1	0.59
Dihydrochamazulene isomer IV	14.16*†	2058.2	[0.29]	13.39	1645.3	0.27
α-Eudesmol	15.10	2151.0	0.10	13.43	1648.7	0.16
(3*E*,5*E*)-7-Hydroxyfarnesene	16.00	2243.8	0.03	13.56	1659.8	0.03
Unknown TAAN IV [m/z 143, 142 (92), 157 (79), 158 (61), 141 (59), 128 (57), 159 (43), 115 (41), 202 (41)]	18.44	2512.6	0.19	14.10	1704.0	0.28
Chamazulene	16.46*	2291.3	[8.19]	14.29	1720.3	8.16
α-Phellandrene dimer II	12.22	1876.6	0.01	15.06	1787.1	0.05
Dehydrochamazulene	17.75	2433.7	0.06	15.30	1808.3	0.02
Phytone	14.46	2086.8	0.06	15.70	1845.0	0.07
meta-Camphorene	15.15*	2156.4	[0.67]	16.82	1948.8	0.11
9-(15,16-Dihydro-15-methyleneneryl)-α-terpinene?	15.52	2193.7	0.16	17.34	1997.9	0.21
9-(15,16-Dihydro-15-methylenegeranyl)-*para*-cymene	16.32	2276.9	0.21	17.41*	2005.2	[0.88]
9-(15,16-Dihydro-15-methylenegeranyl)-α-terpinene	15.56	2197.5	0.70	17.41*	2005.2	[0.88]
Unknown TAAN V analog I	20.80	2797.9	0.15	21.27	2413.3	0.16
Unknown TAAN V [m/z 186, 157 (37), 171 (18), 322 (15)]	21.56	2896.7	0.51	21.86	2481.9	0.51
Unknown TAAN V analog II				22.87	2604.0	0.04
Unknown TAAN V analog III				23.19	2643.7	0.03
Total reported		94.89%			95.34%	

*: 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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