

Date : March 01, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22B22-PTH01


Customer identification : Chamomile Roman ORGANIC - Hungary - CC3105219R

Type : Essential oil

Source : *Chamaemelum nobile*

Customer : Plant Therapy

ANALYSIS

Method: PC-MAT-014  - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.

Analyst : Seydou Ka, Ph. D.

Analysis date : February 28, 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

PHYSICOCHEMICAL DATA

Physical aspect: Clear liquid

Refractive index: 1.4418 ± 0.0003 (20 °C; method PC-MAT-016)

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
Isobutanol	0.04	Aliphatic alcohol
Methallyl alcohol	0.05	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
3-Methyl-2-butanone	0.01	Aliphatic ketone
Isoamyl alcohol	0.19	Aliphatic alcohol
2-Methylbutanol	0.23	Aliphatic alcohol
Ethyl isobutyrate	0.01	Aliphatic ester
Toluene	0.01	Simple phenolic
Ethyl methacrylate	tr	Aliphatic ester
Octene	0.02	Alkene
Hexanal	0.02	Aliphatic aldehyde
Methyl angelate	0.05	Aliphatic ester
3-Methylpentanol	1.22	Aliphatic alcohol
Propyl isobutyrate	0.02	Aliphatic ester
(3Z)-Hexenol	0.11	Aliphatic alcohol
Isobutyl propionate	0.01	Aliphatic ester
Isoamyl acetate	0.18	Aliphatic ester
2-Methylbutyl acetate	0.05	Aliphatic ester
Propyl methacrylate	0.03	Aliphatic ester
Ethyl angelate	0.11	Aliphatic ester
Isobutyl isobutyrate	0.37	Aliphatic ester
Tricyclene	0.03	Monoterpene
Tiglyl acetate?	0.02	Aliphatic ester
α -Thujene	0.01	Monoterpene
α -Pinene	10.78	Monoterpene
Methallyl isobutyrate	0.30	Aliphatic ester
Isobutyl methacrylate	0.24	Aliphatic ester
α -Fenchene	0.03	Monoterpene
Camphene	0.43	Monoterpene
Propyl 2-methylbutyrate	0.07	Aliphatic ester
Thuja-2,4(10)-diene	0.02	Monoterpene
Benzaldehyde	0.03	Simple phenolic
Isobutyl butyrate	3.06	Aliphatic ester
Butyl isobutyrate	0.02	Aliphatic ester
Methallyl methacrylate	0.53	Aliphatic ester
Sabinene	0.05	Monoterpene
β -Pinene	0.41	Monoterpene
2-Methylbutyl propionate	0.03	Aliphatic ester
Butyl methacrylate	0.02	Aliphatic ester
3-Methylpentyl acetate	0.33	Aliphatic ester
Octen-3-ol	0.07	Aliphatic alcohol
Octan-3-one	0.03	Aliphatic ketone
Myrcene	0.09	Monoterpene
Propyl angelate	0.69	Aliphatic ester
Isobutyl 2-methylbutyrate	0.02	Aliphatic ester

Isobutyl isovalerate	0.08	Aliphatic ester
(3Z)-Hexenyl acetate	0.03	Aliphatic ester
Isoamyl isobutyrate	4.01	Aliphatic ester
2-Methylbutyl isobutyrate	1.32	Aliphatic ester
para-Cymene	0.05	Monoterpene
Methallyl 2-methylbutyrate	0.07	Aliphatic ester
Methallyl isovalerate?	0.02	Aliphatic ester
Limonene	0.06	Monoterpene
1,8-Cineole	0.01	Monoterpenic ether
Propyl tiglate	0.01	Aliphatic ester
Unknown	0.01	Unknown
2-Methylbutyl methacrylate	0.58	Aliphatic ester
Isoamyl methacrylate	0.41	Aliphatic ester
Isobutyl angelate	11.11	Aliphatic ester
γ-Terpinene	0.01	Monoterpene
Prenyl isobutyrate	0.02	Aliphatic ester
Tiglyl isobutyrate?	0.05	Aliphatic ester
Unknown	0.02	Unknown
Methallyl angelate	12.76	Aliphatic ester
Isobutyl senecioate	0.07	Aliphatic ester
3-Methylpentyl propionate?	0.24	Aliphatic ester
Tiglyl methacrylate	0.02	Aliphatic ester
Isobutyl tiglate	0.21	Aliphatic ester
Butyl angelate	0.27	Aliphatic ester
2-Methylbutyl isovalerate?	0.01	Aliphatic ester
Linalool	0.02	Monoterpenic alcohol
Isoamyl 2-methylbutyrate	0.14	Aliphatic ester
2-Methylbutyl 2-methylbutyrate	0.15	Aliphatic ester
Methallyl tiglate	0.14	Aliphatic ester
3-Methylpentyl isobutyrate	5.77	Aliphatic ester
α-Campholenal	0.04	Monoterpenic aldehyde
<i>trans</i> -Pinocarveol	5.76	Monoterpenic alcohol
<i>trans</i> -Verbenol	0.03	Monoterpenic alcohol
Camphene hydrate	0.23	Monoterpenic alcohol
3-Methylpentyl methacrylate	1.47	Aliphatic ester
Isoamyl angelate	6.16	Aliphatic ester
Pinocarpone	1.21	Monoterpenic ketone
2-Methylbutyl angelate	6.27	Aliphatic ester
Unknown	0.02	Oxygenated monoterpene
Borneol	0.23	Monoterpenic alcohol
Angelyl angelate?	0.63	Aliphatic ester
Isopinocampone	0.09	Monoterpenic ketone
Terpinen-4-ol	0.05	Monoterpenic alcohol
Isobutyl 3-hydroxy-2-methylenebutyrate	0.09	Aliphatic ester
para-Cymen-8-ol	0.01	Monoterpenic alcohol
Myrtenal	0.58	Monoterpenic aldehyde
Amyl angelate	0.04	Aliphatic ester
Myrtenol	0.42	Monoterpenic alcohol
2-Methylbutyl tiglate	0.11	Aliphatic ester
3-Methylpentyl 2-methylbutyrate?	0.86	Aliphatic ester
3-Methylpentyl isovalerate?	0.04	Aliphatic ester
<i>trans</i> -Carveol	0.02	Monoterpenic alcohol

4-Methylhexyl isobutyrate	0.01	Aliphatic ester
3-Methylpentyl angelate	16.24	Aliphatic ester
(3Z)-Hexenyl angelate	0.01	Aliphatic ester
Hexyl angelate	0.01	Aliphatic ester
<i>trans</i> -Pinocarvyl acetate	0.03	Monoterpenic ester
3-Methylpentyl tiglate	0.07	Aliphatic ester
7 β H-Silphiperfol-5-ene	0.02	Sesquiterpene
β -Caryophyllene	0.01	Sesquiterpene
Myrtenyl propionate?	0.01	Monoterpenic ester
(<i>E</i>)- β -Farnesene	0.01	Sesquiterpene
(3Z,6E)- α -Farnesene	0.01	Sesquiterpene
Consolidated total	98.49%	

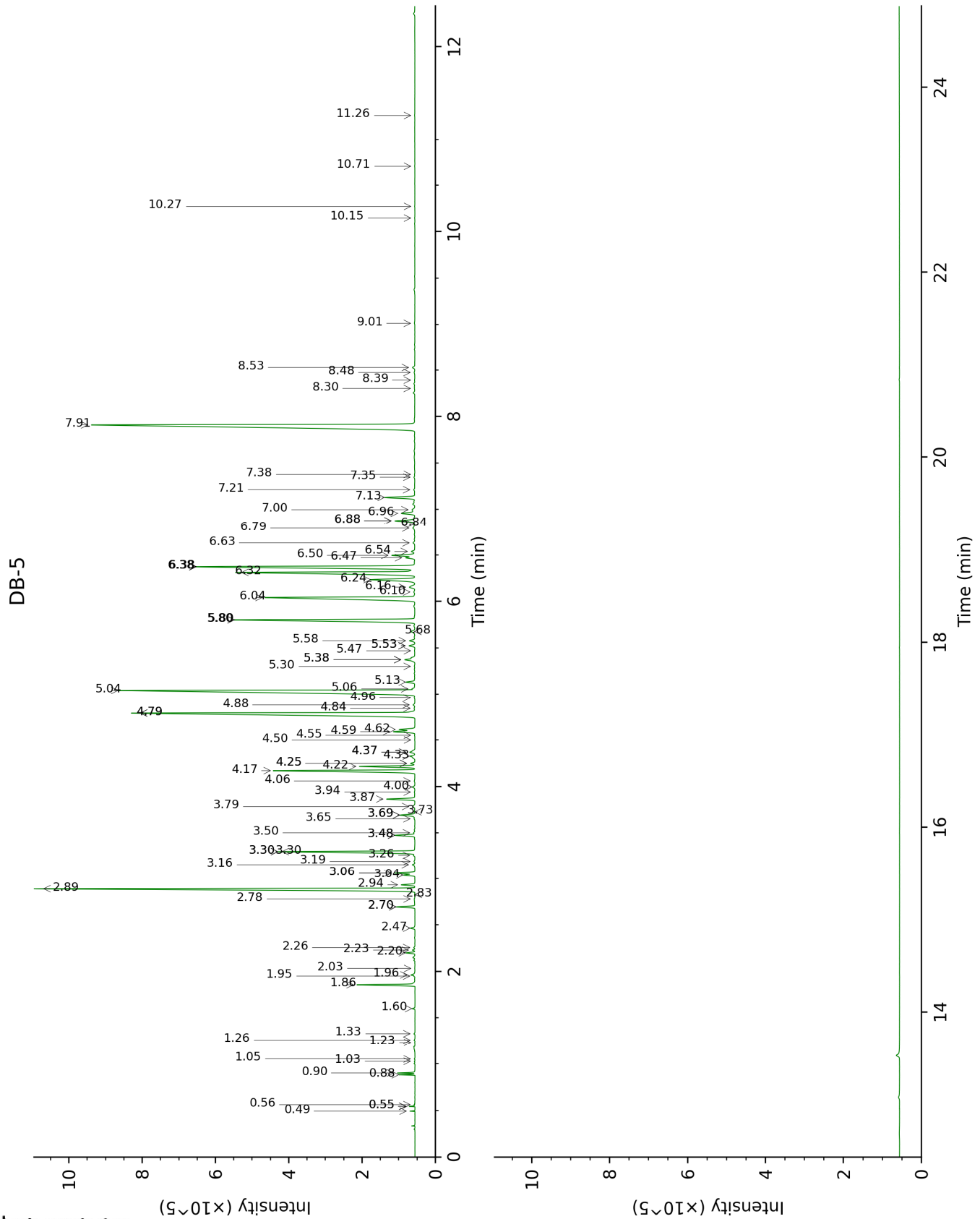
tr: The compound has been detected below 0.005% of total signal.

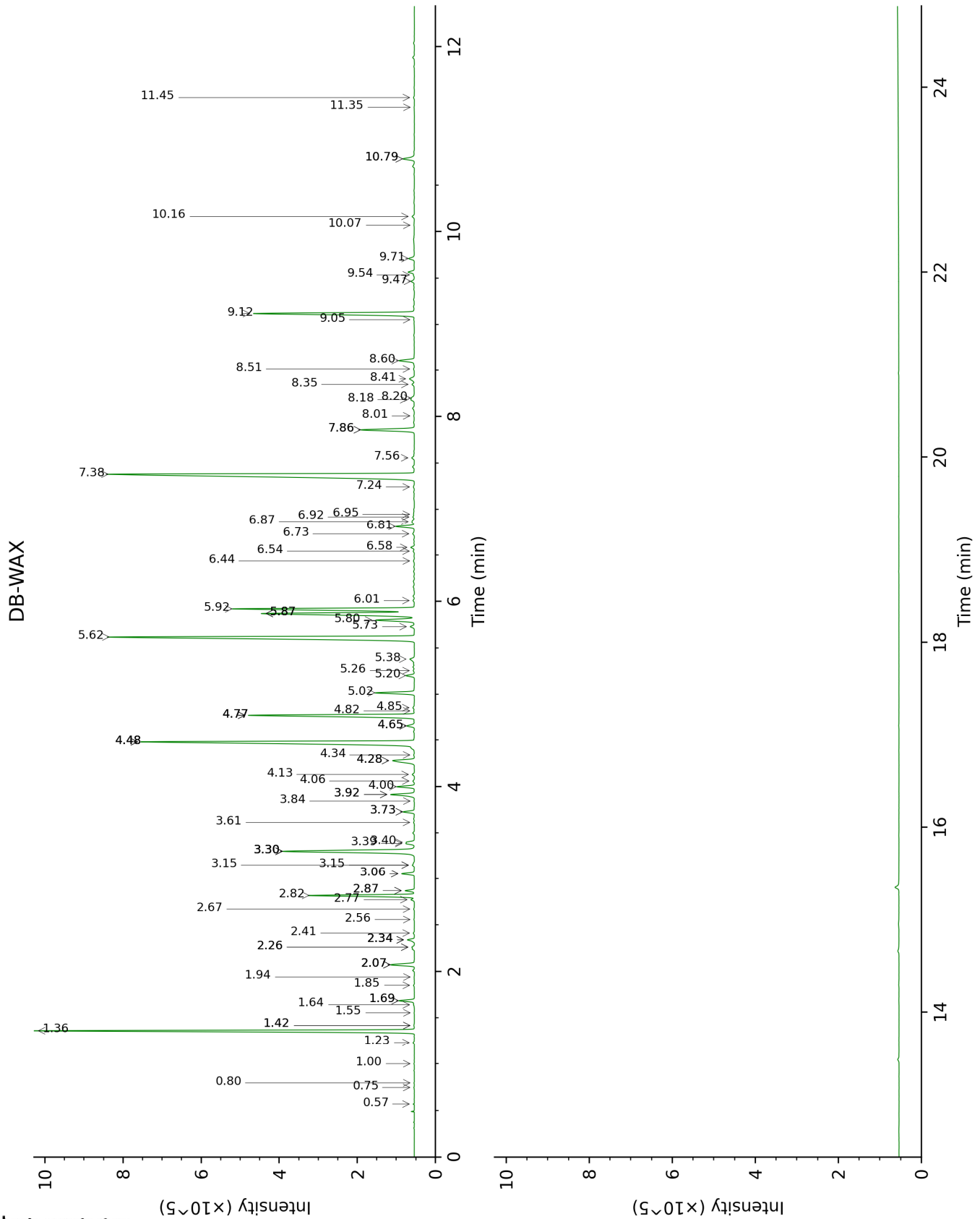
Note: no correction factor was applied

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.

This page was intentionally left blank. The following pages present the complete data of the analysis.





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isobutanol	0.49	619	0.04	2.07*	1066	0.82
Methallyl alcohol	0.54*	639	0.06	3.30*	1170	5.47
Isovaleral	0.54*	639	[0.06]	0.75	887	0.01
3-Methyl-2-butanone	0.56	646	0.01	0.80	903	0.01
Isoamyl alcohol	0.88	731	0.19	3.40	1178	0.19
2-Methylbutanol	0.90	734	0.23	3.39	1177	0.23
Ethyl isobutyrate	1.03	753	0.01	1.00	936	0.01
Toluene	1.05	757	0.01	1.42*	1002	0.02
Ethyl methacrylate	1.23	785	tr	1.56	1015	0.01
Octene	1.26	789	0.02	0.57	824	0.01
Hexanal	1.33	800	0.02	1.85	1044	0.03
Methyl angelate	1.60	825	0.05	2.34*	1093	0.23
3-Methylpentanol	1.86	848	1.22	5.02	1300	1.21
Propyl isobutyrate	1.95	856	0.02	1.69*	1028	0.47
(3Z)-Hexenol	1.96	857	0.11	5.73	1349	0.14
Isobutyl propionate	2.03	863	0.01	1.94	1053	0.01
Isoamyl acetate	2.20	878	0.18	2.34*	1093	[0.23]
2-Methylbutyl acetate	2.23	880	0.05	2.34*	1093	[0.23]
Propyl methacrylate	2.26	883	0.03	2.41	1100	0.03
Ethyl angelate	2.47	901	0.11	2.77	1128	0.10
Isobutyl isobutyrate	2.70*	917	0.41	2.07*	1066	[0.82]
Tricyclene	2.70*	917	[0.41]	1.23	973	0.03
Tiglyl acetate?	2.78	923	0.02	3.84	1212	0.01
α -Thujene	2.83	926	0.01	1.42*	1002	[0.02]
α -Pinene	2.89	930	10.78	1.36	994	10.66
Methallyl isobutyrate	2.94	933	0.30	3.06*	1150	0.37
Isobutyl methacrylate	3.04	940	0.24	2.87*	1136	0.27
α -Fenchene	3.06*	942	0.46	1.64	1024	0.03
Camphene	3.06*	942	[0.46]	1.69*	1028	[0.47]
Propyl 2-methylbutyrate	3.16	948	0.07	2.56	1111	0.01
Thuja-2,4(10)-diene	3.19	951	0.02	2.26*	1085	0.08
Benzaldehyde	3.26	955	0.03	7.24	1459	0.04
Isobutyl butyrate	3.30*	958	3.62	2.82	1132	3.06
Butyl isobutyrate	3.30*	958	[3.62]	2.67	1120	0.02
Methallyl methacrylate	3.30*	958	[3.62]	4.00	1224	0.53
Sabinene	3.48*	970	0.49	2.26*	1085	[0.08]
β -Pinene	3.48*	970	[0.49]	2.07*	1066	[0.82]

2-Methylbutyl propionate	3.50	972	0.03	3.15*	1158	0.09
Butyl methacrylate	3.65	982	0.02	3.61	1194	0.02
3-Methylpentyl acetate	3.69*	985	0.40	3.73*	1204	0.35
Octen-3-ol	3.69*	985	[0.40]	6.73	1421	0.07
Octan-3-one	3.73	987	0.03	3.92*	1217	0.84
Myrcene	3.78	991	0.09	2.87*	1136	[0.27]
Propyl angelate	3.87	996	0.69	3.92*	1217	[0.84]
Isobutyl 2-methylbutyrate	3.94	1002	0.02	3.06*	1150	[0.37]
Isobutyl isovalerate	4.00	1005	0.08	3.30*	1170	[5.47]
(3Z)-Hexenyl acetate	4.06	1009	0.03	4.82	1284	0.02
Isoamyl isobutyrate	4.17	1016	4.01	3.30*	1170	[5.47]
2-Methylbutyl isobutyrate	4.22	1019	1.32	3.30*	1170	[5.47]
para-Cymene	4.25*	1021	0.11	4.06	1228	0.05
Methallyl 2-methylbutyrate	4.25*	1021	[0.11]	4.13	1233	0.07
Methallyl isovalerate?	4.33†	1026	0.38	4.34	1249	0.02
Limonene	4.37*†	1029	[0.38]	3.15*	1158	[0.09]
1,8-Cineole	4.37*†	1029	[0.38]	3.30*	1170	[5.47]
Propyl tiglate	4.50	1037	0.01	4.85	1287	0.06
Unknown [m/z 43, 41 (84), 71 (62), 69 (59), 68 (51), 67 (48), 93 (41)...156 (4)]	4.55	1040	0.01			
2-Methylbutyl methacrylate	4.59	1043	0.58	4.28*	1244	1.04
Isoamyl methacrylate	4.62	1044	0.41	4.28*	1244	[1.04]
Isobutyl angelate	4.79*	1056	11.30	4.48*	1259	11.40
γ-Terpinene	4.79*	1056	[11.30]	3.73*	1204	[0.35]
Prenyl isobutyrate	4.84	1059	0.02	4.77*	1281	5.84
Tiglyl isobutyrate?	4.88	1061	0.05	4.77*	1281	[5.84]
Unknown [m/z 71, 43 (28), 41 (21), 57 (19), 98 (11)... 116 (4), 129 (1), 156 (t)]	4.96	1066	0.02	6.92	1435	0.05
Methallyl angelate	5.04	1072	12.76	5.62	1341	12.68
Isobutyl senecioate	5.06	1073	0.07	5.26	1315	0.04
3-Methylpentyl propionate?	5.13	1077	0.24	4.65*	1272	0.27
Tiglyl methacrylate	5.30	1088	0.02	5.87*	1359	6.11
Isobutyl tiglate	5.38*	1092	0.33	5.38	1324	0.21
Butyl angelate	5.38*	1092	[0.33]	5.20	1311	0.27

2-Methylbutyl isovalerate?	5.47	1099	0.01	4.65*	1272	[0.27]
Linalool	5.52*	1102	0.16	8.01	1517	0.02
Isoamyl 2-methylbutyrate	5.52*	1102	[0.16]	4.48*	1259	[11.40]
2-Methylbutyl 2-methylbutyrate	5.58	1106	0.15	4.48*	1259	[11.40]
Methyl tiglate	5.68	1112	0.14	6.58	1410	0.11
3-Methylpentyl isobutyrate	5.80*	1120	5.87	4.77*	1281	[5.84]
α -Campholenal	5.80*	1120	[5.87]	6.95	1437	0.04
<i>trans</i> -Pinocarveol	6.04	1135	5.76	9.12	1603	5.74
<i>trans</i> -Verbenol	6.10	1139	0.03	9.47	1631	0.12
Camphene hydrate	6.16	1142	0.23	8.41	1548	0.23
3-Methylpentyl methacrylate	6.24	1148	1.47	5.80	1354	1.40
Isoamyl angelate	6.32	1153	6.16	5.87*	1359	[6.11]
Pinocarpone	6.38*	1157	7.50	7.86*	1505	1.90
2-Methylbutyl angelate	6.38*	1157	[7.50]	5.92	1363	6.27
Unknown [m/z 96, 95 (72), 67 (45), 41 (42), 55 (32), 70 (27)... 152 (t)]	6.38*	1157	[7.50]	10.07	1680	0.02
Borneol	6.47	1163	0.23	9.71	1651	0.21
Angelyl angelate?	6.50	1165	0.63	6.81	1427	0.61
Isopinocampone	6.54	1167	0.09	7.56	1482	0.09
Terpinen-4-ol	6.63	1173	0.05	8.51	1556	0.03
Isobutyl 3-hydroxy-2-methylenebutyrate	6.79	1184	0.09	10.79*	1741	0.46
<i>para</i> -Cymen-8-ol	6.84	1186	0.01	11.45	1797	0.02
Myrtenal	6.88*	1189	0.60	8.60	1563	0.58
Amyl angelate	6.88*	1189	[0.60]	6.54	1407	0.04
Myrtenol	6.96	1194	0.42	10.79*	1741	[0.46]
2-Methylbutyl tiglate	7.00	1197	0.11	6.87	1431	0.14
3-Methylpentyl 2-methylbutyrate?	7.13	1205	0.86	5.87*	1359	[6.11]
3-Methylpentyl isovalerate?	7.21	1211	0.04	6.01	1369	0.04
<i>trans</i> -Carveol	7.35	1220	0.02	11.35	1788	0.01
4-Methylhexyl isobutyrate	7.38	1222	0.01			
3-Methylpentyl angelate	7.91	1258	16.24	7.38	1469	16.01
(3 <i>Z</i>)-Hexenyl angelate	8.30	1284	0.01	8.18	1530	0.13
Hexyl angelate	8.39	1290	0.01	7.86*	1505	[1.90]
<i>trans</i> -Pinocarvyl acetate	8.48	1295	0.03	9.05	1598	0.01

3-Methylpentyl tiglate	8.53	1299	0.07	8.20	1532	0.10
7βH-Silphiperfol-5-ene	9.01	1333	0.02	6.44	1400	0.03
β-Caryophyllene	10.15	1414	0.01	8.35	1543	0.08
Myrtenyl propionate?	10.27	1423	0.01			
(E)-β-Farnesene	10.71	1456	0.01	9.54	1637	0.03
(3Z,6E)-α-Farnesene	11.26	1497	0.01	10.16	1688	0.08
Total identified		98.84%			98.09%	
Total reported		98.87%			98.16%	

*: 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