

Date : November 17, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21K08-PTH01

Customer identification : Magnolia Flower - China - MQ0103216R

Type : Essential oil

Source : *Michelia x alba*

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 : November 11, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Light orange liquid

Refractive index: 1.4652 ± 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
3-Methylfuran	0.01	Furan
Methyl propionate	0.05	Aliphatic ester
1,3-Cyclohexadiene	tr	Alkene
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	0.07	Aliphatic aldehyde
Methyl isobutyrate	0.01	Aliphatic ester
Methyl butyrate	0.07	Aliphatic ester
2-Methylbutanenitrile	tr	Aliphatic nitrile
Isoamyl alcohol	0.02	Aliphatic alcohol
2-Methylbutanol	0.04	Aliphatic alcohol
Methyl 2-methylbutyrate	5.22	Aliphatic ester
Ethyl 2-methylbutyrate	0.01	Aliphatic ester
Methyl tiglate	0.02	Aliphatic ester
Isovaleric acid	0.01	Aliphatic acid
Hexanol	0.07	Aliphatic alcohol
2-Methylbutyric acid	0.15	Aliphatic acid
2-Methylhexanoic acid?	0.20	Aliphatic acid
2-Heptanone	0.01	Aliphatic ketone
(4Z)-Heptenal	tr	Aliphatic aldehyde
Heptanal	0.01	Aliphatic aldehyde
Methyl hexanoate	0.01	Aliphatic ester
α -Thujene	0.02	Monoterpene
α -Pinene	0.19	Monoterpene
Methyl (3E)-hexenoate?	0.01	Aliphatic ester
Camphene	0.06	Monoterpene
β -Pinene	0.45	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.11	Monoterpene
α -Terpinene	0.04	Monoterpene
para-Cymene	0.07	Monoterpene
1,8-Cineole	0.50	Monoterpenic ether
Limonene	0.41	Monoterpene
(Z)- β -Ocimene	2.41	Monoterpene
(E)- β -Ocimene	2.64	Monoterpene
γ -Terpinene	0.06	Monoterpene
cis-Linalool oxide (fur.)	0.19	Monoterpenic alcohol
Terpinolene	0.03	Monoterpene
trans-Linalool oxide (fur.)	0.22	Monoterpenic alcohol
Methyl benzoate	0.04	Phenolic ester
Rosefuran	0.02	Monoterpenic ether
Hotrienol	0.08	Monoterpenic alcohol
Linalool	65.18	Monoterpenic alcohol
endo-Fenchol	0.07	Monoterpenic alcohol
Phenylethyl alcohol	0.27	Simple phenolic
Methyl octanoate	0.02	Aliphatic ester

allo-Ocimene	0.06	Monoterpene
Camphor	0.01	Monoterpenic ketone
Camphene hydrate	0.01	Monoterpenic alcohol
Borneol	0.07	Monoterpenic alcohol
<i>cis</i> -Linalool oxide (pyr.)	0.02	Monoterpenic alcohol
Terpinen-4-ol	0.07	Monoterpenic alcohol
<i>trans</i> -Linalool oxide (pyr.)	0.04	Monoterpenic alcohol
α -Terpineol	0.26	Monoterpenic alcohol
Hodiendiol	0.02	Monoterpenic alcohol
Methylchavicol	0.08	Phenylpropanoid
Nerol	0.09	Monoterpenic alcohol
Phenylethyl acetate	0.06	Phenolic ester
Geraniol	0.24	Monoterpenic alcohol
Undec-(5 <i>Z</i>)-en-2-one	0.04	Aliphatic ketone
Safrole	0.13	Phenylpropanoid
1-Nitro-2-phenylethane	0.02	Simple phenolic
Indole	0.02	Indole
δ -Elemene	0.02	Sesquiterpene
Methyl anthranilate	0.03	Phenolic ester
α -Cubebene	0.06	Sesquiterpene
Hodiendiol derivative III	0.01	Oxygenated monoterpene
α -Copaene	0.31	Sesquiterpene
<i>cis</i> - β -Elemene	0.05	Sesquiterpene
β -Cubebene	0.02	Sesquiterpene
β -Elemene	1.62	Sesquiterpene
Phenylethyl isobutyrate	0.02	Phenolic ester
Methyleugenol	2.52	Phenylpropanoid
<i>cis</i> - α -Bergamotene	0.08	Sesquiterpene
β -Caryophyllene	2.50	Sesquiterpene
α -Santalene	0.08	Sesquiterpene
β -Copaene	0.03	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.17*	Sesquiterpene
α -Guaiene	0.17*	Sesquiterpene
9-epi-Isocaryophyllene	0.04	Sesquiterpene
α -Humulene	0.53	Sesquiterpene
allo-Aromadendrene	0.01	Sesquiterpene
(<i>E</i>)- β -Farnesene	0.04	Sesquiterpene
Selina-4,11-diene	0.27	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.08	Sesquiterpene
γ -Murolene	0.11	Sesquiterpene
Germacrene D	0.44	Sesquiterpene
β -Selinene	1.32	Sesquiterpene
Phenylethyl isovalerate	0.22	Phenolic ester
Phenylethyl 2-methylbutyrate	0.07	Phenolic ester
α -Selinene	0.96	Sesquiterpene
α -Murolene	0.04	Sesquiterpene
Methyl (<i>E</i>)-isoeugenol	0.52	Phenylpropanoid
Germacrene A	0.05	Sesquiterpene
δ -Guaiene	0.04	Sesquiterpene
β -Bisabolene	0.26	Sesquiterpene
γ -Cadinene	0.11	Sesquiterpene
Cubebol	0.04	Sesquiterpenic alcohol

(3E,6E)- α -Farnesene	0.14	Sesquiterpene
<i>trans</i> -Calamenene	0.01	Sesquiterpene
δ -Cadinene	0.94	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	0.20	Sesquiterpene
α -Cadinene	0.03	Sesquiterpene
α -Calacorene	0.05	Sesquiterpene
Isocaryophyllene epoxide B	0.06	Sesquiterpenic ether
Elemicin	0.03	Phenylpropanoid
(<i>E</i>)-Nerolidol	0.29	Sesquiterpenic alcohol
Caryophyllene oxide	0.52	Sesquiterpenic ether
Viridiflorol	0.04	Sesquiterpenic alcohol
Humulene epoxide II	0.12	Sesquiterpenic ether
Unknown	0.09	Oxygenated sesquiterpene
Junenol	0.04	Sesquiterpenic alcohol
1- <i>epi</i> -Cubenol	0.12	Sesquiterpenic alcohol
τ -Cadinol	0.41	Sesquiterpenic alcohol
τ -Muurolol	0.29	Sesquiterpenic alcohol
α -Muurolol	0.03	Sesquiterpenic alcohol
Selin-11-en-4 α -ol	0.34	Sesquiterpenic alcohol
α -Cadinol	0.01	Sesquiterpenic alcohol
Phenylethyl hexanoate	0.09	Phenolic ester
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5 β -ol	0.02	Sesquiterpenic alcohol
Heptadecane	0.07	Alkane
Unknown	0.01	Oxygenated sesquiterpene
Phenylethyl octanoate	0.02	Phenolic ester
Unknown	0.11	Aliphatic ester
Unknown	0.15	Aliphatic ester
Nonadecane	0.05	Alkane
Methyl palmitate	0.03	Aliphatic ester
Methyl linoleate	0.36	Aliphatic ester
Methyl α -linolenate	0.20	Aliphatic ester
Heneicosane	0.02	Alkane
Tricosane	0.03	Alkane
Consolidated total	97.86%	

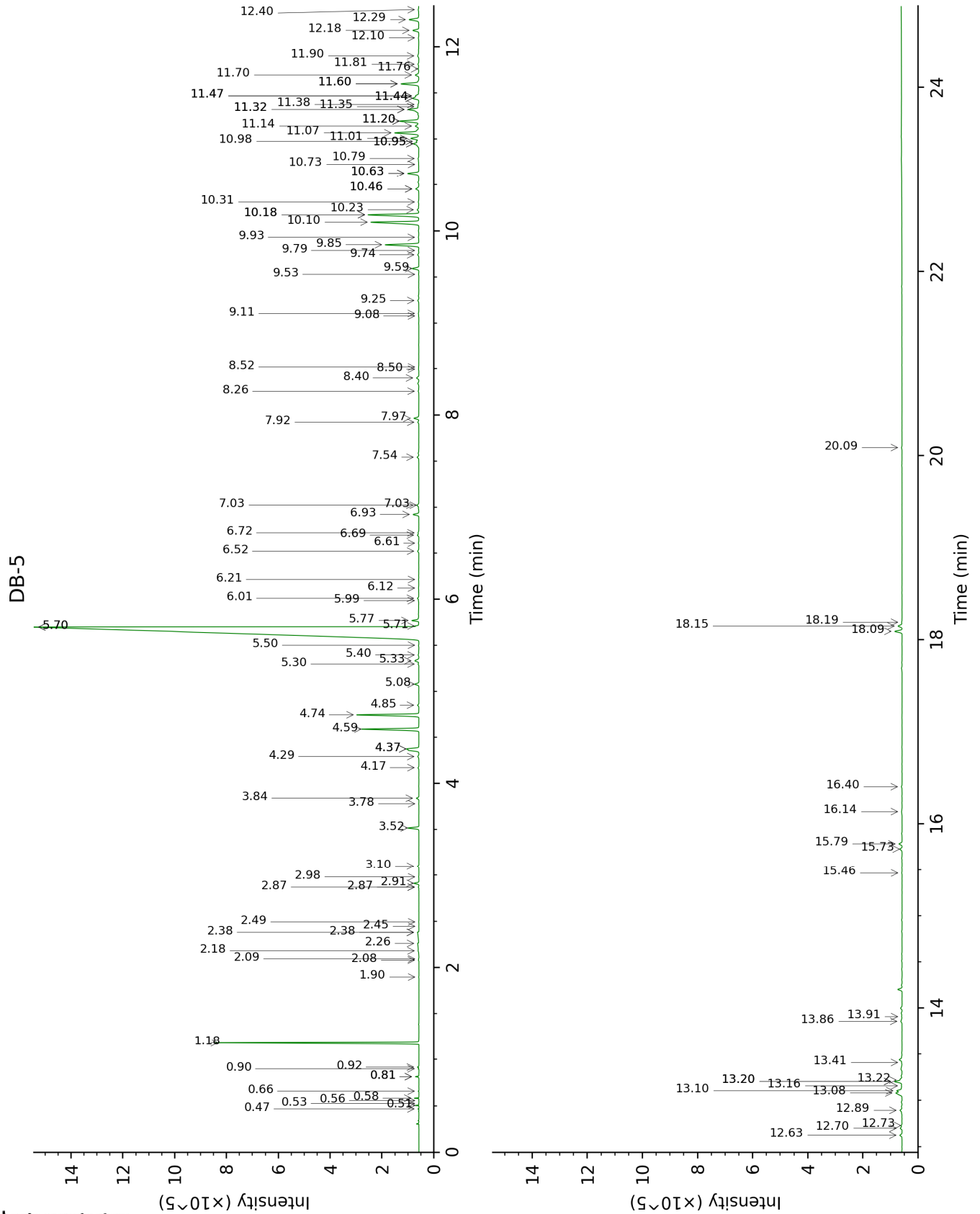
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: The compound has been detected below 0.005% of total signal.

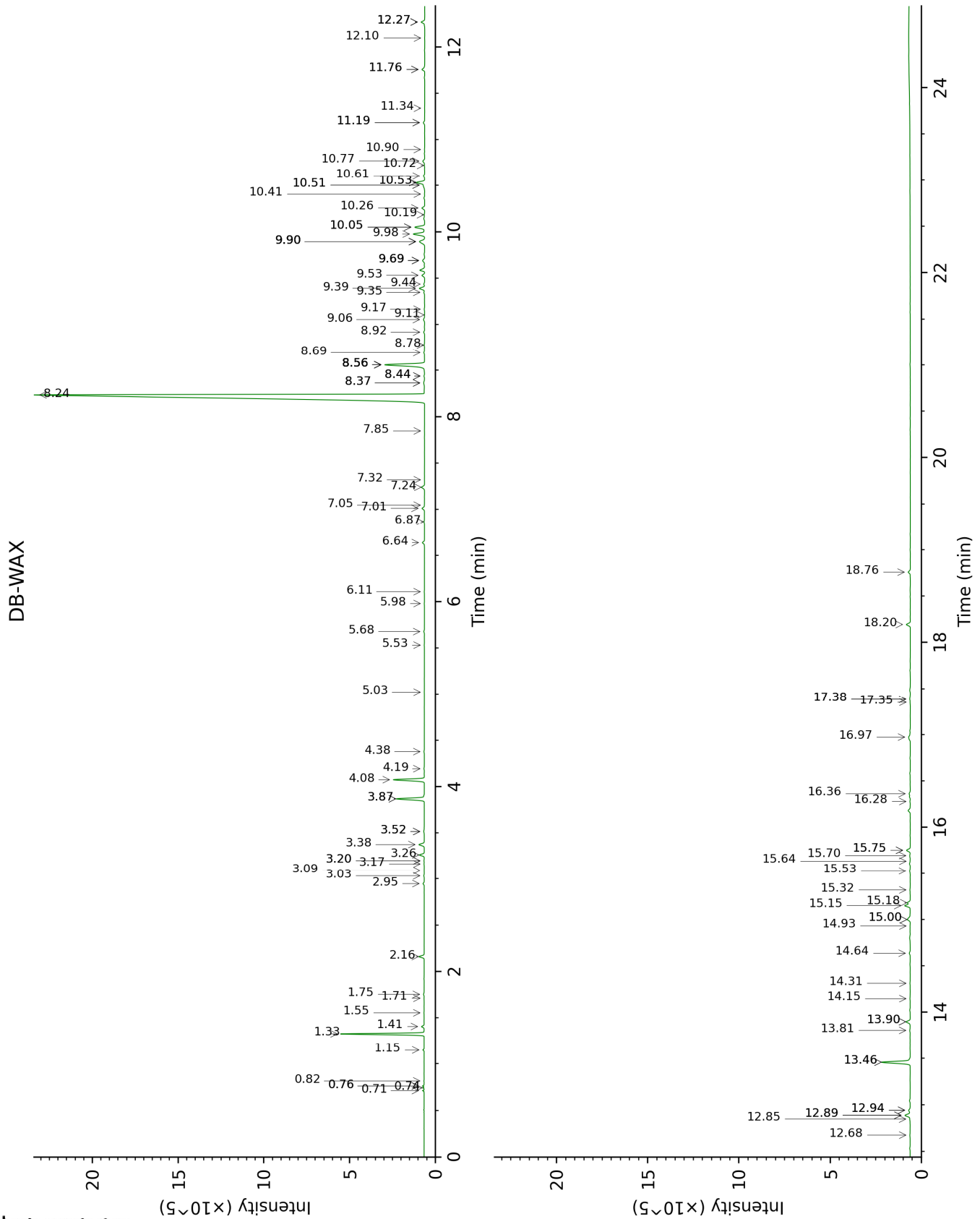
Note: no correction factor was applied

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	%
3-Methylfuran	0.47	606	0.01	0.71	863	0.06
Methyl propionate	0.51	621	0.05	0.74	874	0.05
1,3-Cyclohexadiene	0.53	629	tr			
Isovaleral	0.56	641	tr	0.76*	881	0.07
2-Methylbutyral	0.58	651	0.07	0.76*	881	[0.07]
Methyl isobutyrate	0.66	680	0.01	0.82	896	0.01
Methyl butyrate	0.82*	718	0.08	1.15	949	0.07
2-Methylbutanenitrile	0.82*	718	[0.08]			
Isoamyl alcohol	0.90	731	0.02	3.52*	1178	0.06
2-Methylbutanol	0.92	734	0.04	3.52*	1178	[0.06]
Methyl 2-methylbutyrate	1.18	774	5.22	1.33	978	5.36
Ethyl 2-methylbutyrate	1.90	849	0.01	1.71	1021	0.01
Methyl tiglate	2.08	865	0.02	3.20*	1153	0.03
Isovaleric acid	2.09	866	0.01	9.69*	1634	0.24
Hexanol	2.18	874	0.07	5.53	1324	0.01
2-Methylbutyric acid	2.26	881	0.15	9.90*	1651	0.73
2-Methylhexanoic acid?	2.38*	892	0.21			
2-Heptanone	2.38*	892	[0.21]	3.09	1145	0.01
(4Z)-Heptenal	2.45	897	tr			
Heptanal	2.49	901	0.01	3.17	1150	0.02
Methyl hexanoate	2.87*	927	0.02	3.20*	1153	[0.03]
α -Thujene	2.87*	927	[0.02]	1.56	1006	0.02
α -Pinene	2.91	930	0.19	1.41	991	0.20
Methyl (3E)-hexenoate?	2.98	935	0.01			
Camphene	3.10	943	0.06	1.75	1025	0.06
β -Pinene	3.52	971	0.45	2.16	1065	0.45
6-Methyl-5-hepten-2-one	3.78	989	0.01	5.02	1293	0.01
Myrcene	3.84	993	0.11	2.95	1133	0.10
α -Terpinene	4.17	1014	0.04	3.03	1140	0.04
para-Cymene	4.29	1022	0.07	4.19	1230	0.04
1,8-Cineole	4.37*	1027	0.91	3.38	1167	0.50
Limonene	4.37*	1027	[0.91]	3.26	1158	0.41
(Z)- β -Ocimene	4.59	1041	2.41	3.87*	1206	2.46
(E)- β -Ocimene	4.74	1050	2.64	4.08	1221	2.63
γ -Terpinene	4.85	1057	0.06	3.87*	1206	[2.46]
cis-Linalool oxide (fur.)	5.08	1072	0.19	6.64	1403	0.19
Terpinolene	5.30	1086	0.03	4.38	1244	0.03
trans-Linalool oxide (fur.)	5.34	1088	0.22	7.01	1431	0.24
Methyl benzoate	5.40	1092	0.04	8.78	1563	0.04

Rosefuran	5.50	1099	0.02	6.11	1365	0.02
Hotrienol	5.70*	1111	65.64	8.92	1574	0.08
Linalool	5.70*	1111	[65.64]	8.24	1521	65.18
endo-Fenchol	5.71	1112	0.07	8.56*	1546	4.29
Phenylethyl alcohol	5.77	1116	0.27	12.27*	1850	0.37
Methyl octanoate	5.99	1129	0.02	5.98	1356	0.01
allo-Ocimene	6.01	1131	0.06	5.68	1335	0.05
Camphor	6.12	1138	0.01	7.32	1453	tr
Camphene hydrate	6.21	1144	0.01	8.56*	1546	[4.29]
Borneol	6.52	1164	0.07	9.90*	1651	[0.73]
cis-Linalool oxide (pyr.)	6.61	1169	0.02	10.41	1692	0.02
Terpinen-4-ol	6.69	1175	0.07	8.69	1556	0.08
trans-Linalool oxide (pyr.)	6.72	1176	0.04	10.72	1718	0.03
α-Terpineol	6.93	1190	0.26	9.90*	1651	[0.73]
Hodiendiol	7.03*	1196	0.10	12.94*	1911	0.16
Methylchavicol	7.03*	1196	[0.10]	9.44	1614	0.08
Nerol	7.54	1231	0.09	11.19*	1757	0.14
Phenylethyl acetate	7.92	1256	0.06	11.19*	1757	[0.14]
Geraniol	7.97	1259	0.24	11.76*	1806	0.30
Undec-(5Z)-en-2-one	8.26	1278	0.04	9.06	1584	0.13
Safrole	8.40	1288	0.13	11.76*	1806	[0.30]
1-Nitro-2-phenylethane	8.50	1294	0.02	14.31	2038	0.03
Indole	8.52	1296	0.02	17.38*	2350	0.09
δ-Elemene	9.08	1335	0.02	7.05	1433	0.01
Methyl anthranilate	9.11	1337	0.03	15.53	2157	0.08
α-Cubebene	9.25	1347	0.06	6.87	1420	0.05
Hodiendiol derivative III	9.53	1367	0.01	12.89*	1906	0.57
α-Copaene	9.59	1371	0.31	7.24	1447	0.30
cis-β-Elemene	9.74	1382	0.05	8.44*	1537	0.06
β-Cubebene	9.79	1385	0.02	7.85	1492	0.01
β-Elemene	9.85	1389	1.62	8.56*	1546	[4.29]
Phenylethyl isobutyrate	9.93	1395	0.02	12.10	1835	0.01
Methyleugenol	10.10	1407	2.52	13.46*	1958	2.64
cis-α-Bergamotene	10.18*	1413	2.57	8.36*	1531	0.16
β-Caryophyllene	10.18*	1413	[2.57]	8.56*	1546	[4.29]
α-Santalene	10.23	1417	0.08	8.36*	1531	[0.16]
β-Copaene	10.31	1423	0.03	8.44*	1537	[0.06]
trans-α-Bergamotene	10.46*	1434	0.17	8.56*	1546	[4.29]
α-Guaiene	10.46*	1434	[0.17]	8.56*	1546	[4.29]
9-epi-Isocaryophyllene	10.63*	1446	0.58	9.17	1593	0.04
α-Humulene	10.63*	1446	[0.58]	9.39	1611	0.53
allo-Aromadendrene	10.73	1454	0.01	9.11	1588	0.02
(E)-β-Farnesene	10.79	1459	0.04	9.69*	1634	[0.24]

Selina-4,11-diene	10.95*	1470	0.36	9.53	1622	0.27
<i>trans</i> -Cadina-1(6),4-diene	10.95*	1470	[0.36]	9.35	1607	0.08
γ-Muurolene	10.98	1472	0.11	9.69*	1634	[0.24]
Germacrene D	11.01	1475	0.44	9.90*	1651	[0.73]
β-Selinene	11.07	1479	1.32	9.98	1657	1.21
Phenylethyl isovalerate	11.14	1485	0.22			
Phenylethyl 2-methylbutyrate	11.20*	1489	1.03	12.94*	1911	[0.16]
α-Selinene	11.20*	1489	[1.03]	10.05*	1663	0.99
α-Muurolene	11.32*	1498	0.67	10.18	1674	0.04
Methyl (<i>E</i>)-isoeugenol	11.32*	1498	[0.67]	15.15	2119	0.52
Germacrene A	11.35	1500	0.05	10.50*	1700	0.17
δ-Guaiene	11.38	1502	0.04	10.05*	1663	[0.99]
β-Bisabolene	11.44*	1507	0.37	10.26	1680	0.26
γ-Cadinene	11.44*	1507	[0.37]	10.53*	1702	0.86
Cubebol	11.47*	1509	0.15	12.68	1886	0.04
(3 <i>E</i> ,6 <i>E</i>)-α-Farnesene	11.47*	1509	[0.15]	10.61	1709	0.14
<i>trans</i> -Calamenene	11.60*	1520	0.95	11.34	1770	0.01
δ-Cadinene	11.60*	1520	[0.95]	10.53*	1702	[0.86]
<i>trans</i> -Cadina-1,4-diene	11.70	1527	0.20	10.77	1722	0.21
α-Cadinene	11.76	1532	0.03	10.90	1733	0.02
α-Calacorene	11.81	1536	0.05	12.27*	1850	[0.37]
Isocaryophyllene epoxide B	11.90	1543	0.06	12.27*	1850	[0.37]
Elemicin	12.10	1559	0.03	15.70	2174	0.07
(<i>E</i>)-Nerolidol	12.18	1565	0.29	13.90*	1998	0.40
Caryophyllene oxide	12.30	1574	0.52	12.89*	1906	[0.57]
Viridiflorol	12.40	1583	0.04	14.15	2022	0.04
Humulene epoxide II	12.63	1600	0.12	13.46*	1958	[2.64]
Unknown [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	12.70	1606	0.09	14.64	2069	0.09
Junenol	12.73	1608	0.04	13.81	1990	0.06
1-epi-Cubenol	12.89	1622	0.12	13.90*	1998	[0.40]
τ-Cadinol	13.08	1637	0.41	15.00*	2104	0.37
τ-Muurolol	13.10	1639	0.29	15.18	2122	0.25
α-Muurolol	13.16	1644	0.03	15.32	2136	0.04
Selin-11-en-4α-ol	13.20*	1648	0.38	15.75*	2179	0.37
α-Cadinol	13.20*	1648	[0.38]	15.64	2168	0.01
Phenylethyl hexanoate	13.22	1649	0.09	15.00*	2104	[0.37]
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5β-ol	13.41	1664	0.02	16.97	2306	0.30
Heptadecane	13.86	1702	0.07	10.50*	1700	[0.17]

Unknown [m/z 93, 81 (90), 95 (86), 91 (83), 41 (83), 107 (81)... 220 (29), 238? (4)]	13.91	1706	0.01	17.38*	2350	[0.09]
Phenylethyl octanoate	15.46	1843	0.02	17.35	2347	0.02
Unknown [m/z 43, 67 (85), 81 (70), 79 (53), 95 (46), 55 (39), 41 (37)...]	15.73	1867	0.11	16.28	2234	0.03
Unknown [m/z 79, 43 (84), 67 (55), 93 (50), 95 (41), 80 (35)...]	15.79	1872	0.15	16.36	2242	0.12
Nonadecane	16.14	1904	0.05	12.85	1902	0.03
Methyl palmitate	16.40	1929	0.03	15.75*	2179	[0.37]
Methyl linoleate	18.09	2094	0.36	18.20	2439	0.39
Methyl α -linolenate	18.15	2099	0.20	18.76	2503	0.21
Heneicosane	18.19	2103	0.02	14.93	2097	0.02
Tricosane	20.09	2304	0.03			
Total identified		97.98%			97.12%	
Total reported		98.35%			97.37%	

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

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