Date : 2024-04-26

Certificate of Analysis - GC Profiling

Sample Identification

Internal code : 24D12-PTH05
Customer Identification : Blue Tansy - Morocco - B50112R
Type : Essential Oil
Source : *Tanacetum annuum*
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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

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 : Benoit Roger, Ph. D.
Date : 2024-04-26

Physicochemical data

Refractive index : 1.508 ± 0.0003 (20 °C)
Method : PC-MAT-016 - Measure of the refractive index of a liquid.
Analyst : Cindy Caron B. Sc.
Date : 2024-04-12

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
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	0.01	Aliphatic alcohol
Toluene	tr	Simple phenolic
Unknown	tr	Unknown
Methyl 2-methylbutyrate	tr	Aliphatic ester
Unknown	0.01	Unknown
Ethyl 2-methylbutyrate	0.05	Aliphatic ester
Ethyl isovalerate	0.02	Aliphatic ester
Propyl isobutyrate	tr	Aliphatic ester
Hashishene	0.01	Monoterpene
Tricyclene	0.04	Monoterpene
α-Thujene	0.27	Monoterpene
Ethyl tiglate?	0.01	Aliphatic ester
α-Pinene	2.59	Monoterpene
Camphene	0.81	Monoterpene
α-Fenchene	0.01	Monoterpene
Propyl 2-methylbutyrate	0.06	Aliphatic ester
Thuja-2,4(10)-diene	0.01	Monoterpene
Sabinene	16.38	Monoterpene
β-Pinene	6.12	Monoterpene
6-Methyl-5-hepten-2-one	0.06	Aliphatic ketone
2-Pentylfuran	0.01	Furan
Myrcene	5.88	Monoterpene
α-Phellandrene	5.49	Monoterpene
Octanal	0.03	Aliphatic aldehyde
Menthatriene isomer I	0.01	Monoterpene
Δ3-Carene	0.02	Monoterpene
α-Terpinene	0.51	Monoterpene
Isoamyl isobutyrate	0.02	Aliphatic ester
para-Cymene	4.59	Monoterpene
β-Phellandrene	0.31	Monoterpene
1,8-Cineole	0.28	Monoterpenic ether
Limonene	2.02	Monoterpene
(*Z*)-β-Ocimene	0.01	Monoterpene
Butyl 2-methylbutyrate	0.02	Aliphatic ester
Butyl isovalerate	0.01	Aliphatic ester
(*E*)-β-Ocimene	0.03	Monoterpene

γ-Terpinene	0.90	Monoterpene
Prenyl isobutyrate	0.01	Aliphatic ester
cis-Sabinene hydrate	0.10	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.04	Monoterpenic alcohol
Octanol	0.05	Aliphatic alcohol
para-Cymenene	0.04	Monoterpene
Terpinolene	0.38	Monoterpene
6,7-Epoxymyrcene	0.33	Monoterpenic ether
trans-Sabinene hydrate	0.08	Monoterpenic alcohol
Linalool	0.17	Monoterpenic alcohol
2-Methylbutyl 2-methylbutyrate	0.10	Aliphatic ester
Nonanal	0.02	Aliphatic aldehyde
Amyl isovalerate	0.01	Aliphatic ester
Unknown	0.20	Unknown
(*E*)-4,8-Dimethylnona-1,3,7-triene	0.03	Terpene derivative
cis-para-Menth-2-en-1-ol	0.09	Monoterpenic alcohol
α-Campholenal	0.05	Monoterpenic aldehyde
Limona ketone	0.41	Normonoterpenic ketone
Camphor	9.13	Monoterpenic ketone
trans-Pinocarveol	0.07	Monoterpenic alcohol
α,4-Dimethyl-3-cyclohexene-1-methanol	0.20	Normonoterpenic alcohol
Sabinaketone	0.08	Normonoterpenic ketone
Citronellal	0.02	Monoterpenic aldehyde
Pinocarvone	0.02	Monoterpenic ketone
Borneol	2.70	Monoterpenic alcohol
Unknown	0.03	Oxygenated monoterpene
Unknown	0.09	Oxygenated monoterpene
Terpinen-4-ol	1.77	Monoterpenic alcohol
Unknown	0.08	Unknown
para-Cymen-8-ol	0.05	Monoterpenic alcohol
α-Terpineol	0.22	Monoterpenic alcohol
Myrtenal	0.05	Monoterpenic aldehyde
Myrtenol	0.10	Monoterpenic alcohol
cis-α-Phellandrene epoxide (iPr vs Me)	0.12	Monoterpenic ether
Decanal	0.09	Aliphatic aldehyde
Unknown	0.03	Oxygenated monoterpene
trans-Carveol	0.03	Monoterpenic alcohol
(3*Z*)-Hexenyl 2-methylbutyrate	0.01	Aliphatic ester
Hexyl 2-methylbutyrate	0.08	Aliphatic ester
Cuminal	0.05	Monoterpenic aldehyde
Pulegone	0.05	Monoterpenic ketone
Carvotanacetone	0.07	Monoterpenic ketone
Piperitone	0.02	Monoterpenic ketone
Phellandral	0.06	Monoterpenic aldehyde
α-Terpinen-7-al	0.05	Monoterpenic aldehyde

Bornyl acetate	0.02	Monoterpenic ester
Cuminol	0.04	Monoterpenic alcohol
Perilla alcohol	0.02	Monoterpenic alcohol
Thymol	0.77	Monoterpenic alcohol
4-Methylhexyl 2-methylbutyrate	0.06	Aliphatic ester
Carvacrol	0.07	Monoterpenic alcohol
6-Hydroxycarvotanacetone	0.03	Monoterpenic alcohol
1,4-*para*-Menthadien-7-ol	0.06	Monoterpenic alcohol
Bicycloelemene	0.01	Sesquiterpene
α-Cubebene	0.03	Sesquiterpene
α-Copaene	0.07	Sesquiterpene
Modhephene	0.02	Sesquiterpene
(*E*)-β-Damascenone	0.04	Apocarotenoid
7-epi-Sesquithujene?	0.02	Sesquiterpene
β-Elemene	0.28	Sesquiterpene
α-Cedrene	0.01	Sesquiterpene
β-Caryophyllene	1.67	Sesquiterpene
β-Copaene	0.02	Sesquiterpene
Octyl 2-methylbutyrate	0.06	Aliphatic ester
trans-α-Bergamotene	0.06	Sesquiterpene
Sesquisabinene A	0.85	Sesquiterpene
α-Humulene	0.16	Sesquiterpene
(*E*)-β-Farnesene	0.14	Sesquiterpene
4,5-diepi-Aristolochene	0.10	Sesquiterpene
Dehydrosesquicineole	0.06	Sesquiterpenic ether
γ-Muurolene	0.08	Sesquiterpene
Germacrene D	1.38	Sesquiterpene
γ-Curcumene	0.07	Sesquiterpene
β-Selinene	0.43	Sesquiterpene
ar-Curcumene	0.27	Sesquiterpene
Phenylethyl isovalerate	0.04	Phenolic ester
Bicyclogermacrene	0.04	Sesquiterpene
Phenylethyl 2-methylbutyrate	0.34	Phenolic ester
δ-Guaiene	0.04	Sesquiterpene
β-Curcumene	0.03	Sesquiterpene
3,6-Dihydrochamazulene	3.26	Azulene
Dihydrochamazulene isomer I	0.70	Azulene
δ-Cadinene	0.10	Sesquiterpene
β-Sesquiphellandrene	0.67	Sesquiterpene
Dihydrochamazulene isomer II	0.05	Azulene
Dihydrochamazulene isomer III	0.03	Azulene
Isocaryophyllene epoxide B	0.02	Sesquiterpenic ether
α-Elemol	0.08	Sesquiterpenic alcohol
(*E*)-Nerolidol	0.02	Sesquiterpenic alcohol
Spathulenol	0.09	Sesquiterpenic alcohol

Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
Caryophyllene oxide	0.45	Sesquiterpenic ether
Humulene epoxide II	0.04	Sesquiterpenic ether
5,6-Dihydrochamazulene	0.53	Azulene
Junenol	0.01	Sesquiterpenic alcohol
Unknown	0.02	Sesquiterpene
7,12-Dehydro-5,6,7,8-tetrahydrochamazulene	1.83	Azulene
γ-Eudesmol	0.04	Sesquiterpenic alcohol
Eremoligenol	0.08	Sesquiterpenic alcohol
τ-Cadinol	0.04	Sesquiterpenic alcohol
β-Eudesmol	0.91	Sesquiterpenic alcohol
α-Eudesmol	0.07	Sesquiterpenic alcohol
Dihydrochamazulene isomer IV	1.09	Azulene
(3*E*,5*E*)-7-Hydroxyfarnesene	0.12	Sesquiterpenic alcohol
Unknown	0.17	Azulene
Chamazulene	10.09	Azulene
α-Phellandrene dimer II	0.06	Diterpene
Dehydrochamazulene	0.04	Azulene
Phytone	0.15	Terpenic ketone
9-(15,16-Dihydro-15-methyleneneryl)-*para*-cymene?	0.34	Homoditerpene
9-(15,16-Dihydro-15-methylenegeranyl)-*para*-cymene	0.32	Homoditerpene
9-(15,16-Dihydro-15-methylenegeranyl)-α-terpinene	1.16	Homoditerpene
Unknown	0.31	Unknown
Unknown	1.14	Unknown
Unknown	0.10	Unknown
Unknown	0.06	Unknown
Consolidated total	**95.62**	

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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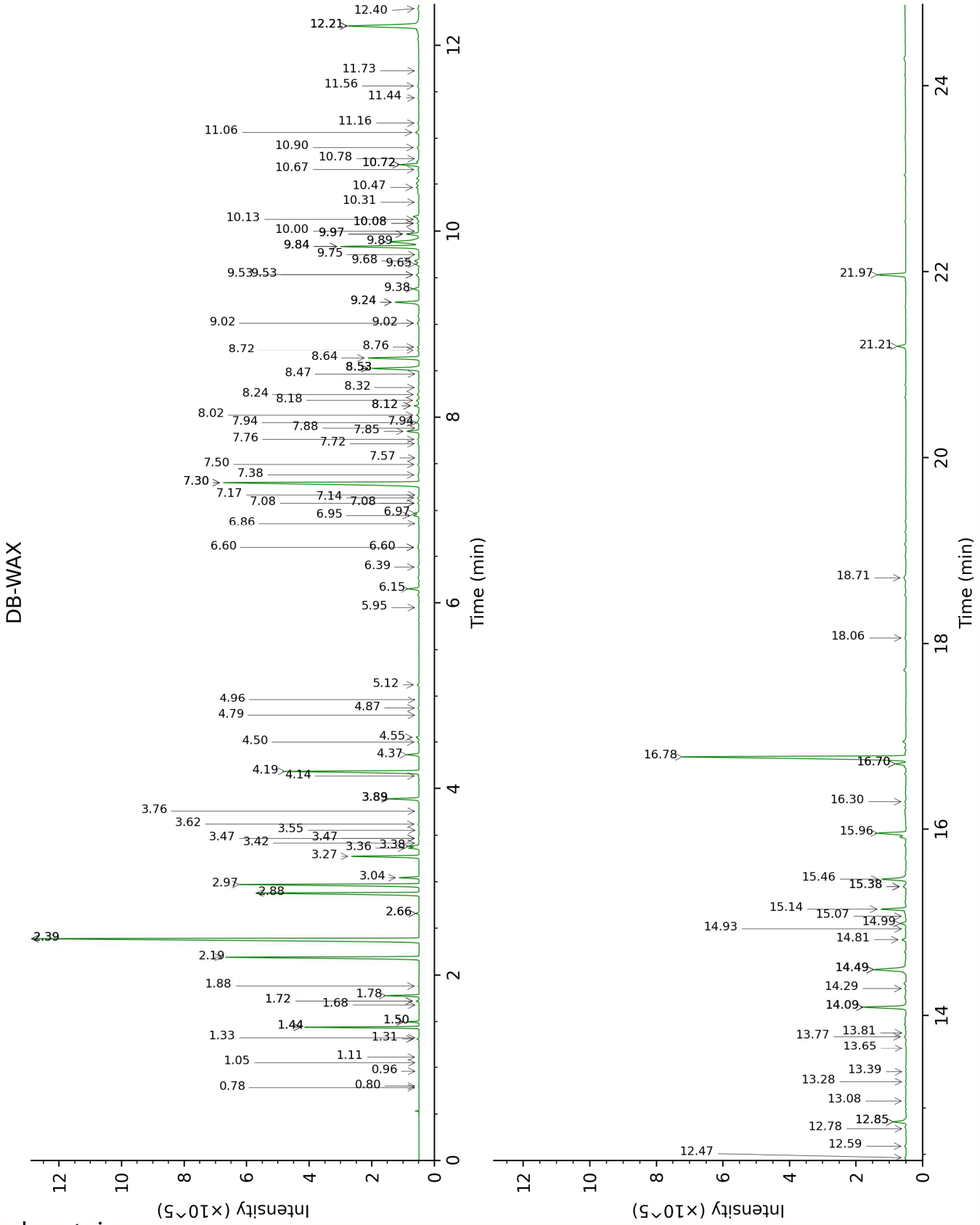
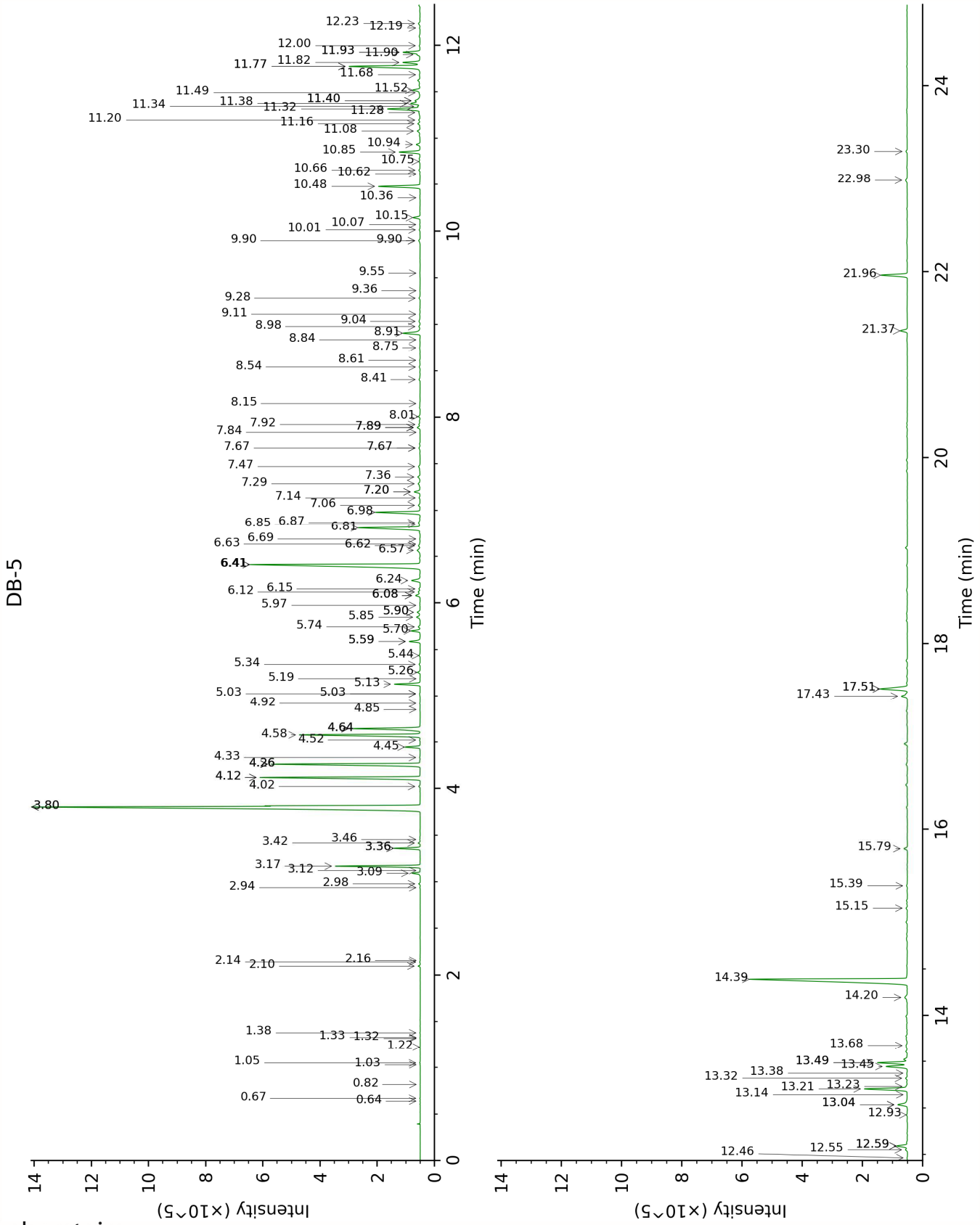

DB-WAX
Time (min)
Intensity (×10^5)
12.40
12.21
11.73
11.56
11.44
11.16
11.06
10.90
10.78
10.72
10.67
10.47
10.31
10.13
10.08
10.00
9.97
9.89
9.84
9.75
9.68
9.65
9.53
9.38
9.24
9.02
8.76
8.72
8.64
8.53
8.47
8.32
8.24
8.18
8.12
8.02
7.94
7.88
7.85
7.76
7.72
7.57
7.50
7.38
7.30
7.17
7.14
7.08
6.97
6.95
6.86
6.60
6.39
6.15
5.95
5.12
4.96
4.87
4.79
4.55
4.50
4.37
4.19
4.14
3.89
3.76
3.62
3.55
3.47
3.42
3.36
3.38
3.27
3.04
2.97
2.88
2.66
2.39
2.19
1.88
1.78
1.72
1.68
1.50
1.44
1.33
1.31
1.11
1.05
0.96
0.80
0.78
21.97
21.21
18.71
18.06
16.78
16.70
16.30
15.96
15.46
15.38
15.14
15.07
14.99
14.93
14.81
14.49
14.29
14.09
13.81
13.77
13.65
13.39
13.28
13.08
12.85
12.78
12.59
12.47


DB-5
Time (min)
Intensity (×10^5)
12.23
12.19
12.00
11.93
11.90
11.77
11.82
11.68
11.49
11.52
11.34
11.38
11.32
11.40
11.28
11.20
11.16
11.08
10.85
10.94
10.75
10.66
10.62
10.48
10.36
10.15
10.01
10.07
9.90
9.90
9.55
9.36
9.28
9.11
9.04
8.98
8.91
8.84
8.75
8.61
8.54
8.41
8.15
8.01
7.92
7.89
7.84
7.67
7.67
7.47
7.36
7.29
7.20
7.14
7.06
6.98
6.85
6.87
6.81
6.63
6.69
6.62
6.57
6.41
6.24
6.12
6.15
6.08
5.97
5.90
5.85
5.74
5.70
5.59
5.44
5.34
5.26
5.19
5.13
5.03
5.03
4.92
4.85
4.64
4.58
4.52
4.45
4.33
4.26
4.12
4.02
3.80
3.46
3.42
3.36
3.17
3.12
3.09
2.98
2.94
2.16
2.14
2.10
1.38
1.33
1.32
1.22
1.05
1.03
0.82
0.67
0.64
23.30
22.98
21.96
21.37
17.51
17.43
15.79
15.39
15.15
14.39
14.20
13.68
13.49
13.45
13.32
13.38
13.21
13.23
13.14
13.04
12.93
12.46
12.55
12.59

FULL ANALYSIS DATA

Isovaleral	**Column DB-WAX**			**Column DB-5**		
	0.80	887.2	tr	0.64	641.0	tr
2-Methylbutyral	0.78	881.2	0.01	0.67	651.1	0.01
2-Ethylfuran	0.96	924.6	tr	0.82	701.0	tr
Isoamyl alcohol	3.55	1181.2	0.01	1.03	733.2	0.01
2-Methylbutanol	3.47*	1174.6	[0.03]	1.05	736.0	0.01
Toluene	1.50*	1004.5	[0.25]	1.22	759.9	tr
Unknown HEIT III [m/z 73, 41 (54), 87 (50), 56 (47), 54 (29), 55 (25), 100 (23)... 115? (6)]	1.05	938.2	tr	1.32	772.9	tr
Methyl 2-methylbutyrate	1.33	979.1	tr	1.33	774.3	tr
Unknown HEIT II [m/z 73, 87 (52), 41 (45), 56 (42), 100 (29)...]	1.11	947.0	0.01	1.38	781.3	0.01
Ethyl 2-methylbutyrate	1.72*	1027.3	[0.06]	2.10	850.2	0.05
Ethyl isovalerate	1.88	1042.3	0.02	2.14	853.7	0.02
Propyl isobutyrate	1.68	1023.4	tr	2.16	855.2	tr
Hashishene	1.44*	995.9	[2.58]	2.94	916.7	0.01
Tricyclene	1.32	977.2	0.04	2.98	919.4	0.04
α-Thujene	1.50*	1004.5	[0.25]	3.09	926.8	0.27
Ethyl tiglate?	3.62	1186.1	0.03	3.12	928.8	0.01
α-Pinene	1.44*	995.9	[2.58]	3.17	931.9	2.59
Camphene	1.78	1032.8	0.81	3.36*	944.5	[0.82]
α-Fenchene	1.72*	1027.3	[0.06]	3.36*	944.5	[0.82]
Propyl 2-methylbutyrate	2.66*	1114.0	[0.08]	3.42	948.2	0.06
Thuja-2,4(10)-diene	2.39*	1090.0	[16.32]	3.46	950.7	0.01
Sabinene	2.39*	1090.0	[16.32]	3.80*†	973.7	[20.05]
β-Pinene	2.19	1071.3	6.12	3.80*†	973.7	[20.05]
6-Methyl-5-hepten-2-one	5.12	1294.0	0.06	4.02	988.2	0.06
2-Pentylfuran	3.76	1196.6	0.01	4.12*	994.6	[5.88]
Myrcene	2.97	1137.3	5.88	4.12*	994.6	[5.88]
α-Phellandrene	2.88	1130.4	5.49	4.26*	1004.0	[5.54]
Octanal	4.50	1249.9	0.03	4.26*	1004.0	[5.54]
Menthatriene isomer I	3.47*	1174.6	[0.03]	4.26*	1004.0	[5.54]
Δ3-Carene	2.66*	1114.0	[0.08]	4.34	1008.6	0.02
α-Terpinene	3.04	1142.8	0.51	4.45	1015.5	0.51
Isoamyl isobutyrate	3.42	1170.8	0.02	4.52	1020.3	0.02
para-Cymene	4.19	1227.6	4.59	4.58	1023.7	4.59
β-Phellandrene	3.36	1166.7	0.31	4.64*	1028.0	[2.61]
1,8-Cineole	3.38	1168.3	0.28	4.64*	1028.0	[2.61]
Limonene	3.28	1160.1	2.02	4.64*	1028.0	[2.61]
(*Z*)-β-Ocimene	3.89*	1206.6	[0.94]	4.85	1040.8	0.01

Butyl 2-methylbutyrate	3.89*	1206.6	[0.94]	4.92	1045.1	0.02
Butyl isovalerate				5.02*	1051.7	[0.04]
(*E*)-β-Ocimene	4.14	1224.1	0.03	5.02*	1051.7	[0.04]
γ-Terpinene	3.89*	1206.6	[0.94]	5.13	1058.3	0.90
Prenyl isobutyrate	4.96	1282.2	0.01	5.19	1061.9	0.01
cis-Sabinene hydrate	6.97	1429.7	0.14	5.26	1066.2	0.10
cis-Linalool oxide (fur.)	6.60*	1401.8	[0.06]	5.34	1071.6	0.04
Octanol	8.24	1526.2	0.07	5.44	1077.5	0.05
para-Cymenene	6.39	1386.4	0.04	5.59*	1086.9	[0.42]
Terpinolene	4.36	1240.3	0.38	5.59*	1086.9	[0.42]
6,7-Epoxymyrcene	6.15	1369.4	0.35	5.70	1094.0	0.33
trans-Sabinene hydrate	8.02	1509.0	0.09	5.74	1096.8	0.08
Linalool	8.12*	1516.8	[0.15]	5.85	1103.3	0.17
2-Methylbutyl 2-methylbutyrate	4.55	1253.5	0.10	5.90*	1106.6	[0.14]
Nonanal	5.95	1354.8	0.02	5.90*	1106.6	[0.14]
Amyl isovalerate	4.79	1270.4	0.01	5.98	1111.3	0.01
Unknown TAAN I [m/z 71, 43 (95), 81 (82), 79 (73), 67 (67), 41 (49), 109 (14)...]	6.95	1427.9	0.20	6.08*	1118.0	[0.21]
(*E*)-4,8-Dimethylnona-1,3,7-triene	4.87	1275.8	0.03	6.08*	1118.0	[0.21]
cis-para-Menth-2-en-1-ol	8.18	1521.3	0.11	6.12	1120.4	0.09
α-Campholenal	7.08*	1437.8	[0.05]	6.15	1122.6	0.05
Limona ketone	7.85	1495.9	0.43	6.24	1128.3	0.41
Camphor	7.30*	1454.4	[9.09]	6.41*	1139.2	[9.20]
trans-Pinocarveol	9.24*	1604.3	[0.91]	6.41*	1139.2	[9.20]
α,4-Dimethyl-3-cyclohexene-1-methanol				6.57	1149.0	0.20
Sabinaketone	8.76	1566.8	0.05	6.62	1152.2	0.08
Citronellal	7.08*	1437.8	[0.05]	6.63	1153.3	0.02
Pinocarvone	7.94*	1502.8	[0.10]	6.69	1156.8	0.02
Borneol	9.84*	1652.9	[2.91]	6.81	1164.6	2.70
Unknown CALU II [m/z 95, 110 (38), 81 (21), 79 (16)... 152 (7)]	7.72	1485.9	0.04	6.85	1167.0	0.03
Unknown CALU III [m/z 95, 110 (43), 81 (28), 41 (15)... 152 (8)]	7.76	1489.4	0.05	6.87	1168.2	0.09
Terpinen-4-ol	8.64	1557.0	1.76	6.98	1175.5	1.77
Unknown EUDI I [m/z 69, 68 (65), 110 (51), 67 (39), 41 (27), 83 (26)...]	7.94*	1502.8	[0.10]	7.06	1180.3	0.08
para-Cymen-8-ol	11.56	1798.3	0.06	7.14	1185.4	0.05

α-Terpineol	9.84*	1652.9	[2.91]	7.20*	1189.6	[0.27]
Myrtenal	8.72	1563.8	0.05	7.20*	1189.6	[0.27]
Myrtenol	10.90	1741.7	0.07	7.29	1195.1	0.10
cis-α-Phellandrene epoxide (iPr vs Me)	11.06	1755.5	0.15	7.36	1199.7	0.12
Decanal	7.38	1460.7	0.06	7.47	1206.9	0.09
Unknown TAAN II [m/z 93, 41 (68), 79 (67), 91 (66), 92 (57), 67 (42), 77 (41)... 150 (12)]				7.67*	1220.2	[0.06]
trans-Carveol	11.44	1787.4	0.03	7.67*	1220.2	[0.06]
(3*Z*)-Hexenyl 2-methylbutyrate	7.17	1444.5	0.01	7.84	1231.5	0.01
Hexyl 2-methylbutyrate	6.60*	1401.8	[0.06]	7.89*	1234.9	[0.13]
Cuminal	10.67	1721.4	0.05	7.89*	1234.9	[0.13]
Pulegone	9.02*	1586.8	[0.06]	7.92	1237.1	0.05
Carvotanacetone	9.53*	1628.1	[0.13]	8.01	1242.7	0.07
Piperitone	9.97*	1663.8	[0.50]	8.15	1252.2	0.02
Phellandral	10.08*	1673.2	[0.07]	8.41	1269.4	0.06
α-Terpinen-7-al	10.78	1731.5	0.02	8.54	1278.4	0.05
Bornyl acetate	8.32	1532.1	0.03	8.61	1283.3	0.02
Cuminol	14.29	2048.6	0.04	8.75	1292.6	0.04
Perilla alcohol	13.28	1953.1	0.02	8.84	1298.3	0.02
Thymol	15.14	2131.8	0.85	8.91	1303.1	0.77
4-Methylhexyl 2-methylbutyrate	7.50	1469.1	0.04	8.98	1307.9	0.06
Carvacrol	15.38*	2156.2	[0.14]	9.04	1311.9	0.07
6-Hydroxycarvotanacetone	11.73	1812.2	0.03	9.11	1317.2	0.03
1,4-*para*-Menthadien-7-ol	13.77	1998.9	0.08	9.28	1329.3	0.06
Bicycloelemene	7.14	1442.2	0.05	9.36	1335.0	0.01
α-Cubebene	6.86	1421.2	0.03	9.55	1348.2	0.03
α-Copaene	7.30*	1454.4	[9.09]	9.90*	1372.7	[0.08]
Modhephene	7.56	1474.4	0.02	9.90*	1372.7	[0.08]
(*E*)-β-Damascenone	11.16	1764.2	0.05	10.01	1380.8	0.04
7-epi-Sesquithujene?	7.88	1498.4	0.01	10.07	1384.8	0.02
β-Elemene	8.52*	1548.2	[1.93]	10.15	1390.1	0.28
α-Cedrene	8.12*	1516.8	[0.15]	10.36	1405.1	0.01
β-Caryophyllene	8.52*	1548.2	[1.93]	10.48	1414.1	1.67
β-Copaene	8.47	1543.6	0.01	10.62	1424.4	0.02
Octyl 2-methylbutyrate	9.02*	1586.8	[0.06]	10.66	1427.4	0.06
trans-α-Bergamotene	8.52*	1548.2	[1.93]	10.75	1434.4	0.06
Sesquisabinene A	9.24*	1604.3	[0.91]	10.85	1442.0	0.85
α-Humulene	9.38	1615.8	0.22	10.94	1448.0	0.16

(*E*)-β-Farnesene	9.65	1637.4	0.13	11.08	1458.8	0.14
4,5-diepi-Aristolochene	9.53*	1628.1	[0.13]	11.16	1464.6	0.10
Dehydrosesquicineole	10.13	1676.7	0.06	11.20	1467.5	0.06
γ-Muurolene	9.68	1640.2	0.18	11.28	1473.5	0.08
Germacrene D	9.89	1657.1	1.62	11.32	1476.4	1.38
γ-Curcumene	9.75	1645.8	0.01	11.34	1478.4	0.07
β-Selinene	9.97*	1663.8	[0.50]	11.38	1480.7	0.43
ar-Curcumene	10.72*	1726.0	[0.69]	11.40*	1483.0	[0.30]
Phenylethyl isovalerate	13.08	1933.8	0.04	11.40*	1483.0	[0.30]
Bicyclogermacrene	10.08*	1673.2	[0.07]	11.49	1489.4	0.04
Phenylethyl 2-methylbutyrate	12.85*	1912.9	[0.47]	11.52	1491.5	0.34
δ-Guaiene	10.00	1666.4	0.02	11.68	1503.8	0.04
β-Curcumene	10.31	1691.8	0.03	11.77*	1510.6	[3.29]
3,6-Dihydrochamazulene	12.21*	1855.3	[3.72]	11.77*	1510.6	[3.29]
Dihydrochamazulene isomer I	12.21*	1855.3	[3.72]	11.82	1513.9	0.70
δ-Cadinene	10.47	1704.7	0.12	11.90	1520.6	0.10
β-Sesquiphellandrene	10.72*	1726.0	[0.69]	11.92*	1522.5	[0.72]
Dihydrochamazulene isomer II	12.47	1878.4	0.05	11.92*	1522.5	[0.72]
Dihydrochamazulene isomer III	12.40	1872.3	0.04	12.00	1528.1	0.03
Isocaryophyllene epoxide B	12.21*	1855.3	[3.72]	12.19	1543.0	0.02
α-Elemol	14.09*	2029.1	[1.70]	12.23	1546.7	0.08
(*E*)-Nerolidol	13.82	2002.7	0.02	12.46	1564.8	0.02
Spathulenol	14.49*	2068.2	[1.70]	12.55	1571.7	0.09
Caryophyllene oxide isomer	12.78	1906.3	0.02	12.59*	1574.9	[0.46]
Caryophyllene oxide	12.85*	1912.9	[0.47]	12.59*	1574.9	[0.46]
Humulene epoxide II	13.39	1963.1	0.02	12.93	1601.1	0.04
5,6-Dihydrochamazulene	14.49*	2068.2	[1.70]	13.04*	1609.9	[0.55]
Junenol	13.65	1987.0	0.01	13.04*	1609.9	[0.55]
Unknown TAAN III [m/z 145, 173 (83), 159 (57), 174 (47), 129 (47), 115 (44), 128 (43), 91 (43), 157 (36), 202 (30)]				13.14	1618.7	0.02
7,12-Dehydro-5,6,7,8-tetrahydrochamazulene	14.09*	2029.1	[1.70]	13.21	1623.9	1.83
γ-Eudesmol	14.99	2116.3	0.23	13.23	1626.0	0.04
Eremoligenol	15.07	2124.0	0.04	13.32	1633.3	0.08
τ-Cadinol	14.93	2110.6	0.03	13.38	1637.9	0.04
β-Eudesmol	15.46	2164.4	1.04	13.45	1643.8	0.91

α-Eudesmol	15.38*	2156.2	[0.14]	13.49*	1647.2	[1.16]
Dihydrochamazulene isomer IV	14.49*	2068.2	[1.70]	13.49*	1647.2	[1.16]
(3*E*,5*E*)-7-Hydroxyfarnesene	16.30	2249.6	0.06	13.68	1662.9	0.12
Unknown TAAN IV [m/z 143, 142 (92), 157 (79), 158 (61), 141 (59), 128 (57), 159 (43), 115 (41), 202 (41)]	18.71	2512.5	0.19	14.20	1705.6	0.17
Chamazulene	16.78	2300.0	10.11	14.39	1722.5	10.09
α-Phellandrene dimer II	12.59	1889.5	0.05	15.15	1788.7	0.06
Dehydrochamazulene	18.06	2439.8	0.06	15.39	1809.7	0.04
Phytone	14.82	2099.3	0.17	15.79	1845.9	0.15
9-(15,16-Dihydro-15-methyleneneryl)-*para*-cymene?	16.70*	2292.1	[0.38]	17.43	1999.4	0.34
9-(15,16-Dihydro-15-methylenegeranyl)-*para*-cymene	16.70*	2292.1	[0.38]	17.51*	2006.9	[1.47]
9-(15,16-Dihydro-15-methylenegeranyl)-α-terpinene	15.96	2214.1	1.16	17.51*	2006.9	[1.47]
Unknown TAAN V analog I	21.21	2813.0	0.38	21.37	2414.6	0.31
Unknown TAAN V [m/z 186, 157 (37), 171 (18), 322 (15)]	21.97	2910.7	1.17	21.96	2484.0	1.14
Unknown TAAN V analog II				22.98	2606.2	0.10
Unknown TAAN V analog III				23.30	2645.4	0.06
Total reported		94.26%			95.62%	

*: 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