

Date : April 20, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21D16-PTH08


Customer identification : Chamomile Roman ORGANIC - Hungary - CC3103203R

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 : Sylvain Mercier, M. Sc., Chimiste

Analysis date : April 18, 2021

Checked and approved by :



Alexis St-Gelais, M. Sc., chimiste 2013-174

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PHYSICOCHEMICAL DATA

Physical aspect: Clear liquid

Refractive index: 1.4372 ± 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
Methacrolein	tr	Aliphatic aldehyde
Isobutanol	0.07	Aliphatic alcohol
Methallyl alcohol	0.09	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
3-Methyl-2-butanone	tr	Aliphatic ketone
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	0.24	Aliphatic alcohol
2-Methylbutanol	0.30	Aliphatic alcohol
Ethyl isobutyrate	0.01	Aliphatic ester
Isobutyric acid	0.08	Aliphatic acid
Isobutyl acetate	tr	Aliphatic ester
Hexanal	0.03	Aliphatic aldehyde
Methyl angelate	0.03	Aliphatic ester
3-Methylpentanol	1.13	Aliphatic alcohol
Propyl isobutyrate	0.09	Aliphatic ester
(3Z)-Hexenol	0.03	Aliphatic alcohol
Isobutyl propionate	0.01	Aliphatic ester
(2E)-Hexenol	0.05	Aliphatic alcohol
Hexanol	0.06	Aliphatic alcohol
Isoamyl acetate	0.18	Aliphatic ester
2-Methylbutyl acetate	0.06	Aliphatic ester
Propyl methacrylate	0.02	Aliphatic ester
Ethyl angelate	0.05	Aliphatic ester
Heptanal	0.01	Aliphatic aldehyde
Tiglic acid	0.08	Aliphatic acid
Tricyclene	0.03	Monoterpene
Isobutyl isobutyrate	0.49	Aliphatic ester
α -Pinene	8.30	Monoterpene
Methallyl isobutyrate	0.35	Aliphatic ester
Camphene	0.25	Monoterpene
Isobutyl methacrylate	0.24	Aliphatic ester
α -Fenchene	0.02	Monoterpene
Propyl 2-methylbutyrate	0.02	Aliphatic ester
Thuja-2,4(10)-diene	0.01	Monoterpene
Propyl isovalerate	0.03	Aliphatic ester
Benzaldehyde	0.04	Simple phenolic
Butyl isobutyrate	0.03	Aliphatic ester
Methallyl methacrylate	0.52	Aliphatic ester
Isobutyl butyrate	8.12	Aliphatic ester
Sabinene	0.06	Monoterpene
β -Pinene	0.01	Monoterpene
2-Methylbutyl propionate	0.03	Aliphatic ester
Butyl methacrylate	0.03	Aliphatic ester
Octen-3-ol	0.07	Aliphatic alcohol
3-Methylpentyl acetate	0.36	Aliphatic ester

Octan-3-one	0.02	Aliphatic ketone
Myrcene	0.04	Monoterpene
Propyl angelate	0.68	Aliphatic ester
Isobutyl 2-methylbutyrate	0.01	Aliphatic ester
Isobutyl isovalerate	0.10	Aliphatic ester
(3Z)-Hexenyl acetate	0.03	Aliphatic ester
Isoamyl isobutyrate	8.39	Aliphatic ester
2-Methylbutyl isobutyrate	1.74	Aliphatic ester
para-Cymene	0.04	Monoterpene
Methallyl 2-methylbutyrate	0.09	Aliphatic ester
Methallyl isovalerate?	0.02	Aliphatic ester
Limonene	0.06	Monoterpene
1,8-Cineole	0.02	Monoterpenic ether
Propyl tiglate	0.01	Aliphatic ester
Unknown	0.01	Unknown
2-Methylbutyl methacrylate	0.52	Aliphatic ester
Isoamyl methacrylate	0.39	Aliphatic ester
Isobutyl angelate	3.62	Aliphatic ester
γ-Terpinene	0.03	Monoterpene
Prenyl isobutyrate	0.01	Aliphatic ester
Tiglyl isobutyrate?	0.03	Aliphatic ester
Unknown	0.02	Unknown
Methallyl angelate	11.90	Aliphatic ester
Isobutyl senecioate	0.04	Aliphatic ester
3-Methylpentyl propionate?	0.27	Aliphatic ester
Tiglyl methacrylate	0.01	Aliphatic ester
Isobutyl tiglate	0.10	Aliphatic ester
Butyl angelate	0.25	Aliphatic ester
Linalool	0.02	Monoterpenic alcohol
Isoamyl 2-methylbutyrate	0.17	Aliphatic ester
2-Methylbutyl 2-methylbutyrate	0.21	Aliphatic ester
Methallyl tiglate	0.17	Aliphatic ester
3-Methylpentyl isobutyrate	6.76	Aliphatic ester
α-Campholenal	0.04	Monoterpenic aldehyde
<i>trans</i> -Pinocarveol	5.18	Monoterpenic alcohol
<i>trans</i> -Verbenol	0.04	Monoterpenic alcohol
Camphene hydrate	0.19	Monoterpenic alcohol
3-Methylpentyl methacrylate	1.18	Aliphatic ester
Isoamyl angelate	6.17	Aliphatic ester
Pinocarvone	2.26	Monoterpenic ketone
2-Methylbutyl angelate	5.74	Aliphatic ester
Borneol	0.24	Monoterpenic alcohol
Angelyl angelate?	0.68	Aliphatic ester
Isopinocampone	0.17	Monoterpenic ketone
Terpinen-4-ol	0.03	Monoterpenic alcohol
Isobutyl 3-hydroxy-2-methylenebutyrate	0.08	Aliphatic ester
para-Cymen-8-ol	0.02	Monoterpenic alcohol
Myrtenal	0.71	Monoterpenic aldehyde
Amyl angelate	0.03	Aliphatic ester
Myrtenol	0.42	Monoterpenic alcohol
Tiglyl angelate	0.05	Aliphatic ester
2-Methylbutyl tiglate	0.12	Aliphatic ester

3-Methylpentyl 2-methylbutyrate?	0.98	Aliphatic ester
3-Methylpentyl isovalerate?	0.03	Aliphatic ester
<i>trans</i> -Carveol	0.01	Monoterpenic alcohol
4-Methylhexyl isobutyrate	0.02	Aliphatic ester
3-Methylpentyl angelate	15.44	Aliphatic ester
Linalyl acetate	0.09	Monoterpenic ester
(3 <i>Z</i>)-Hexenyl angelate	0.04	Aliphatic ester
Hexyl angelate	0.03	Aliphatic ester
<i>trans</i> -Pinocarvyl acetate	0.02	Monoterpenic ester
3-Methylpentyl tiglate	0.11	Aliphatic ester
Benzyl isobutyrate	0.01	Phenolic ester
7 β H-Silphiperfol-5-ene	0.03	Sesquiterpene
Eugenol	0.02	Phenylpropanoid
α -Copaene	0.01	Sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.01	Unknown
Consolidated total	97.69%	

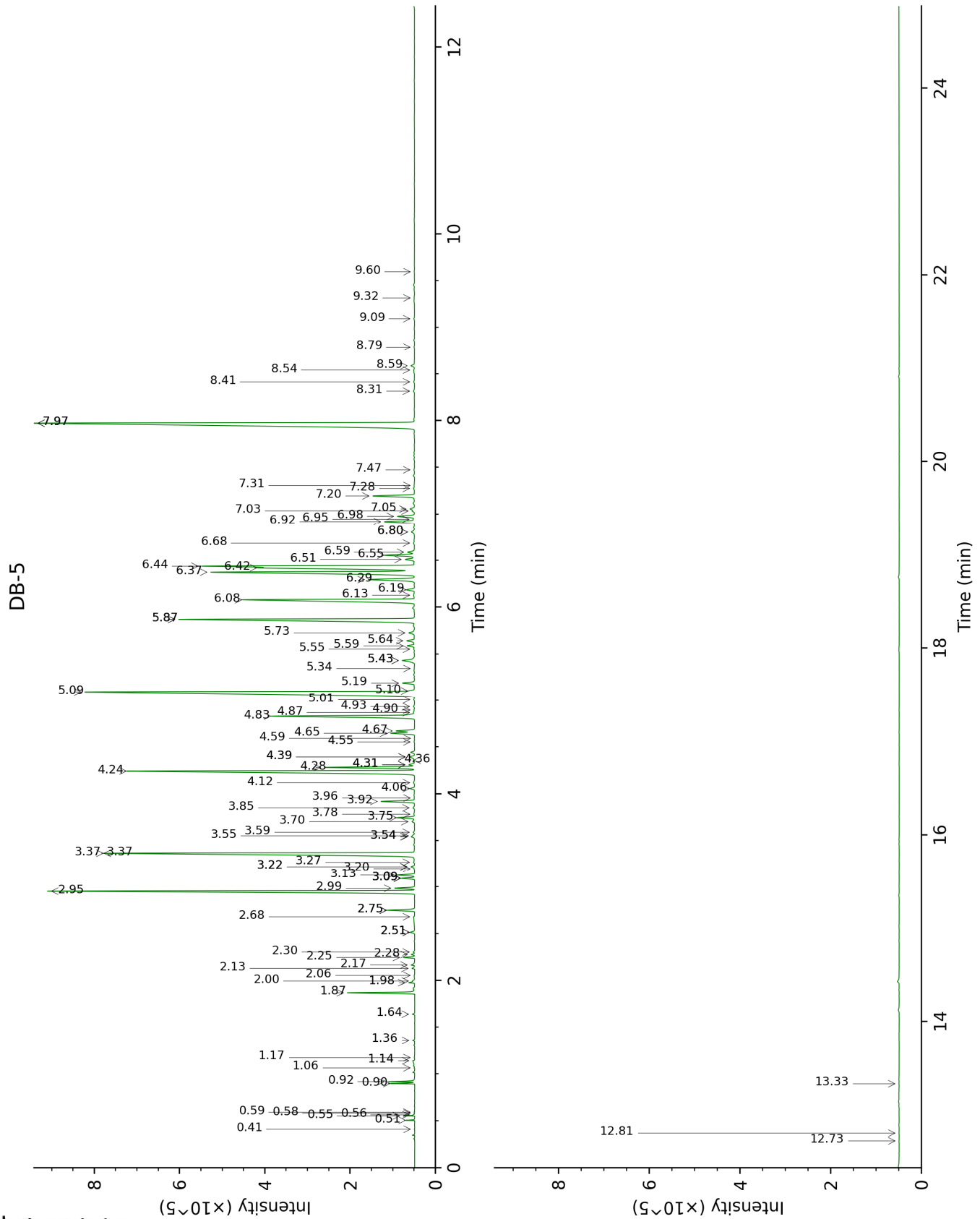
tr: The compound has been detected below 0.005% of total signal.

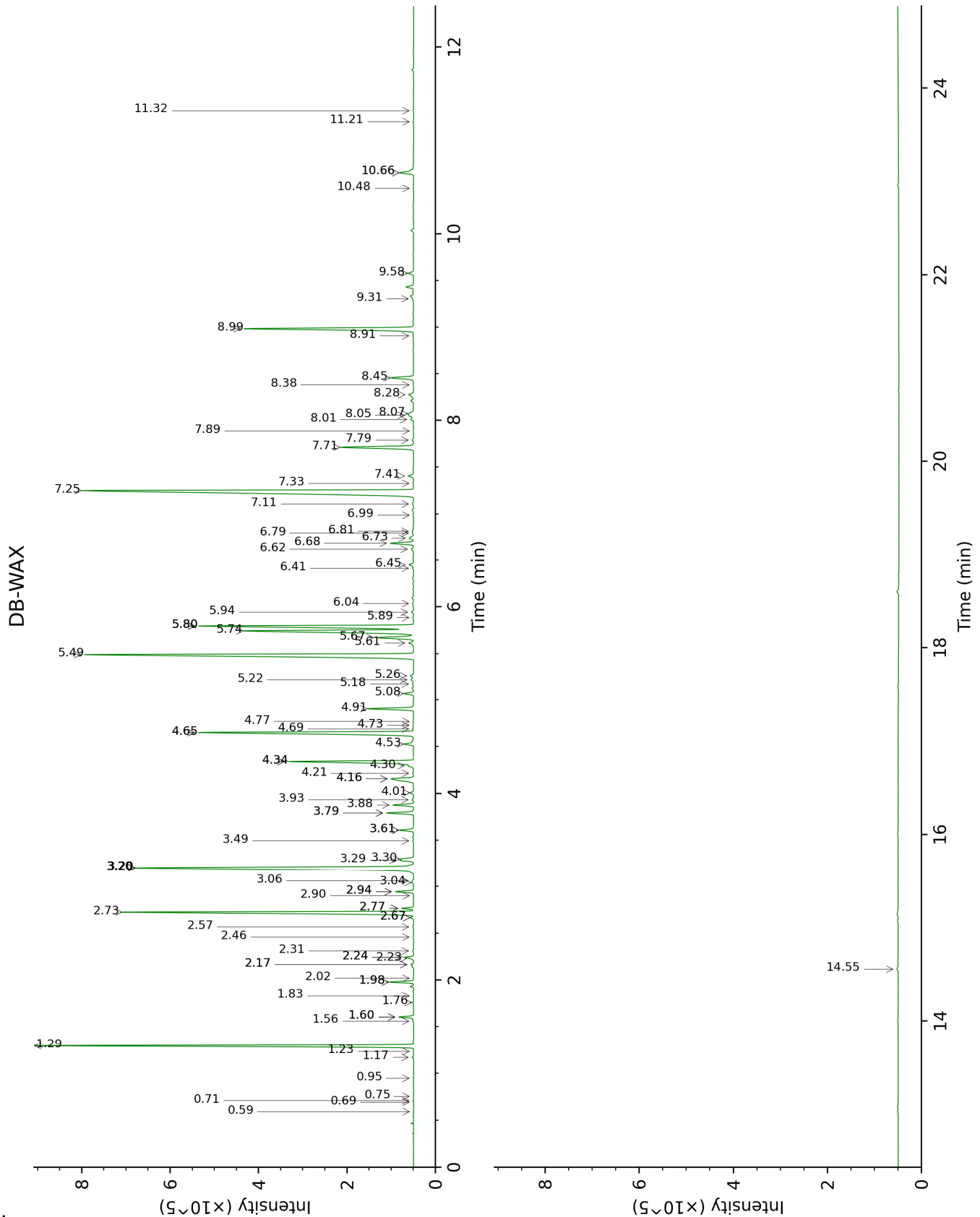
Note: no correction factor was applied

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	%
Methacrolein	0.41	543	tr	0.59	842	tr
Isobutanol	0.51	616	0.07	1.98*	1065	0.56
Methallyl alcohol	0.55	635	0.09	3.20*	1170	10.34
Isovaleral	0.56	639	0.01	0.71	888	0.01
3-Methyl-2-butanone	0.58	646	tr	0.75	902	0.01
2-Methylbutyral	0.59	650	tr	0.69	881	tr
Isoamyl alcohol	0.90	730	0.24	3.29†	1177	0.61
2-Methylbutanol	0.92	733	0.30	3.30†	1178	[0.61]
Ethyl isobutyrate	1.06	755	0.01	0.95	934	0.01
Isobutyric acid	1.14	767	0.08			
Isobutyl acetate	1.17	772	tr	1.23	983	tr
Hexanal	1.36	801	0.03	1.76	1043	0.03
Methyl angelate	1.64	827	0.03	2.23	1091	0.04
3-Methylpentanol	1.87	847	1.13	4.91	1300	1.22
Propyl isobutyrate	1.98	856	0.09	1.60*	1028	0.34
(3Z)-Hexenol	2.00	858	0.03	5.61	1348	0.16
Isobutyl propionate	2.06	863	0.01	1.83	1050	0.01
(2E)-Hexenol	2.13	869	0.05	5.94	1372	0.06
Hexanol	2.17	872	0.06	5.26	1322	0.11
Isoamyl acetate	2.25	879	0.18	2.24*	1092	0.21
2-Methylbutyl acetate	2.28	882	0.06	2.24*	1092	[0.21]
Propyl methacrylate	2.30	884	0.02	2.31	1099	0.03
Ethyl angelate	2.51*	902	0.09	2.67*	1128	0.08
Heptanal	2.51*	902	[0.09]	2.90	1146	0.01
Tiglic acid	2.68	914	0.08			
Tricyclene	2.75*	919	0.52	1.17	972	0.03
Isobutyl isobutyrate	2.75*	919	[0.52]	1.98*	1065	[0.56]
α-Pinene	2.95	933	8.30	1.29	994	8.31
Methallyl isobutyrate	2.99	935	0.35	2.94*	1150	0.46
Camphene	3.09*†	942	0.58	1.60*	1028	[0.34]
Isobutyl methacrylate	3.09*†	942	[0.58]	2.77*	1136	0.27
α-Fenchene	3.09*†	942	[0.58]	1.56	1023	0.02
Propyl 2-methylbutyrate	3.13†	944	[0.58]	2.46	1111	0.02
Thuja-2,4(10)-diene	3.20	949	0.01	2.17*†	1084	0.11
Propyl isovalerate	3.22*	951	0.07	2.67*	1128	[0.08]
Benzaldehyde	3.22*	951	[0.07]	7.11	1458	0.04
Butyl isobutyrate	3.27	954	0.03	2.57	1120	0.03
Methallyl methacrylate	3.37*	961	8.70	3.88	1223	0.52

Isobutyl butyrate	3.37*	961	[8.70]	2.72	1132	8.12
Sabinene	3.54*†	972	0.11	2.17*†	1084	[0.11]
β-Pinene	3.54*†	972	[0.11]	2.02	1069	0.01
2-Methylbutyl propionate	3.55†	973	[0.11]	3.06	1159	0.03
Butyl methacrylate	3.59	976	0.03	3.49	1194	0.02
Octen-3-ol	3.70	983	0.07	6.62	1421	0.07
3-Methylpentyl acetate	3.75	986	0.36	3.61*	1203	0.37
Octan-3-one	3.78	989	0.02	3.79*	1216	0.70
Myrcene	3.85	993	0.04	2.77*	1136	[0.27]
Propyl angelate	3.92	998	0.68	3.79*	1216	[0.70]
Isobutyl 2-methylbutyrate	3.96	1000	0.01	2.94*	1150	[0.46]
Isobutyl isovalerate	4.06	1007	0.10	3.20*	1170	[10.34]
(3Z)-Hexenyl acetate	4.12	1011	0.03	4.69	1283	0.03
Isoamyl isobutyrate	4.24	1019	8.39	3.20*	1170	[10.34]
2-Methylbutyl isobutyrate	4.28	1021	1.74	3.20*	1170	[10.34]
para-Cymene	4.31*	1023	0.13	3.93	1227	0.04
Methallyl 2-methylbutyrate	4.31*	1023	[0.13]	4.01	1232	0.09
Methallyl isovalerate?	4.36	1026	0.02	4.22	1248	0.03
Limonene	4.39*	1028	0.14	3.04	1158	0.06
1,8-Cineole	4.39*	1028	[0.14]	3.20*	1170	[10.34]
Propyl tiglate	4.55	1039	0.01	4.77	1289	0.02
Unknown [m/z 43, 41 (84), 71 (62), 69 (59), 68 (51), 67 (48), 93 (41)...156 (4)]	4.59	1041	0.01			
2-Methylbutyl methacrylate	4.65	1044	0.52	4.16*	1244	0.98
Isoamyl methacrylate	4.67	1046	0.39	4.16*	1244	[0.98]
Isobutyl angelate	4.83	1056	3.62	4.34*	1257	3.65
γ-Terpinene	4.87	1058	0.03	3.61*	1203	[0.37]
Prenyl isobutyrate	4.90	1060	0.01	4.73	1286	0.03
Tiglyl isobutyrate?	4.93	1063	0.03	4.65*	1280	6.79
Unknown [m/z 71, 43 (28), 41 (21), 57 (19), 98 (11)... 116 (4), 129 (1), 156 (t)]	5.01	1067	0.02	6.79	1434	0.03
Methallyl angelate	5.09†	1073	12.01	5.49	1339	11.90
Isobutyl senecioate	5.10†	1074	[12.01]	5.18	1316	0.04
3-Methylpentyl propionate?	5.19	1079	0.27	4.53	1271	0.27

Tiglyl methacrylate	5.34	1089	0.01	5.80*	1361	6.74
Isobutyl tiglate	5.43*	1094	0.38	5.22	1319	0.10
Butyl angelate	5.43*	1094	[0.38]	5.08	1309	0.25
Linalool	5.55	1102	0.02	7.89	1517	0.01
Isoamyl 2-methylbutyrate	5.59	1104	0.17	4.30	1254	0.14
2-Methylbutyl 2-methylbutyrate	5.64	1108	0.21	4.34*	1257	[3.65]
Methallyl tiglate	5.73	1113	0.17	6.45	1409	0.13
3-Methylpentyl isobutyrate	5.87*	1122	6.85	4.65*	1280	[6.79]
α-Campholenal	5.87*	1122	[6.85]	6.81	1436	0.04
trans-Pinocarveol	6.08	1136	5.18	8.99	1603	5.16
trans-Verbenol	6.13	1139	0.04	9.31	1629	0.04
Camphene hydrate	6.19	1142	0.19	8.28	1547	0.16
3-Methylpentyl methacrylate	6.30	1150	1.18	5.67	1352	1.14
Isoamyl angelate	6.37	1155	6.17	5.74	1357	6.01
Pinocarpone	6.42†	1158	8.27	7.71	1503	2.26
2-Methylbutyl angelate	6.44†	1159	[8.27]	5.80*	1361	[6.74]
Borneol	6.51	1163	0.24	9.58	1651	0.17
Angelyl angelate?	6.56	1166	0.68	6.68	1426	0.65
Isopinocampone	6.59	1168	0.17	7.41	1480	0.17
Terpinen-4-ol	6.68	1175	0.03	8.38	1555	0.02
Isobutyl 3-hydroxy-2-methylenebutyrate	6.80*	1182	0.10	10.66*	1742	0.54
para-Cymen-8-ol	6.80*	1182	[0.10]	11.32	1798	0.02
Myrtenal	6.92	1190	0.71	8.45	1561	0.72
Amyl angelate	6.94	1191	0.03	6.41	1406	0.03
Myrtenol	6.98	1193	0.42	10.66*	1742	[0.54]
Tiglyl angelate	7.03	1197	0.05	7.33	1474	0.03
2-Methylbutyl tiglate	7.06	1198	0.12	6.73	1430	0.18
3-Methylpentyl 2-methylbutyrate?	7.20	1208	0.98	5.80*	1361	[6.74]
3-Methylpentyl isovalerate?	7.28	1213	0.03	5.89	1368	0.03
trans-Carveol	7.31	1215	0.01	11.20	1788	0.01
4-Methylhexyl isobutyrate	7.47	1226	0.02			
3-Methylpentyl angelate	7.97*	1260	15.80	7.25	1469	15.44
Linalyl acetate	7.97*	1260	[15.80]	8.01	1526	0.09
(3Z)-Hexenyl angelate	8.31	1283	0.04	8.07	1531	0.17
Hexyl angelate	8.41	1290	0.03	7.79	1509	0.05
trans-Pinocarvyl acetate	8.54	1298	0.02	8.91	1597	0.04
3-Methylpentyl tiglate	8.58	1301	0.11	8.05	1530	0.17

Benzyl isobutyrate	8.79	1315	0.01	10.48	1727	0.01
7βH-Silphiperfol-5-ene	9.09	1337	0.03	6.04	1378	0.04
Eugenol	9.32	1353	0.02	14.55	2098	0.06
α-Copaene	9.60	1372	0.01	6.99	1449	0.03
Unknown [m/z 105, 131 (96), 91 (95), 93 (84), 159 (82), 43 (70)...220 (6)]	12.73	1610	0.01			
Unknown [m/z 43, 79 (41), 93 (39), 41 (39), 91 (38), 81 (36)... 220 (3)]	12.81	1617	0.01			
Unknown [m/z 81, 41 (46), 79 (46), 93 (39), 91 (33), 107 (33)... 206 (8)]	13.33	1660	0.01			
Total identified		98.53%			97.73%	
Total reported		98.59%			97.76%	

*: 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