

Date : September 28, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21114-PTH01

Customer identification : Lavandin - France - L20107207R

Type : Essential oil

Source : *Lavandula x intermedia* cv. Grosso

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 : Sarah-Eve Tremblay, M. Sc. A., Chimiste

Analysis date : September 27, 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: 1.4603 ± 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
Ethanol	tr	Aliphatic alcohol
Isobutyral	tr	Aliphatic aldehyde
Methacrolein	tr	Aliphatic aldehyde
3-Buten-2-one	tr	Aliphatic ketone
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	tr	Aliphatic alcohol
Toluene	tr	Simple phenolic
Hexanal	0.01	Aliphatic aldehyde
Methyl hexyl ether	0.03	Aliphatic ether
(2E)-Hexenal	0.01	Aliphatic aldehyde
(3Z)-Hexenol	0.04	Aliphatic alcohol
Hexanol	0.10	Aliphatic alcohol
Hashishene	tr	Monoterpene
Tricyclene	0.01	Monoterpene
α -Thujene	0.07	Monoterpene
α -Pinene	0.34	Monoterpene
Camphene	0.26	Monoterpene
α -Fenchene	tr	Monoterpene
Thuja-2,4(10)-diene	0.01	Monoterpene
Butyl isobutyrate	0.01	Aliphatic ester
β -Pinene	0.27	Monoterpene
Sabinene	0.09	Monoterpene
Octen-3-ol	0.19	Aliphatic alcohol
Dehydro-1,8-cineole	0.03	Monoterpenic ether
Myrcene	0.42	Monoterpene
Butyl butyrate	0.03	Aliphatic ester
Octan-3-ol	0.01	Aliphatic alcohol
α -Phellandrene	0.03	Monoterpene
Δ^3 -Carene	0.07	Monoterpene
α -Terpinene	0.03	Monoterpene
Hexyl acetate	0.14	Aliphatic ester
ortho-Cymene	0.01	Monoterpene
para-Cymene	0.10	Monoterpene
1,8-Cineole	4.04	Monoterpenic ether
Limonene	0.63	Monoterpene
Lavender lactone	0.02	Aliphatic lactone
(Z)- β -Ocimene	0.85	Monoterpene
(E)- β -Ocimene	0.22	Monoterpene
γ -Terpinene	0.10	Monoterpene
cis-Sabinene hydrate	0.13	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.13	Monoterpenic alcohol
Octanol	0.04	Aliphatic alcohol
α -Pinene oxide analog	0.06	Monoterpenic ether
Terpinolene	0.08	Monoterpene

<i>trans</i> -Linalool oxide (fur.)	0.24	Monoterpenic alcohol
para-Cymenene	0.01	Monoterpene
<i>trans</i> -Sabinene hydrate	0.02	Monoterpenic alcohol
Rosefuran	0.04	Monoterpenic ether
Linalool	30.12	Monoterpenic alcohol
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	0.03	Aliphatic ketone
Octen-3-yl acetate	0.28	Aliphatic ester
Unknown	0.02	Unknown
α -Campholenal	0.03	Monoterpenic aldehyde
Octan-3-yl acetate	0.03	Aliphatic ester
Camphor	7.34	Monoterpenic ketone
Camphene hydrate	0.06	Monoterpenic alcohol
Hexyl isobutyrate	0.11	Aliphatic ester
Nerol oxide	0.07	Aliphatic ether
Borneol	2.71	Monoterpenic alcohol
δ -Terpineol	0.07	Monoterpenic alcohol
Lavandulol	0.48	Monoterpenic alcohol
Terpinen-4-ol	3.19	Monoterpenic alcohol
(<i>3E,5Z</i>)-Undeca-1,3,5-triene	0.02	Alkene
meta-Cymen-8-ol	0.03	Monoterpenic alcohol
para-Cymen-8-ol	0.05	Monoterpenic alcohol
α -Terpineol	0.63	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
Myrtenol	0.02	Monoterpenic alcohol
Hodiendiol	0.02	Monoterpenic alcohol
Hexyl butyrate	0.35	Aliphatic ester
Verbenone	0.02	Monoterpenic ketone
Unknown	0.04	Unknown
(<i>3E,5E</i>)-2,6-Dimethylocta-3,5,7-trien-2-ol	0.01	Monoterpenic alcohol
Octyl acetate	0.03	Aliphatic ester
Bornyl formate	0.04	Monoterpenic ester
Nerol	0.10	Monoterpenic alcohol
Hexyl 2-methylbutyrate	0.02	Aliphatic ester
Neral	0.09	Monoterpenic aldehyde
Hexyl isovalerate	0.17	Aliphatic ester
Linalyl acetate	33.59	Monoterpenic ester
Geraniol	0.26	Monoterpenic alcohol
<i>trans</i> -Ascaridole glycol	0.01	Monoterpenic alcohol
Geranial	tr	Monoterpenic aldehyde
Bornyl acetate	0.04	Monoterpenic ester
Lavandulyl acetate	2.16	Monoterpenic ester
Car-3-en-5-one	0.01	Monoterpenic ketone
Hexyl tiglate	0.18	Aliphatic ester
Hodiendiol derivative	0.03	Oxygenated monoterpene
Unknown	0.04	Oxygenated monoterpene
Unknown	0.03	Oxygenated monoterpene
Neryl acetate	0.16	Monoterpenic ester
α -Copaene	0.01	Sesquiterpene
7-Cubebene epimer?	0.09	Aliphatic alcohol
Daucene	0.07	Sesquiterpene
β -Bourbonene	0.05	Sesquiterpene
Geranyl acetate	0.27	Monoterpenic ester

7-epi-Sesquithujene	0.06	Sesquiterpene
Hexyl hexanoate	0.05	Aliphatic ester
α -Funebrene	0.01	Sesquiterpene
Sesquithujene	0.09	Sesquiterpene
β -Caryophyllene	1.51	Sesquiterpene
α -Santalene	0.23	Sesquiterpene
Lavandulyl isobutyrate	0.01	Monoterpenic ester
Coumarin	0.06	Coumarin
<i>trans</i> - α -Bergamotene	0.15	Sesquiterpene
Isogermacrene D	0.01	Sesquiterpene
Sesquisabinene A	0.09	Sesquiterpene
α -Humulene	0.06	Sesquiterpene
Lavandulyl butyrate?	0.10	Monoterpenic ester
(<i>E</i>)- β -Farnesene	1.14	Sesquiterpene
β -Santalene	0.05	Sesquiterpene
Dauca-5,8-diene?	0.08	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.09	Sesquiterpene
Germacrene D	0.78	Sesquiterpene
<i>trans</i> - β -Bergamotene	0.05	Sesquiterpene
Isodaucene	0.10	Sesquiterpene
α -Muurolene	0.05	Sesquiterpene
β -Bisabolene	0.22	Sesquiterpene
Lavandulyl isovalerate	0.34	Monoterpenic ester
Cubebol	0.02	Sesquiterpenic alcohol
γ -Cadinene	0.25	Sesquiterpene
δ -Cadinene	0.01	Sesquiterpene
β -Sesquiphellandrene	0.25	Sesquiterpene
(<i>E</i>)- α -Bisabolene	0.01	Sesquiterpene
<i>cis</i> -Sesquisabinene hydrate	0.01	Sesquiterpenic alcohol
(<i>E</i>)-Nerolidol	0.01	Sesquiterpenic alcohol
Germacrene D-4-ol	0.01	Sesquiterpenic alcohol
Caryophyllene oxide	0.09	Sesquiterpenic ether
Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
Neryl valerate?	0.03	Aliphatic ester
τ -Cadinol	0.16	Sesquiterpenic alcohol
(3 <i>Z</i>)-Caryophylla-3,8(13)-dien-5 β -ol	0.01	Sesquiterpenic alcohol
<i>cis</i> -14-nor-Muurool-5-en-4-one?	tr	Norsesquiterpenic ketone
α -Bisabolol	0.34	Sesquiterpenic alcohol
Consolidated total	98.67%	

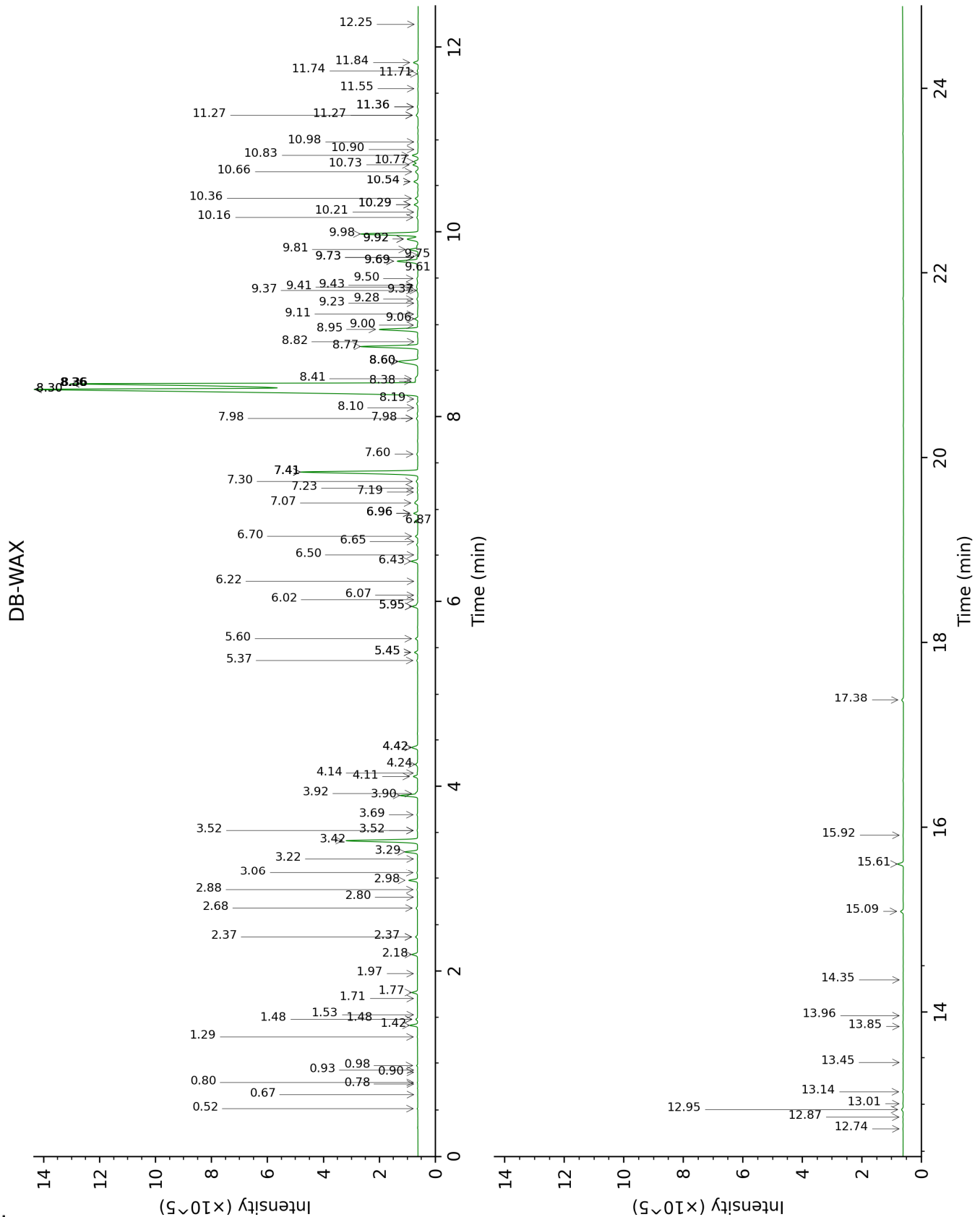
tr: The compound has been detected below 0.005% of total signal.

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	%
Ethanol	0.36	506	tr	0.90	908	tr
Isobutyral	0.39	539	tr	0.52	784	0.02
Methacrolein	0.40	552	tr	0.66	843	tr
3-Buten-2-one	0.43	577	tr	0.93	912	tr
Isovaleral	0.56	642	0.01	0.80	890	0.01
2-Methylbutyral	0.58	652	tr	0.78	884	tr
Isoamyl alcohol	0.90	732	tr	3.52*	1176	0.02
Toluene	1.07	758	tr	1.53	1001	tr
Hexanal	1.34	800	0.01	1.97	1045	tr
Methyl hexyl ether	1.63	826	0.03	0.98	919	0.03
(2E)-Hexenal	1.89	849	0.01	3.52*	1176	[0.02]
(3Z)-Hexenol	1.98	857	0.04	5.95*	1350	0.34
Hexanol	2.16	873	0.10	5.60	1325	0.12
Hashishene	2.72	917	tr	1.48*	996	0.07
Tricyclene	2.73	918	0.01	1.29	970	0.01
α-Thujene	2.84	925	0.07	1.48*	996	[0.07]
α-Pinene	2.91	930	0.34	1.42	990	0.34
Camphene	3.10*	942	0.26	1.77	1025	0.26
α-Fenchene	3.10*	942	[0.26]	1.70	1018	tr
Thuja-2,4(10)-diene	3.20	949	0.01	2.37*	1084	0.10
Butyl isobutyrate	3.28	955	0.01	2.80	1119	0.01
β-Pinene	3.51*	971	0.36	2.18	1065	0.27
Sabinene	3.51*	971	[0.36]	2.37*	1084	[0.10]
Octen-3-ol	3.71	984	0.19	6.87	1417	0.17
Dehydro-1,8-cineole	3.76	987	0.03	3.22	1152	0.01
Myrcene	3.84	992	0.42	2.98	1133	0.41
Butyl butyrate	3.94*	999	0.04	3.69	1190	0.03
Octan-3-ol	3.94*	999	[0.04]	6.22	1369	0.01
α-Phellandrene	3.97	1001	0.03	2.88	1126	0.02
Δ3-Carene	4.06	1007	0.07	2.68	1110	0.07
α-Terpinene	4.17	1014	0.03	3.06	1140	0.03
Hexyl acetate	4.23	1018	0.14	4.42*	1244	0.35
ortho-Cymene	4.25	1019	0.01	4.14	1223	0.02
para-Cymene	4.29	1022	0.10	4.24	1230	0.12
1,8-Cineole	4.38*	1027	4.59	3.42	1168	4.04
Limonene	4.38*	1027	[4.59]	3.29	1158	0.63
Lavender lactone	4.50	1035	0.02	9.37*	1606	0.07
(Z)-β-Ocimene	4.58	1040	0.85	3.90	1206	0.87
(E)-β-Ocimene	4.73	1050	0.22	4.11	1221	0.21
γ-Terpinene	4.84	1056	0.10	3.92	1207	0.08
cis-Sabinene hydrate	4.98	1065	0.13	6.96*	1423	0.20
cis-Linalool oxide (fur.)	5.07	1071	0.13	6.70	1404	0.13
Octanol	5.17	1077	0.04	8.36*†	1527	[64.06]
α-Pinene oxide analog	5.19	1078	0.06	5.45*	1314	0.16

Terpinolene	5.30*†	1085	0.33	4.42*	1244	[0.35]
<i>trans</i> -Linalool oxide (fur.)	5.30*†	1085	[0.33]	7.07	1431	0.24
para-Cymenene	5.30*†	1085	[0.33]	6.50	1389	0.01
<i>trans</i> -Sabinene hydrate	5.48	1097	0.02	8.10	1508	0.01
Rosefuran	5.50	1098	0.04	6.07	1358	0.02
Linalool	5.65	1108	30.12	8.30*†	1523	64.06
(<i>Z</i>)-6-Methyl-3,5-heptadien-2-one	5.67	1109	0.03	8.38	1530	0.13
Octen-3-yl acetate	5.80	1117	0.28	5.95*	1350	[0.34]
Unknown [m/z 82, 81 (72), 43 (64), 54 (32), 41 (20)...]	5.85	1120	0.02	9.75	1637	0.02
α-Campholenal	5.89	1122	0.03	7.19	1440	0.03
Octan-3-yl acetate	6.00	1130	0.03	5.36	1308	0.05
Camphor	6.14	1138	7.34	7.40*	1456	7.35
Camphene hydrate	6.20	1143	0.06	8.60*	1546	1.64
Hexyl isobutyrate	6.35*	1152	0.18	5.45*	1314	[0.16]
Nerol oxide	6.35*	1152	[0.18]	6.96*	1423	[0.20]
Borneol	6.53	1164	2.71	9.98†	1655	[4.12]
δ-Terpineol	6.56	1165	0.07	9.61	1625	tr
Lavandulol	6.62	1170	0.48	9.81	1642	0.47
Terpinen-4-ol	6.71	1175	3.19	8.77	1559	3.14
(3 <i>E</i> ,5 <i>Z</i>)-Undeca-1,3,5-triene	6.74	1177	0.02	6.02	1355	0.01
meta-Cymen-8-ol	6.82	1183	0.03	11.71	1799	0.03
para-Cymen-8-ol	6.86	1185	0.05	11.74	1802	0.06
α-Terpineol	6.92*	1189	0.67	9.92*†	1650	4.12
Myrtenal	6.92*	1189	[0.67]	8.82	1563	0.01
Myrtenol	7.02*	1195	0.37	10.98	1737	0.02
Hodiendiol	7.02*	1195	[0.37]	13.01	1914	0.02
Hexyl butyrate	7.02*	1195	[0.37]	6.44	1384	0.35
Verbenone	7.13	1202	0.02	9.73*	1635	0.06
Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.15	1204	0.04	11.36*	1769	0.05
(3 <i>E</i> ,5 <i>E</i>)-2,6-Dimethylocta-3,5,7-trien-2-ol	7.29	1213	0.01	11.55	1785	0.03
Octyl acetate	7.33	1216	0.03	7.23	1443	0.03
Bornyl formate	7.43	1222	0.04	8.19	1515	0.02
Nerol	7.55	1230	0.10	11.27*	1761	0.14
Hexyl 2-methylbutyrate	7.61	1234	0.02	6.65	1400	0.01
Neral	7.69	1240	0.09	9.69*	1631	1.23
Hexyl isovalerate	7.77	1245	0.17	6.96*	1423	[0.20]
Linalyl acetate	8.04*	1263	34.38	8.36*†	1527	[64.06]
Geraniol	8.04*	1263	[34.38]	11.84	1810	0.26
<i>trans</i> -Ascaridole glycol	8.15	1270	0.01	14.35	2038	0.01
Geranial	8.22	1275	tr	10.30*	1680	0.22

Bornyl acetate	8.34	1282	0.04	8.41	1532	0.23
Lavandulyl acetate	8.51	1294	2.16	8.95	1573	2.16
Car-3-en-5-one	8.65	1304	0.01	12.25	1846	0.01
Hexyl tiglate	9.06	1332	0.18	9.06	1582	0.17
Hodiendiol derivative	9.21	1343	0.03	13.14	1925	0.04
Unknown [m/z 43, 79 (47), 71 (31), 94 (27), 81 (23), 41 (22)... 197 (0)]	9.35	1353	0.04	11.27*	1761	[0.14]
Unknown [m/z 43, 79 (46), 71 (30), 94 (25), 41 (23), 81 (21)... 197 (0)]	9.40	1356	0.03	11.36*	1769	[0.05]
Neryl acetate	9.54	1366	0.16	10.36	1686	0.17
α -Copaene	9.60	1371	0.01	7.30	1448	0.10
7-Cubebene epimer?	9.66	1375	0.09	7.40*	1456	[7.35]
Daucene	9.71	1378	0.07	7.40*	1456	[7.35]
β -Bourbonene	9.78	1383	0.05	7.60	1470	0.07
Geranyl acetate	9.81	1385	0.27	10.73	1717	0.29
7-epi-Sesquithujene	9.86*	1389	0.11	7.98*	1499	0.09
Hexyl hexanoate	9.86*	1389	[0.11]	9.00	1577	0.05
α -Funebrene	9.91	1392	0.01	7.98*	1499	[0.09]
Sesquithujene	10.08	1405	0.09	8.30*†	1523	[64.06]
β -Caryophyllene	10.18	1412	1.51	8.60*	1546	[1.64]
α -Santalene	10.24	1416	0.23	8.36*†	1527	[64.06]
Lavandulyl isobutyrate	10.32	1422	0.01	9.50	1616	0.07
Coumarin	10.34	1424	0.06	17.38	2342	0.10
<i>trans</i> - α -Bergamotene	10.46	1433	0.15	8.60*	1546	[1.64]
Isogermacrene D	10.52	1437	0.01	9.11	1586	0.03
Sesquisabinene A	10.56	1440	0.09	9.28	1599	0.07
α -Humulene	10.63	1445	0.06	9.42	1610	0.04
Lavandulyl butyrate?	10.75	1454	0.10	10.66	1710	0.18
(<i>E</i>)- β -Farnesene	10.80*	1458	1.20	9.69*	1631	[1.23]
β -Santalene	10.80*	1458	[1.20]	9.37*	1606	[0.07]
Dauca-5,8-diene?	10.86	1462	0.08	9.23	1595	0.01
<i>trans</i> -Cadina-1(6),4-diene	10.92	1467	0.09	9.41	1609	0.09
Germacrene D	11.01	1474	0.78	9.92*†	1650	[4.12]
<i>trans</i> - β -Bergamotene	11.10	1480	0.05	9.73*	1635	[0.06]
Isodaucene	11.23	1490	0.10	10.16	1669	0.08
α -Muurolene	11.31	1496	0.05	10.21	1674	0.03
β -Bisabolene	11.46*†	1507	0.88	10.30*	1680	[0.22]
Lavandulyl isovalerate	11.46*†	1507	[0.88]	10.83	1725	0.34
Cubebol	11.51*†	1511	[0.88]	12.74	1889	0.02

γ-Cadinene	11.51*†	1511	[0.88]	10.54*	1701	0.26
δ-Cadinene	11.60	1518	0.01	10.54*	1701	[0.26]
β-Sesquiphellandrene	11.63	1521	0.25	10.77	1720	0.24
(E)-α-Bisabolene	11.92	1543	0.01	10.90	1730	0.01
cis-Sesquisabinene hydrate	12.02	1551	0.01	13.45	1954	0.01
(E)-Nerolidol	12.18	1564	0.01	13.96	2001	0.01
Germacrene D-4-ol	12.24	1569	0.01	13.85	1990	tr
Caryophyllene oxide	12.29*	1572	0.11	12.95	1908	0.09
Caryophyllene oxide isomer	12.29*	1572	[0.11]	12.87	1901	0.02
Neryl valerate?	12.73	1607	0.03			
τ-Cadinol	13.06	1634	0.16	15.09	2109	0.16
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	13.44	1666	0.01			
cis-14-nor-Muurool-5-en-4-one?	13.54	1674	tr	15.92	2191	0.03
α-Bisabolol	13.61	1680	0.34	15.61	2160	0.31
Total identified		99.04%			98.72%	
Total reported		99.17%			98.73%	

*: 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