

Date : September 20, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 22114-PTH05

Customer identification : Chamomile Roman ORGANIC - Hungary - CC3106R

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 : Amélie Simard, Analyste

Analysis date : September 20, 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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: 1.4406 ± 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	0.05	Aliphatic alcohol
Methallyl alcohol	0.07	Aliphatic alcohol
Isovaleral	0.02	Aliphatic aldehyde
3-Methyl-2-butanone	0.01	Aliphatic ketone
2-Methylbutyral	0.01	Aliphatic aldehyde
3-Methyl-3-buten-2-one	tr	Aliphatic ketone
Methyl isobutyrate	tr	Aliphatic ester
Valeral	tr	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Methyl methacrylate	tr	Aliphatic ester
Isoamyl alcohol	0.21	Aliphatic alcohol
2-Methylbutanol	0.20	Aliphatic alcohol
Ethyl isobutyrate	0.01	Aliphatic ester
Toluene	0.01	Simple phenolic
Isobutyl acetate	0.05	Aliphatic ester
Methyl isovalerate	0.06	Aliphatic ester
Ethyl methacrylate	0.01	Aliphatic ester
Octene	0.04	Alkene
Hexanal	0.03	Aliphatic aldehyde
Methyl angelate	0.05	Aliphatic ester
3-Methylpentanol	0.89	Aliphatic alcohol
Ethyl 2-methylbutyrate	0.06	Aliphatic ester
Propyl isobutyrate	0.02	Aliphatic ester
(3Z)-Hexenol	0.03	Aliphatic alcohol
(2E)-Hexenol	0.04	Aliphatic alcohol
Isobutyl propionate	0.01	Aliphatic ester
Hexanol	0.06	Aliphatic alcohol
Isoamyl acetate	0.28	Aliphatic ester
2-Methylbutyl acetate	0.07	Aliphatic ester
Propyl methacrylate	0.04	Aliphatic ester
Ethyl angelate	0.10	Aliphatic ester
Heptanal	0.01	Aliphatic aldehyde
Isobutyl isobutyrate	0.56	Aliphatic ester
Tricyclene	0.04	Monoterpene
Tiglyl acetate?	0.02	Aliphatic ester
α -Thujene	0.02	Monoterpene
α -Pinene	10.42	Monoterpene
Methallyl isobutyrate	0.46	Aliphatic ester
Isobutyl methacrylate	0.28	Aliphatic ester
Camphene	0.44	Monoterpene
α -Fenchene	0.03	Monoterpene
Propyl 2-methylbutyrate	0.02	Aliphatic ester
Thuja-2,4(10)-diene	0.09	Monoterpene
Benzaldehyde	0.03	Simple phenolic

Butyl isobutyrate	0.03	Aliphatic ester
Methallyl methacrylate	0.79	Aliphatic ester
Isobutyl butyrate	3.09	Aliphatic ester
β-Pinene	0.29	Monoterpene
Sabinene	0.03	Monoterpene
2-Methylbutyl propionate	0.04	Aliphatic ester
Butyl methacrylate	0.03	Aliphatic ester
Octen-3-ol	0.06	Aliphatic alcohol
3-Methylpentyl acetate	0.53	Aliphatic ester
Octan-3-one	0.02	Aliphatic ketone
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
2-Pentylfuran	0.05	Furan
Myrcene	0.03	Monoterpene
Propyl angelate	0.69	Aliphatic ester
Isobutyl 2-methylbutyrate	0.09	Aliphatic ester
Isobutyl isovalerate	0.04	Aliphatic ester
Isoamyl isobutyrate	4.25	Aliphatic ester
2-Methylbutyl isobutyrate	1.64	Aliphatic ester
Methallyl 2-methylbutyrate	0.10	Aliphatic ester
para-Cymene	0.04	Monoterpene
Methallyl isovalerate?	0.04	Aliphatic ester
Limonene	0.04	Monoterpene
1,8-Cineole	0.01	Monoterpenic ether
Propyl tiglate	0.01	Aliphatic ester
Unknown	0.01	Unknown
2-Methylbutyl methacrylate	0.63	Aliphatic ester
Isoamyl methacrylate	0.39	Aliphatic ester
Isobutyl angelate	10.78	Aliphatic ester
γ-Terpinene	0.22	Monoterpene
Prenyl isobutyrate	0.04	Aliphatic ester
Tiglyl isobutyrate?	0.01	Aliphatic ester
Unknown	0.02	Unknown
Methallyl angelate	13.29	Aliphatic ester
Isobutyl senecioate	0.10	Aliphatic ester
3-Methylpentyl propionate?	0.34	Aliphatic ester
para-Cymenene	0.03	Monoterpene
Tiglyl methacrylate	0.02	Aliphatic ester
Butyl angelate	0.27	Aliphatic ester
Isobutyl tiglate	0.11	Aliphatic ester
2-Methylbutyl isovalerate?	0.02	Aliphatic ester
Isoamyl 2-methylbutyrate	0.14	Aliphatic ester
Linalool	0.03	Monoterpenic alcohol
2-Methylbutyl 2-methylbutyrate	0.18	Aliphatic ester
Methallyl tiglate	0.16	Aliphatic ester
3-Methylpentyl isobutyrate?	0.04	Aliphatic ester
3-Methylpentyl isobutyrate	7.39	Aliphatic ester
α-Campholenal	0.02	Monoterpenic aldehyde
trans-Pinocarveol	5.10	Monoterpenic alcohol
trans-Verbenol	0.04	Monoterpenic alcohol
Camphene hydrate	0.19	Monoterpenic alcohol
3-Methylpentyl methacrylate	1.47	Aliphatic ester
Isoamyl angelate	5.60	Aliphatic ester

Pinocarvone	1.96	Monoterpenic ketone
2-Methylbutyl angelate	4.51	Aliphatic ester
Unknown	0.01	Oxygenated monoterpene
Benzyl acetate	0.02	Phenolic ester
Borneol	0.20	Monoterpenic alcohol
Angelyl angelate?	0.60	Aliphatic ester
Isopinocampone	0.05	Monoterpenic ketone
Terpinen-4-ol	0.04	Monoterpenic alcohol
Isobutyl 3-hydroxy-2-methylenebutyrate	0.06	Aliphatic ester
para-Cymen-8-ol	0.04	Monoterpenic alcohol
trans-Isocarveol	0.02	Monoterpenic alcohol
Amyl angelate	0.04	Aliphatic ester
Myrtenal	0.64	Monoterpenic aldehyde
Myrtenol	0.34	Monoterpenic alcohol
2-Methylbutyl tiglate	0.07	Aliphatic ester
Tiglyl angelate	0.04	Aliphatic ester
Isoamyl tiglate	0.01	Aliphatic ester
Verbenone	0.05	Monoterpenic ketone
3-Methylpentyl 2-methylbutyrate?	0.94	Aliphatic ester
3-Methylpentyl isovalerate?	0.04	Aliphatic ester
trans-Carveol	0.01	Monoterpenic alcohol
4-Methylhexyl isobutyrate	0.03	Aliphatic ester
Carvone	0.01	Monoterpenic ketone
2-Hydroxy-2-methylbut-3-enyl angelate	0.02	Aliphatic ester
Linalyl acetate	0.01	Monoterpenic ester
3-Methylpentyl angelate	14.46	Aliphatic ester
(3Z)-Hexenyl angelate	0.02	Aliphatic ester
Hexyl angelate	0.02	Aliphatic ester
trans-Pinocarvyl acetate	0.01	Monoterpenic ester
3-Methylpentyl tiglate	0.07	Aliphatic ester
Benzyl isobutyrate	0.02	Phenolic ester
7βH-Silphiperfol-5-ene	0.02	Sesquiterpene
Cyclosativene II	0.04	Sesquiterpene
α-Copaene	0.01	Sesquiterpene
Isobutyl phenylacetate	0.01	Phenolic ester
Consolidated total	97.88%	

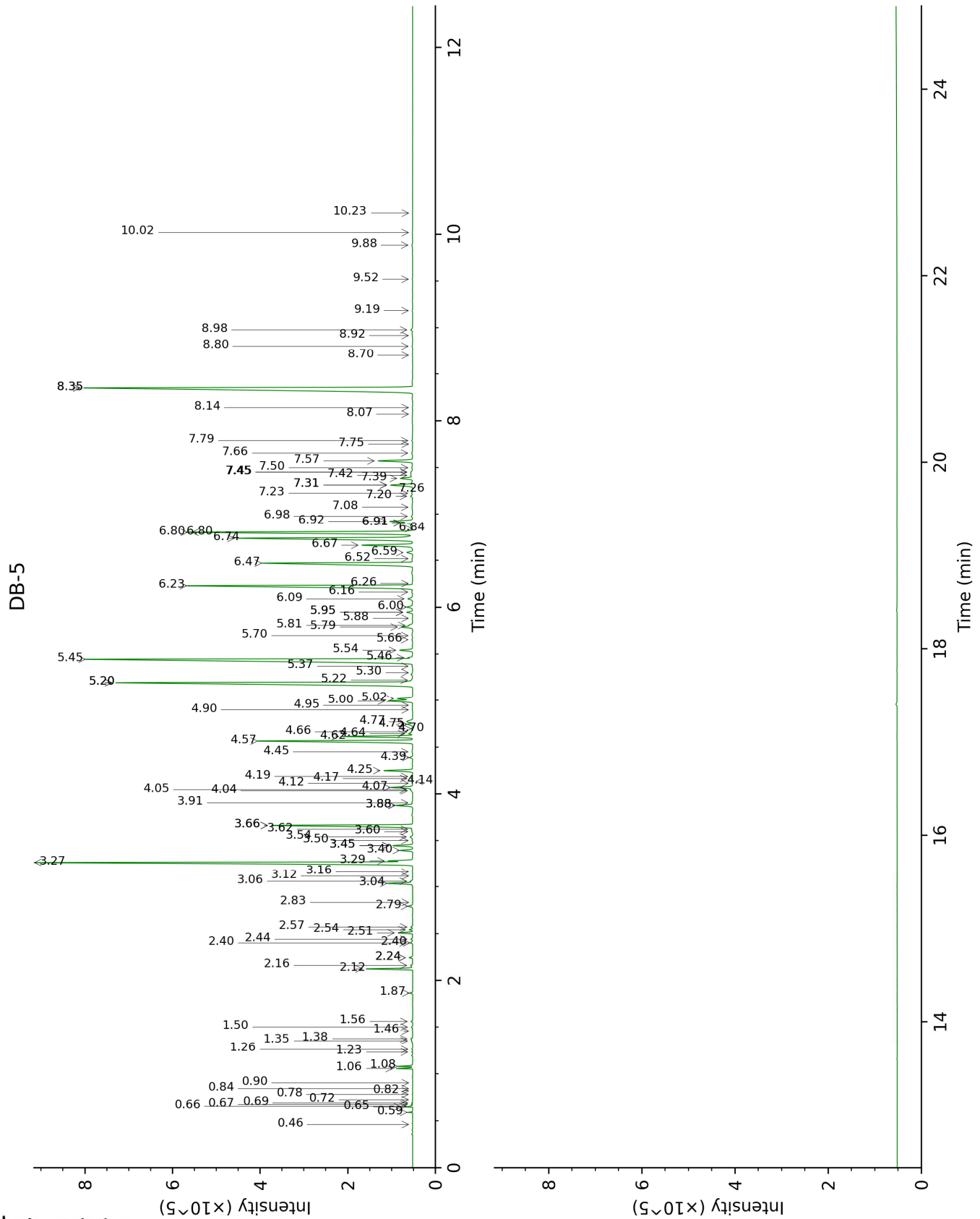
tr: The compound has been detected below 0.005% of total signal.

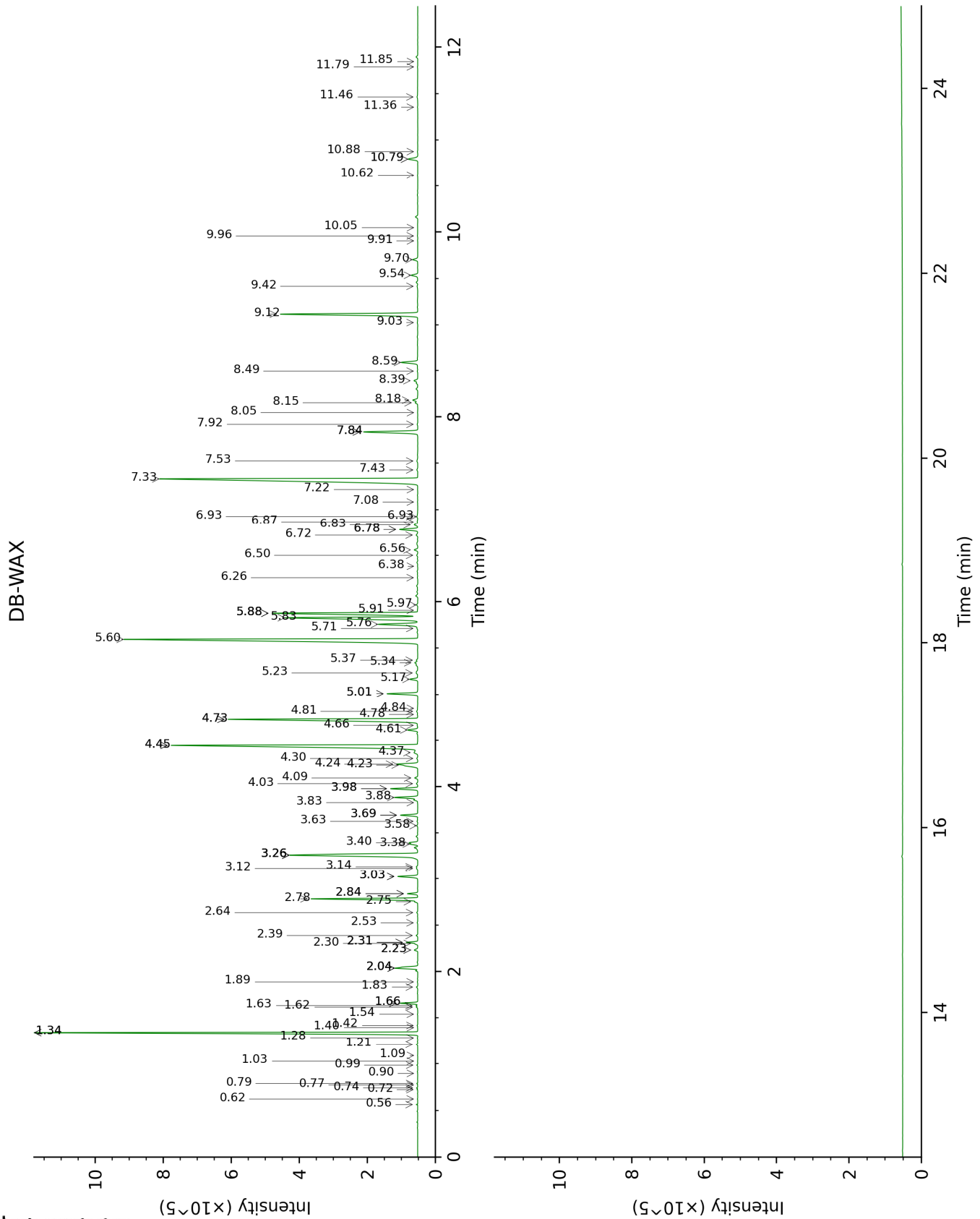
Note: no correction factor was applied

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	0.46	548	tr	0.62	842	tr
Isobutanol	0.59	621	0.05	2.04*	1065	0.90
Methallyl alcohol	0.65	639	0.07	3.26*	1168	6.01
Isovaleral	0.66	641	0.02	0.74	888	0.02
3-Methyl-2-butanone	0.67	647	0.01	0.79	900	0.01
2-Methylbutyral	0.69	652	0.01	0.72	881	0.01
3-Methyl-3-buten-2-one	0.72	663	tr	1.09	952	tr
Methyl isobutyrate	0.78	680	tr	0.77	897	tr
Valeral	0.82	692	tr	1.03	941	tr
2-Ethylfuran	0.84	699	tr	0.90	919	tr
Methyl methacrylate	0.90	709	tr			
Isoamyl alcohol	1.06	730	0.21	3.38†	1178	0.44
2-Methylbutanol	1.08	733	0.20	3.40†	1179	[0.44]
Ethyl isobutyrate	1.23	754	0.01	0.99	934	0.01
Toluene	1.26	758	0.01	1.42	1003	0.01
Isobutyl acetate	1.35	770	0.05	1.28	985	0.01
Methyl isovalerate	1.38	773	0.06	1.34*	995	10.41
Ethyl methacrylate	1.46	785	0.01	1.54	1015	0.01
Octene	1.50	790	0.04	0.56	819	0.01
Hexanal	1.56	798	0.03	1.83	1044	0.03
Methyl angelate	1.87	825	0.05	2.30†	1092	0.36
3-Methylpentanol	2.12	846	0.89	5.01*	1297	0.94
Ethyl 2-methylbutyrate	2.16	849	0.06	1.63	1024	0.04
Propyl isobutyrate	2.24*	856	0.06	1.66*	1027	0.46
(3Z)-Hexenol	2.24*	856	[0.06]	5.71	1348	0.03
(2E)-Hexenol	2.40*	869	0.07	5.97	1366	0.04
Isobutyl propionate	2.40*	869	[0.07]	1.89	1050	0.01
Hexanol	2.44	872	0.06	5.37	1323	0.05
Isoamyl acetate	2.51	877	0.28	2.32*†	1093	[0.36]
2-Methylbutyl acetate	2.54	880	0.07	2.32*†	1093	[0.36]
Propyl methacrylate	2.57	882	0.04	2.39	1099	0.04
Ethyl angelate	2.79	900	0.10	2.75	1128	0.08
Heptanal	2.84	904	0.01	3.03*	1150	0.62
Isobutyl isobutyrate	3.04	917	0.56	2.04*	1065	[0.90]
Tricyclene	3.06	919	0.04	1.21	972	0.03
Tiglyl acetate?	3.12	922	0.02	3.83	1211	0.01
α-Thujene	3.16	925	0.02	1.40	1000	tr
α-Pinene	3.27	932	10.42	1.34*	995	[10.41]
Methallyl isobutyrate	3.28	933	0.46	3.03*	1150	[0.62]

Isobutyl methacrylate	3.40	941	0.28	2.84*	1135	0.29
Camphene	3.45*	944	0.47	1.66*	1027	[0.46]
α-Fenchene	3.45*	944	[0.47]	1.62	1023	0.03
Propyl 2-methylbutyrate	3.50	948	0.02	2.53	1110	0.02
Thuja-2,4(10)-diene	3.54	950	0.09	2.23*	1085	0.12
Benzaldehyde	3.60	954	0.03	7.22	1459	0.01
Butyl isobutyrate	3.62	956	0.03	2.64	1119	0.03
Methallyl methacrylate	3.66*	958	3.88	3.98*	1222	0.82
Isobutyl butyrate	3.66*	958	[3.88]	2.78	1130	3.09
β-Pinene	3.88*	972	0.43	2.04*	1065	[0.90]
Sabinene	3.88*	972	[0.43]	2.23*	1085	[0.12]
2-Methylbutyl propionate	3.91	974	0.04	3.12	1157	0.04
Butyl methacrylate	4.04	982	0.03	3.58	1193	0.03
Octen-3-ol	4.05	983	0.06	6.72	1422	0.06
3-Methylpentyl acetate	4.07	985	0.53	3.69*	1202	0.52
Octan-3-one	4.12	988	0.02	3.98*	1222	[0.82]
6-Methyl-5-hepten-2-one	4.14	989	0.01	5.01*	1297	[0.94]
2-Pentylfuran	4.16	991	0.05	3.63	1197	0.02
Myrcene	4.19	993	0.03	2.84*	1135	[0.29]
Propyl angelate	4.25	997	0.69	3.88	1215	0.73
Isobutyl 2-methylbutyrate	4.39	1006	0.09	3.03*	1150	[0.62]
Isobutyl isovalerate	4.45	1010	0.04	3.26*	1168	[6.01]
Isoamyl isobutyrate	4.57	1017	4.25	3.26*	1168	[6.01]
2-Methylbutyl isobutyrate	4.62	1020	1.64	3.26*	1168	[6.01]
Methallyl 2-methylbutyrate	4.64	1022	0.10	4.10	1231	0.10
para-Cymene	4.66	1023	0.04	4.03	1226	0.04
Methallyl isovalerate?	4.70	1025	0.04	4.30	1246	0.04
Limonene	4.74†	1028	0.38	3.14	1158	0.04
1,8-Cineole	4.77†	1030	[0.38]	3.26*	1168	[6.01]
Propyl tiglate	4.90	1038	0.01	4.84	1285	0.01
Unknown [m/z 43, 41 (84), 71 (62), 69 (59), 68 (51), 67 (48), 93 (41)...156 (4)]	4.95	1041	0.01			
2-Methylbutyl methacrylate	5.00	1044	0.63	4.24†	1241	[1.10]
Isoamyl methacrylate	5.02	1045	0.39	4.23†	1241	1.10

Isobutyl angelate	5.20*	1056	11.00	4.45*	1256	10.92
γ-Terpinene	5.20*	1056	[11.00]	3.69*	1202	[0.52]
Prenyl isobutyrate	5.22	1058	0.04	4.81	1283	0.05
Tiglyl isobutyrate?	5.30	1063	0.01	4.78	1280	0.02
Unknown [m/z 71, 43 (28), 41 (21), 57 (19), 98 (11)... 116 (4), 129 (1), 156 (t)]	5.37	1067	0.02	6.87	1433	0.03
Methallyl angelate	5.45	1072	13.29	5.60	1339	13.42
Isobutyl senecioate	5.46	1073	0.10	5.23	1313	0.05
3-Methylpentyl propionate?	5.54	1078	0.34	4.61	1268	0.34
para-Cymenene	5.66	1085	0.03	6.26	1388	0.02
Tiglyl methacrylate	5.70	1088	0.02	5.91	1362	0.02
Butyl angelate	5.79†	1093	0.41	5.17	1308	0.27
Isobutyl tiglate	5.81†	1094	[0.41]	5.34	1321	0.11
2-Methylbutyl isovalerate?	5.88	1099	0.02	4.66	1272	0.02
Isoamyl 2-methylbutyrate	5.95*	1103	0.17	4.45*	1256	[10.92]
Linalool	5.95*	1103	[0.17]	7.92	1512	0.03
2-Methylbutyl 2-methylbutyrate	6.00	1107	0.18	4.37	1250	0.21
Methallyl tiglate	6.09	1112	0.16	6.56	1410	0.12
3-Methylpentyl isobutyrate?	6.16	1117	0.04	4.73*	1276	7.40
3-Methylpentyl isobutyrate	6.23	1121	7.39	4.73*	1276	[7.40]
α-Campholenal	6.26	1123	0.02	6.93*	1437	0.05
trans-Pinocarveol	6.47	1137	5.10	9.12	1605	5.12
trans-Verbenol	6.52	1140	0.04	9.42	1630	0.04
Camphene hydrate	6.59	1144	0.19	8.39	1548	0.15
3-Methylpentyl methacrylate	6.66	1149	1.47	5.76	1351	1.47
Isoamyl angelate	6.74	1154	5.60	5.83	1356	5.44
Pinocarpone	6.80*	1158	6.72	7.84*	1506	1.98
2-Methylbutyl angelate	6.80*	1158	[6.72]	5.88*	1360	5.49
Unknown [m/z 96, 95 (72), 67 (45), 41 (42), 55 (32), 70 (27)... 152 (t)]	6.84	1160	0.01	10.05	1681	0.01
Benzyl acetate	6.91*†	1164	0.82	9.96	1674	0.02
Borneol	6.91*†	1164	[0.82]	9.70	1653	0.20
Angelyl angelate?	6.92†	1166	[0.82]	6.78*	1426	0.61
Isopinocampone	6.98	1169	0.05	7.53	1482	0.05
Terpinen-4-ol	7.08	1175	0.04	8.50	1556	0.02
Isobutyl 3-hydroxy-2-methylenebutyrate	7.20	1183	0.06	10.80*	1744	0.40
para-Cymen-8-ol	7.23	1185	0.04	11.46	1801	0.05

<i>trans</i> -Isocarveol	7.26	1187	0.02	10.88	1750	0.02
Amyl angelate	7.31*	1190	0.65	6.50	1405	0.04
Myrtenal	7.31*	1190	[0.65]	8.59	1564	0.64
Myrtenol	7.39	1195	0.34	10.80*	1744	[0.40]
2-Methylbutyl tiglate	7.42	1197	0.07	6.83	1430	0.14
Tiglyl angelate	7.45*	1199	0.07	7.43	1474	0.04
Isoamyl tiglate	7.45*	1199	[0.07]	6.78*	1426	[0.61]
Verbenone	7.50	1202	0.05	9.54	1639	0.26
3-Methylpentyl 2-methylbutyrate?	7.57	1207	0.94	5.88*	1360	[5.49]
3-Methylpentyl isovalerate?	7.66	1212	0.04	5.88*	1360	[5.49]
<i>trans</i> -Carveol	7.75	1219	0.01	11.36	1791	0.01
4-Methylhexyl isobutyrate	7.79	1221	0.03			
Carvone	8.07	1240	0.01	9.91	1669	0.01
2-Hydroxy-2-methylbut-3-enyl angelate	8.14	1245	0.02	11.79	1830	0.02
Linalyl acetate	8.35*	1259	14.70	8.05	1522	0.01
3-Methylpentyl angelate	8.35*	1259	[14.70]	7.33	1467	14.46
(3 <i>Z</i>)-Hexenyl angelate	8.70	1282	0.02	8.15	1530	0.09
Hexyl angelate	8.80	1289	0.02	7.84*	1506	[1.98]
<i>trans</i> -Pinocarvyl acetate	8.92	1297	0.01	9.03	1598	0.03
3-Methylpentyl tiglate	8.98	1301	0.07	8.18	1532	0.20
Benzyl isobutyrate	9.18	1313	0.02	10.62	1729	0.01
7βH-Silphiperfol-5-ene	9.52	1337	0.02	6.38	1396	0.01
Cyclosativene II	9.88	1362	0.04	6.93*	1437	[0.05]
α-Copaene	10.02	1372	0.01	7.08	1449	0.01
Isobutyl phenylacetate	10.23	1386	0.01	11.85	1835	0.01
Total identified		98.79%			97.86%	
Total reported		98.84%			97.90%	

*: 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