

Date : 2024-10-21

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24J04-PTH03

Customer Identification : Roman Chamomile - China - C90116R

Type : Essential Oil

Source : *Chamaemelum nobile*

Customer : Plant Therapy

Checked and approved by:

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

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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 : 2024-10-16

PHYSICOCHEMICAL DATA

Refractive index : 1.4451 ± 0.0003 (20 °C)

Method : PC-MAT-016 - Measure of the refractive index of a liquid.

Analyst : Cindy Caron B. Sc.

Date : 2024-10-08

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

ANALYSIS SUMMARY - CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
Isobutyral	tr	Aliphatic aldehyde
Methacrolein	tr	Aliphatic aldehyde
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Isobutanol	tr	Aliphatic alcohol
Methallyl alcohol	0.02	Aliphatic alcohol
3-Methyl-2-butanone	tr	Aliphatic ketone
2-Methylbutyral	0.01	Aliphatic aldehyde
3-Methyl-3-buten-2-one	tr	Aliphatic ketone
2-Ethylfuran	0.01	Furan
Isoamyl alcohol	0.01	Aliphatic alcohol
2-Methylbutanol	0.02	Aliphatic alcohol
Ethyl isobutyrate	0.01	Aliphatic ester
Toluene	tr	Simple phenolic
Isobutyl acetate	0.02	Aliphatic ester
Methyl isovalerate	0.01	Aliphatic ester
Ethyl methacrylate	tr	Aliphatic ester
Octene	0.03	Alkene
Hexanal	0.02	Aliphatic aldehyde
Methyl angelate	0.03	Aliphatic ester
3-Methylpentanol	0.03	Aliphatic alcohol
Ethyl 2-methylbutyrate	0.07	Aliphatic ester
7-Methyloctene	tr	Alkene
(3Z)-Hexenol	0.05	Aliphatic alcohol
Propyl isobutyrate	0.08	Aliphatic ester
Isobutyl propionate	0.01	Aliphatic ester
Hexanol	tr	Aliphatic alcohol
Isoamyl acetate	0.06	Aliphatic ester
2-Methylbutyl acetate	0.07	Aliphatic ester
Propyl methacrylate	0.09	Aliphatic ester
Nonene	0.02	Alkene
Ethyl angelate	0.05	Aliphatic ester
Tricyclene	0.01	Monoterpene
Isobutyl isobutyrate	1.94	Aliphatic ester
Tiglyl acetate?	0.34	Aliphatic ester
α -Pinene	5.93	Monoterpene
Methallyl isobutyrate	0.85	Aliphatic ester
Isobutyl methacrylate	1.83	Aliphatic ester
Camphene	0.54	Monoterpene
Propyl 2-methylbutyrate	0.08	Aliphatic ester
Thuja-2,4(10)-diene	0.05	Monoterpene

Benzaldehyde	0.01	Simple phenolic
Butyl isobutyrate	0.05	Aliphatic ester
Methallyl methacrylate	1.93	Aliphatic ester
β -Pinene	0.62	Monoterpene
Sabinene	0.07	Monoterpene
2-Methylbutyl propionate	0.04	Aliphatic ester
Butyl methacrylate	0.08	Aliphatic ester
Octen-3-ol	0.05	Aliphatic alcohol
3-Methylpentyl acetate	0.02	Aliphatic ester
Dehydro-1,8-cineole	tr	Monoterpenic ether
Octan-3-one	0.02	Aliphatic ketone
2-Pentylfuran	0.05	Furan
Myrcene	0.04	Monoterpene
Propyl angelate	0.88	Aliphatic ester
Isobutyl 2-methylbutyrate	0.95	Aliphatic ester
(3Z)-Hexenyl acetate	tr	Aliphatic ester
Isobutyl isovalerate	0.18	Aliphatic ester
Isoamyl isobutyrate	0.51	Aliphatic ester
2-Methylbutyl isobutyrate	2.25	Aliphatic ester
Methallyl 2-methylbutyrate	0.49	Aliphatic ester
<i>para</i> -Cymene	0.10	Monoterpene
1,8-Cineole	0.01	Monoterpenic ether
Limonene	0.72	Monoterpene
Methallyl isovalerate?	0.03	Aliphatic ester
Propyl tiglate	0.01	Aliphatic ester
Unknown	0.04	Unknown
2-Methylbutyl methacrylate	1.21	Aliphatic ester
Isoamyl methacrylate	1.83	Aliphatic ester
(E)- β -Ocimene	0.04	Monoterpene
Isobutyl angelate	10.61	Aliphatic ester
γ -Terpinene	0.04	Monoterpene
Tiglyl isobutyrate?	0.01	Aliphatic ester
Prenyl isobutyrate	1.16	Aliphatic ester
Unknown	0.03	Unknown
Methallyl angelate	12.21	Aliphatic ester
Isobutyl senecioate	0.14	Aliphatic ester
3-Methylpentyl propionate?	0.06	Aliphatic ester
<i>para</i> -Cymenene	0.01	Monoterpene
Tiglyl methacrylate	0.94	Aliphatic ester
Butyl angelate	0.49	Aliphatic ester
α -Pinene oxide	0.04	Monoterpenic ether
Isobutyl tiglate	0.09	Aliphatic ester
2-Methylbutyl isovalerate?	0.03	Aliphatic ester
Linalool	0.02	Monoterpenic alcohol
Isoamyl 2-methylbutyrate	0.23	Aliphatic ester

2-Methylbutyl 2-methylbutyrate	0.95	Aliphatic ester
Methyl tiglate	0.19	Aliphatic ester
2-Methylbutyl isovalerate	0.27	Aliphatic ester
3-Methylpentyl isobutyrate	1.28	Aliphatic ester
α -Campholenal	0.14	Monoterpenic aldehyde
<i>trans</i> -Pinocarveol	3.54	Monoterpenic alcohol
<i>trans</i> -Verbenol	0.05	Monoterpenic alcohol
Camphene hydrate	0.21	Monoterpenic alcohol
3-Methylpentyl methacrylate	2.89	Aliphatic ester
Isoamyl angelate	5.21	Aliphatic ester
2-Methylbutyl angelate	9.13	Aliphatic ester
Pinocarvone	4.20	Monoterpenic ketone
Unknown	0.04	Oxygenated monoterpene
Angelyl angelate?	0.60	Aliphatic ester
Borneol	0.15	Monoterpenic alcohol
Isopinocampone	0.19	Monoterpenic ketone
Terpinen-4-ol	0.04	Monoterpenic alcohol
Hexyl methacrylate?	0.05	Aliphatic ester
Isobutyl 3-hydroxy-2-methylenebutyrate	0.06	Aliphatic ester
<i>para</i> -Cymen-8-ol	0.04	Monoterpenic alcohol
α -Terpineol	0.01	Monoterpenic alcohol
Amyl angelate	0.10	Aliphatic ester
Myrtenal	0.70	Monoterpenic aldehyde
Myrtenol	0.28	Monoterpenic alcohol
Tiglyl angelate	2.30	Aliphatic ester
2-Methylbutyl tiglate	0.11	Aliphatic ester
Verbenone	0.09	Monoterpenic ketone
3-Methylpentyl 2-methylbutyrate?	0.58	Aliphatic ester
3-Methylpentyl isovalerate?	0.11	Aliphatic ester
<i>trans</i> -Carveol	0.02	Monoterpenic alcohol
4-Methylhexyl isobutyrate	0.01	Aliphatic ester
Myrtenyl formate?	0.02	Monoterpenic ester
Carvone	0.02	Monoterpenic ketone
2-Hydroxy-2-methylbut-3-enyl angelate	0.27	Aliphatic ester
Lepalone	0.03	Monoterpenic ketone
3-Methylpentyl angelate	9.52	Aliphatic ester
Linalyl acetate	0.16	Monoterpenic ester
(3Z)-Hexenyl angelate	0.06	Aliphatic ester
2-Methylbutyl 3-hydroxy-2-methylenebutyrate	0.03	Aliphatic ester
Isoamyl 3-hydroxy-2-methylenebutyrate	0.05	Aliphatic ester
Hexyl angelate	0.09	Aliphatic ester
<i>trans</i> -Pinocarvyl acetate	0.05	Monoterpenic ester
3-Methylpentyl tiglate	0.08	Aliphatic ester
Benzyl isobutyrate	0.03	Phenolic ester
(2E,4E)-Decadienal	0.01	Aliphatic aldehyde

Unknown	0.02	Unknown
7βH-Silphiperfol-5-ene	0.01	Sesquiterpene
Cyclosativene I	0.02	Sesquiterpene
Cyclosativene II	0.04	Sesquiterpene
α-Copaene	0.06	Sesquiterpene
4-Methylpentyl 3-hydroxy-2-methylenbutyrate	0.04	Aliphatic ester
Isobutyl phenylacetate	0.03	Phenolic ester
β-Elemene	0.03	Sesquiterpene
Phenylethyl isobutyrate	0.02	Phenolic ester
β-Caryophyllene	0.14	Sesquiterpene
Unknown	0.01	Sesquiterpene
Myrtenyl propionate?	0.01	Monoterpenic ester
<i>trans</i> -α-Bergamotene	0.02	Sesquiterpene
Benzyl angelate	0.04	Phenolic ester
α-Humulene	0.03	Sesquiterpene
(<i>E</i>)-β-Farnesene	0.47	Sesquiterpene
Myrtenyl isobutyrate	0.03	Monoterpenic ester
Germacrene D	1.18	Sesquiterpene
ar-Curcumene	0.08	Sesquiterpene
β-Selinene	0.06	Sesquiterpene
Bicyclogermacrene	0.11	Sesquiterpene
α-Selinene	0.02	Sesquiterpene
(3 <i>Z</i> ,6 <i>E</i>)-α-Farnesene	0.05	Sesquiterpene
(3 <i>E</i> ,6 <i>E</i>)-α-Farnesene	0.26	Sesquiterpene
Presilphiperfolan-9α-ol	0.02	Sesquiterpenic alcohol
δ-Cadinene	0.06	Sesquiterpene
(2 <i>Z</i> ?,8 <i>Z</i> ?) <i>-</i> Matricaria ester	0.04	Polyne ester
Spathulenol	0.05	Sesquiterpenic alcohol
Caryophyllene oxide	0.03	Sesquiterpenic ether
Phenylethyl tiglate	0.02	Phenolic ester
Copaborneol	0.11	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.01	Unknown
Xanthoxylene	0.05	Simple phenolic
Chamazulene	0.08	Azulene
Neophytadiene	0.05	Diterpene
Phytone	0.07	Terpenic ketone
Phytadiene isomer II	0.01	Diterpene
Phytol	0.02	Diterpenic alcohol
Consolidated total	98.03	

tr: The compound has been detected below 0.005% of the total signal

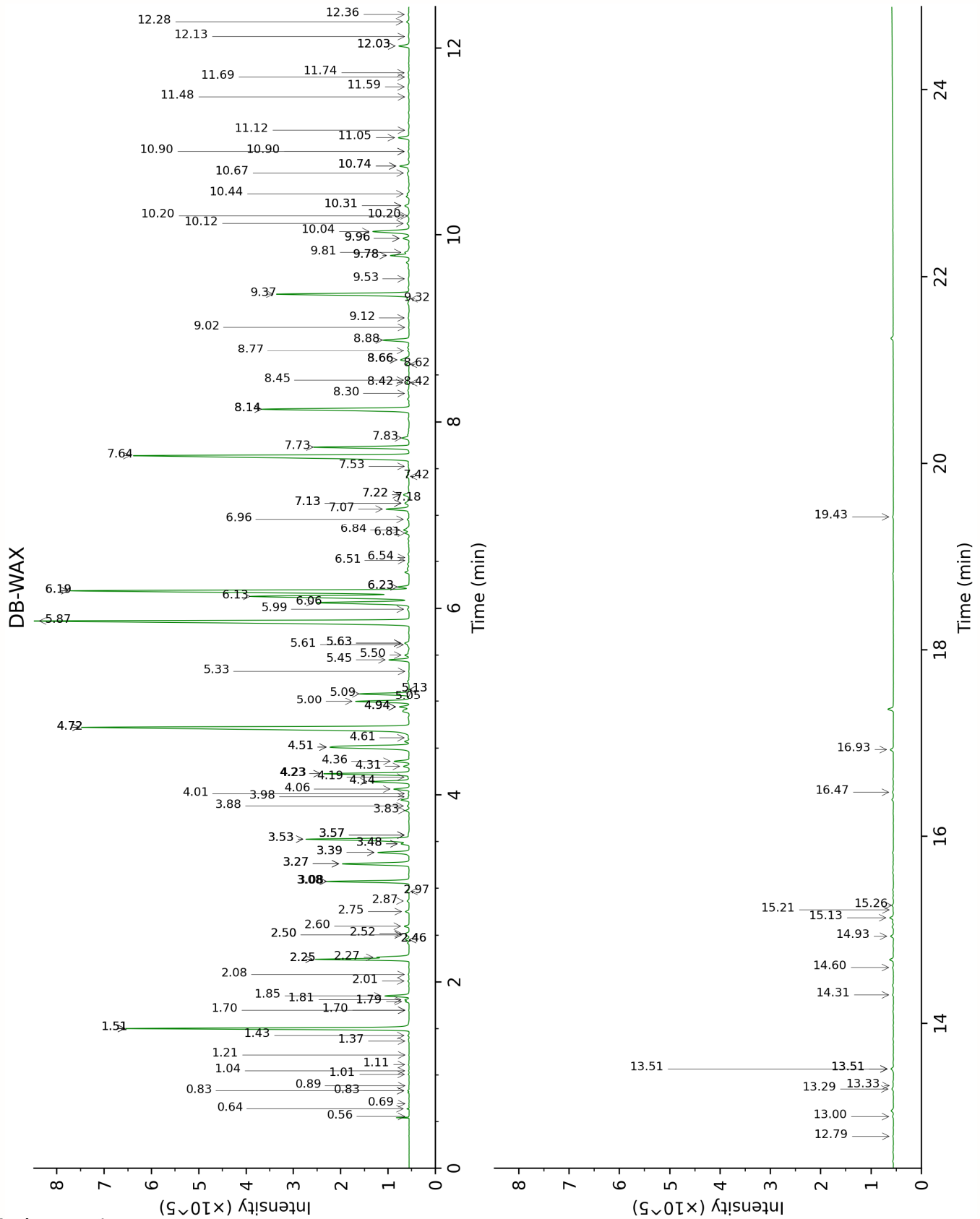
Note: no correction factor was applied

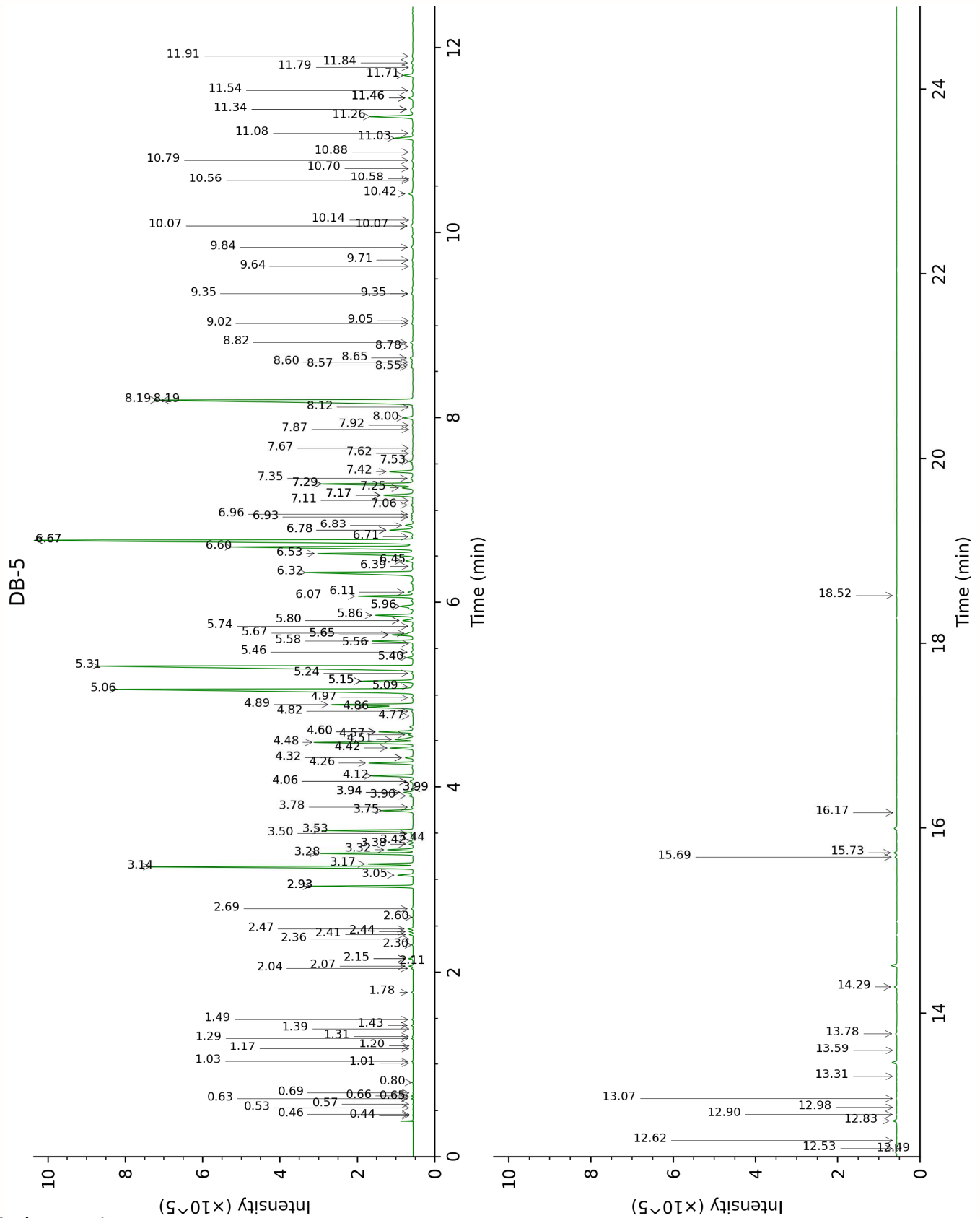
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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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FULL ANALYSIS DATA

Isobutyral	Column DB-WAX			Column DB-5		
	0.56	781.1	tr	0.44	535.9	tr
Methacrolein	0.69	835.5	tr	0.46	548.6	tr
2-Methyl-3-buten-2-ol	1.70*	1013.9	[0.01]	0.53	605.9	tr
Isobutanol	2.24*	1065.8	[1.97]	0.57	619.5	tr
Methallyl alcohol	3.57*	1172.4	[0.04]	0.63	640.0	0.02
3-Methyl-2-butanone	0.89	898.6	tr	0.65	646.0	tr
2-Methylbutyral	0.83*	883.4	[0.02]	0.66	650.4	0.01
3-Methyl-3-buten-2-one	1.21	949.5	tr	0.69	661.9	tr
2-Ethylfuran	1.01	917.3	0.01	0.80	700.9	0.01
Isoamyl alcohol	3.57*	1172.4	[0.04]	1.01	731.7	0.01
2-Methylbutanol	3.57*	1172.4	[0.04]	1.03	734.5	0.02
Ethyl isobutyrate	1.11	933.6	0.01	1.17	753.9	0.01
Toluene	1.51*	994.4	[5.93]	1.20	758.2	tr
Isobutyl acetate	1.43	982.8	0.03	1.29	770.3	0.02
Methyl isovalerate	1.51*	994.4	[5.93]	1.31	773.5	0.01
Ethyl methacrylate	1.70*	1013.9	[0.01]	1.39	784.8	tr
Octene	0.64	816.8	0.02	1.43	790.2	0.03
Hexanal	2.01	1043.7	0.03	1.49	799.0	0.02
Methyl angelate	2.52*†	1091.9	[0.08]	1.78	825.1	0.03
3-Methylpentanol	5.33	1299.4	0.01	2.04	846.6	0.03
Ethyl 2-methylbutyrate	1.79	1022.7	0.07	2.07	848.7	0.07
7-Methyloctene	0.83*	883.4	[0.02]	2.11	852.4	tr
(3Z)-Hexenol	5.99	1346.9	0.05	2.15*	855.5	[0.07]
Propyl isobutyrate	1.81	1024.5	0.08	2.15*	855.5	[0.07]
Isobutyl propionate	2.08	1050.4	0.02	2.30	867.7	0.01
Hexanol	5.63*†	1321.0	[0.11]	2.36	873.0	tr
Isoamyl acetate	2.50*†	1090.5	[0.07]	2.41	877.0	0.06
2-Methylbutyl acetate	2.50*†	1090.5	[0.07]	2.44	879.6	0.07
Propyl methacrylate	2.60	1098.8	0.11	2.47	882.0	0.09
Nonene	1.04	923.3	0.01	2.60	892.5	0.02
Ethyl angelate	2.97	1127.0	0.06	2.69	900.1	0.05
Tricyclene	1.37	973.6	0.01	2.93*	916.9	[1.95]
Isobutyl isobutyrate	2.24*	1065.8	[1.97]	2.93*	916.9	[1.95]
Tiglyl acetate?	4.06	1208.5	0.34	3.05	924.8	0.34
α-Pinene	1.51*	994.4	[5.93]	3.14	930.8	5.93

Methallyl isobutyrate	3.26*	1149.3	[1.82]	3.17	932.7	0.85
Isobutyl methacrylate	3.08*	1135.1	[1.88]	3.28	940.3	1.83
Camphene	1.85	1028.5	0.55	3.32	942.9	0.54
Propyl 2-methylbutyrate	2.75	1110.6	0.09	3.38	946.8	0.08
Thuja-2,4(10)-diene	2.46*	1085.8	[0.09]	3.42	949.1	0.05
Benzaldehyde	7.53	1458.8	0.03	3.44	950.8	0.01
Butyl isobutyrate	2.87	1119.2	0.05	3.50	954.5	0.05
Methallyl methacrylate	4.23*	1220.0	[1.95]	3.53	956.8	1.93
β-Pinene	2.27	1067.8	0.62	3.75*	970.8	[0.69]
Sabinene	2.46*	1085.8	[0.09]	3.75*	970.8	[0.69]
2-Methylbutyl propionate	3.39*	1158.4	[0.76]	3.78	973.3	0.04
Butyl methacrylate	3.83	1192.2	0.08	3.90	981.4	0.08
Octen-3-ol	6.96	1416.9	0.05	3.94*	983.8	[0.25]
3-Methylpentyl acetate	4.01	1205.0	0.02	3.94*	983.8	[0.25]
Dehydro-1,8-cineole	3.26*	1149.3	[1.82]	3.99*	986.7	[0.03]
Octan-3-one	4.19	1217.4	0.02	3.99*	986.7	[0.03]
2-Pentylfuran	3.88	1195.8	0.05	4.06*	991.6	[0.09]
Myrcene	3.08*	1135.1	[1.88]	4.06*	991.6	[0.09]
Propyl angelate	4.14	1214.1	0.92	4.12	995.7	0.88
Isobutyl 2-methylbutyrate	3.26*	1149.3	[1.82]	4.26	1004.7	0.95
(3Z)-Hexenyl acetate	5.14*	1283.3	[0.01]	4.32*	1008.4	[0.18]
Isobutyl isovalerate	3.48*	1165.4	[0.19]	4.32*	1008.4	[0.18]
Isoamyl isobutyrate	3.53*	1169.1	[2.77]	4.42	1014.9	0.51
2-Methylbutyl isobutyrate	3.53*	1169.1	[2.77]	4.48	1018.7	2.25
Methallyl 2-methylbutyrate	4.36	1229.3	0.35	4.51	1020.6	0.49
para-Cymene	4.31	1225.5	0.13	4.56	1023.9	0.10
1,8-Cineole	3.48*	1165.4	[0.19]	4.60*	1025.9	[0.76]
Limonene	3.39*	1158.4	[0.76]	4.60*	1025.9	[0.76]
Methallyl isovalerate?	4.61	1246.8	0.03	4.60*	1025.9	[0.76]
Propyl tiglate	5.14*	1283.3	[0.01]	4.77	1036.5	0.01

Unknown CHNO I [m/z 43, 41 (84), 71 (62), 69 (59), 68 (51), 67 (48), 93 (41)...156 (4)]				4.82	1039.7	0.04
2-Methylbutyl methacrylate	4.51*	1239.9	[3.09]	4.86	1042.5	1.21
Isoamyl methacrylate	4.51*	1239.9	[3.09]	4.89	1044.3	1.83
(E)-β-Ocimene	4.23*	1220.0	[1.95]	4.97	1049.2	0.04
Isobutyl angelate	4.72*	1254.7	[11.48]	5.06	1055.1	10.61
γ-Terpinene	3.98	1202.6	0.02	5.09	1056.8	0.04
Tiglyl isobutyrate?	5.05	1277.3	0.01	5.15*	1060.6	[1.17]
Prenyl isobutyrate	5.09	1280.1	1.16	5.15*	1060.6	[1.17]
Unknown CHNO II [m/z 71, 43 (28), 41 (21), 57 (19), 98 (11)... 116 (4), 129 (1), 156 (t)]						
	7.18	1433.2	0.01	5.24	1065.9	0.03
Methallyl angelate	5.87	1337.9	12.17	5.31	1070.8	12.21
Isobutyl senecioate	5.50	1311.8	0.11	5.40	1076.5	0.14
3-Methylpentyl propionate?	4.94*	1269.9	[0.24]	5.46	1080.3	0.06
<i>para</i> -Cymenene	6.51	1384.1	0.01	5.56	1086.1	0.01
Tiglyl methacrylate	6.19*†	1361.1	[10.49]	5.58	1087.7	0.94
Butyl angelate	5.45	1308.2	0.49	5.65*	1092.0	[0.52]
α-Pinene oxide	5.63*†	1321.0	[0.11]	5.65*	1092.0	[0.52]
Isobutyl tiglate	5.61*†	1319.8	[0.04]	5.67	1093.1	0.09
2-Methylbutyl isovalerate?	4.94*	1269.9	[0.24]	5.74	1097.8	0.03
Linalool	8.30	1517.4	0.02	5.80*	1101.6	[0.25]
Isoamyl 2- methylbutyrate	4.72*	1254.7	[11.48]	5.80*	1101.6	[0.25]
2-Methylbutyl 2- methylbutyrate	4.72*	1254.7	[11.48]	5.86	1105.2	0.95
Methallyl tiglate	6.84	1408.0	0.19	5.96*	1111.4	[0.46]
2-Methylbutyl isovalerate	4.94*	1269.9	[0.24]	5.96*	1111.4	[0.46]
3-Methylpentyl isobutyrate	5.00	1274.0	1.29	6.07	1118.4	1.28
α-Campholenal	7.22*	1436.4	[0.18]	6.11	1121.1	0.14
<i>trans</i> -Pinocarveol	9.37	1600.1	3.47	6.32	1134.7	3.54
<i>trans</i> -Verbenol	9.78*	1633.3	[0.48]	6.39	1138.9	0.05
Camphene hydrate	8.66*†	1545.2	[0.32]	6.45	1142.7	0.21

3-Methylpentyl methacrylate	6.06	1351.9	2.68	6.53	1147.7	2.89
Isoamyl angelate	6.13	1356.8	5.13	6.60	1152.3	5.21
2-Methylbutyl angelate	6.19*†	1361.1	[10.49]	6.67*	1156.9	[13.33]
Pinocarvone	8.14*	1504.5	[4.18]	6.67*	1156.9	[13.33]
Unknown CHNO III [m/z 96, 95 (72), 67 (45), 41 (42), 55 (32), 70 (27)... 152 (t)]	10.31*	1676.0	[0.15]	6.71	1159.4	0.04
Angelyl angelate?	7.07	1425.0	0.60	6.78*	1163.9	[0.74]
Borneol	9.96*	1648.0	[0.16]	6.78*	1163.9	[0.74]
Isopinocampone	7.83	1481.3	0.21	6.83	1167.2	0.19
Terpinen-4-ol	8.77	1553.0	0.04	6.93	1173.4	0.04
Hexyl methacrylate?				6.96	1175.3	0.05
Isobutyl 3-hydroxy-2-methylenebutyrate	11.12	1744.0	0.02	7.06	1181.7	0.06
<i>para</i> -Cymen-8-ol	11.74	1795.9	0.03	7.11	1184.9	0.04
α -Terpineol	9.96*	1648.0	[0.16]	7.16*	1188.5	[0.80]
Amyl angelate	6.81	1405.5	0.10	7.16*	1188.5	[0.80]
Myrtenal	8.88	1562.0	0.70	7.16*	1188.5	[0.80]
Myrtenol	11.05	1737.3	0.28	7.24	1193.6	0.28
Tiglyl angelate	7.73	1474.0	2.30	7.29*	1196.3	[2.41]
2-Methylbutyl tiglate	7.13*	1429.7	[0.16]	7.29*	1196.3	[2.41]
Verbenone	9.82	1635.9	0.13	7.35	1200.1	0.09
3-Methylpentyl 2-methylbutyrate?	6.23*†	1364.0	[0.26]	7.42	1204.8	0.58
3-Methylpentyl isovalerate?	6.23*†	1364.0	[0.26]	7.53	1212.3	0.11
<i>trans</i> -Carveol	11.59	1783.1	0.03	7.62	1217.9	0.02
4-Methylhexyl isobutyrate				7.67	1221.7	0.01
Myrtenyl formate?	9.12	1580.2	0.03	7.87	1235.2	0.02
Carvone	10.20*	1667.3	[0.05]	7.92	1238.3	0.02
2-Hydroxy-2-methylbut-3-enyl angelate	12.02*	1821.3	[0.26]	8.00	1243.7	0.27
Lepalone	11.69	1792.0	0.02	8.12	1251.4	0.03
3-Methylpentyl angelate	7.64	1467.3	9.52	8.19*	1256.5	[9.68]
Linalyl acetate	8.42*	1526.3	[0.07]	8.19*	1256.5	[9.68]

(3Z)-Hexenyl angelate	8.42*	1526.3	[0.07]	8.55	1280.3	0.06
2-Methylbutyl 3-hydroxy-2-methylenebutyrate	12.36	1851.0	0.03	8.57	1281.9	0.03
Isoamyl 3-hydroxy-2-methylenebutyrate	12.28	1844.1	0.07	8.60	1283.9	0.05
Hexyl angelate	8.14*	1504.5	[4.18]	8.65	1286.9	0.09
<i>trans</i> -Pinocarvyl acetate	9.32	1596.0	0.06	8.78	1295.6	0.05
3-Methylpentyl tiglate	8.45	1528.4	0.06	8.82	1298.6	0.08
Benzyl isobutyrate	10.90*	1724.7	[0.03]	9.02	1312.7	0.03
(2E,4E)-Decadienal	11.48	1774.0	0.02	9.05	1314.8	0.01
Unknown CHNO V [m/z 83, 55 (79), 82 (26), 43 (25), 45 (18), 69 (15)...166 (8)]	14.31	2029.9	0.02	9.34*	1335.3	[0.06]
7βH-Silphiperfol-5-ene	6.54	1386.5	0.01	9.34*	1335.3	[0.06]
Cyclosativene I	7.13*	1429.7	[0.16]	9.64	1356.0	0.02
Cyclosativene II	7.22*	1436.4	[0.18]	9.71	1360.8	0.04
α-Copaene	7.42	1450.9	0.08	9.84	1370.5	0.06
4-Methylpentyl 3-hydroxy-2-methylenebutyrate	13.51*	1954.7	[0.08]	10.07*	1386.6	[0.10]
Isobutyl phenylacetate	12.13	1830.2	0.03	10.07*	1386.6	[0.10]
β-Elemene	8.62*†	1541.5	[0.07]	10.07*	1386.6	[0.10]
Phenylethyl isobutyrate	12.02*	1821.3	[0.26]	10.14	1391.1	0.02
β-Caryophyllene	8.66*†	1545.2	[0.32]	10.42	1411.5	0.14
Unknown EUMA X [m/z 121, 93 (72), 107 (50), 105 (47), 91 (47), 119 (39), 79 (34), 133 (33)... 204 (14)]	9.02	1572.5	0.01	10.56	1422.2	0.01
Myrtenyl propionate?				10.58	1423.5	0.01
<i>trans</i> -α-Bergamotene	8.66*†	1545.2	[0.32]	10.70	1432.4	0.02
Benzyl angelate	13.29	1934.9	0.05	10.79	1438.9	0.04

α -Humulene	9.53	1613.2	0.04	10.88	1445.6	0.03
(E)- β -Farnesene	9.78*	1633.3	[0.48]	11.03	1456.8	0.47
Myrtenyl isobutyrate	10.74*	1711.6	[0.27]	11.08	1460.6	0.03
Germacrene D	10.04	1653.9	1.17	11.26	1474.1	1.18
α -Curcumene	10.90*	1724.7	[0.03]	11.34*†	1479.8	[0.08]
β -Selinene	10.12	1660.8	0.06	11.34*†	1479.8	[0.08]
Bicyclogermacrene	10.31*	1676.0	[0.15]	11.46*	1489.0	[0.13]
α -Selinene	10.20*	1667.3	[0.05]	11.46*	1489.0	[0.13]
(3Z,6E)- α -Farnesene	10.44	1686.3	0.05	11.54	1495.0	0.05
(3E,6E)- α -Farnesene	10.74*	1711.6	[0.27]	11.70	1507.5	0.26
Presilphiperfolan-9 α -ol	13.51*	1954.7	[0.08]	11.79	1514.1	0.02
δ -Cadinene	10.67	1705.3	0.08	11.84	1518.0	0.06
(2Z?,8Z?)-Matricaria ester	16.47	2245.6	0.03	11.91	1523.7	0.04
Spathulenol	14.60	2058.0	0.03	12.49	1569.2	0.05
Caryophyllene oxide	13.00	1907.8	0.03	12.53	1572.5	0.03
Phenylethyl tiglate	15.26	2123.0	0.03	12.62	1579.2	0.02
Copaborneol	15.13	2109.8	0.11	12.83	1596.0	0.11
Unknown ARAN XXXV [m/z 203, 218 (33), 161 (22), 91 (20), 204 (16)]	13.33	1938.3	0.01	12.90	1601.3	0.02
Unknown CHNO VII [m/z 105, 131 (96), 91 (95), 93 (84), 159 (82), 43 (70)...220 (6)]				12.98	1607.6	0.01
Unknown POCA XXI [m/z 43, 79 (41), 93 (39), 41 (39), 91 (38), 81 (36)... 220 (3)]	15.22	2118.1	0.02	13.07	1615.6	0.02
Unknown CHNO VIII [m/z 43, 79 (65), 91 (64), 80 (63), 93 (60), 81 (59)...220 (5)]				13.31	1635.3	0.01
Unknown SASC VIII [m/z 81, 41 (46), 79 (46), 93 (39), 91				13.59	1658.5	0.01

(33), 107 (33)... 206 (8)]						
Xanthoxyline				13.78	1673.9	0.05
Chamazulene	16.93	2293.0	0.08	14.29	1716.4	0.08
Neophytadiene	12.79	1888.5	0.01	15.68	1839.4	0.05
Phytone	14.93	2090.1	0.08	15.73	1843.8	0.07
Phytadiene isomer II	13.51*	1954.7	[0.08]	16.17	1883.1	0.01
Phytol	19.43	2571.3	0.02	18.52	2110.6	0.02
Total reported		96.65%			98.16%	

*: 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