

Date : February 24, 2021

CERTIFICATE OF ANALYSIS – GC PROFILING & CARRIER OIL DETERMINATION

SAMPLE IDENTIFICATION

Internal code : 21B23-PTH10


Customer identification : Ylang Ylang Complete ORG - Y801062012R

Type : Essential oil

Source : *Cananga odorata* var. *genuina* (Ylang-ylang)

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. Carrier oil determination by PC-MAT-010 – GC-FID quantitation of fatty acid methyl esters after derivatization, against an internal standard of tridecanoic acid.

Analyst : Sylvain Mercier, M. Sc., Chimiste

Analysis date : February 23, 2021

Checked and approved by :

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

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PHYSICOCHEMICAL DATA

Physical aspect: Faintly yellow liquid

Refractive index: 1.5074 ± 0.0003 (20 °C; method PC-MAT-016)

CARRIER OIL DETERMINATION

After derivatization, less than 0.1% of fatty acids were found (i.e. none detected). The oil is therefore undiluted with a carrier oil.

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method. The oil is not diluted with a carrier oil.

ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

New readers of similar reports are encouraged to read table footnotes at least once.

Identification	%	Class
2-Methyl-3-buten-2-ol	0.02	Aliphatic alcohol
Toluene	0.01	Simple phenolic
Prenol	tr	Aliphatic alcohol
Butyl acetate	tr	Aliphatic ester
2-Methylbutyl acetate	tr	Aliphatic ester
3-Methyl-3-butenyl acetate	0.18	Aliphatic ester
Isobutyl isobutyrate	tr	Aliphatic ester
Prenyl acetate	0.45	Aliphatic ester
α -Pinene	0.10	Monoterpene
Benzaldehyde	0.01	Simple phenolic
β -Pinene	0.04	Monoterpene
6-Methyl-5-hepten-2-one	0.01	Aliphatic ketone
Myrcene	0.03	Monoterpene
(3Z)-Hexenyl acetate	0.03	Aliphatic ester
Hexyl acetate	0.01	Aliphatic ester
para-Methylanisole	2.28	Simple phenolic
Limonene	0.01	Monoterpene
1,8-Cineole	0.06	Monoterpenic ether
Benzyl alcohol	0.03	Simple phenolic
(E)- β -Ocimene	0.01	Monoterpene
cis-Sabinene hydrate	0.01	Monoterpenic alcohol
cis-Linalool oxide (fur.)	0.01	Monoterpenic alcohol
para-Cresol	0.02	Simple phenolic
Terpinolene	0.01	Monoterpene
Methyl benzoate	1.42	Phenolic ester
Linalool	2.90	Monoterpenic alcohol
Nonanal	0.03	Aliphatic aldehyde
2-Nonanol	0.03	Aliphatic alcohol
Benzeneacetonitrile	0.01	Simple phenolic
ortho-Dimethoxybenzene	0.03	Simple phenolic
Benzyl acetate	3.82	Phenolic ester
para-Cresyl acetate	0.10	Phenolic ester
Ethyl benzoate	0.07	Phenolic ester
Terpinen-4-ol	0.02	Monoterpenic alcohol
α -Terpineol	0.07	Monoterpenic alcohol
Methylchavicol	0.01	Phenylpropanoid
Nerol	0.01	Monoterpenic alcohol
Phenylethyl acetate	0.03	Phenolic ester
Geraniol	0.14	Monoterpenic alcohol
(E)-Anethole	0.10	Phenylpropanoid
1-Nitro-2-phenylethane	0.02	Simple phenolic
(E)-Cinnamyl alcohol	0.02	Phenylpropanoid
4-Vinylguaiacol	0.01	Simple phenolic
Bicycloelemene	0.14	Sesquiterpene
δ -Elemene	0.06	Sesquiterpene

α-Cubebene	0.21	Sesquiterpene
Eugenol	0.04	Phenylpropanoid
Neryl acetate	0.04	Monoterpenic ester
α-Ylangene	0.26	Sesquiterpene
α-Copaene	1.38	Sesquiterpene
β-Bourbonene	0.07	Sesquiterpene
β-Cubebene	0.17	Sesquiterpene
Geranyl acetate	2.20	Monoterpenic ester
β-Elemene	0.41	Sesquiterpene
Cyperene	0.02	Sesquiterpene
Vanillin	0.03	Simple phenolic
Isocaryophyllene	0.01	Sesquiterpene
Methyleugenol	0.01	Phenylpropanoid
α-Gurjunene	0.02	Sesquiterpene
β-Caryophyllene	5.73	Sesquiterpene
β-Ylangene	0.13	Sesquiterpene
β-Copaene	0.31	Sesquiterpene
Caryophylla-4(12),8(13)-diene	0.10	Sesquiterpene
Aromadendrene	0.04	Sesquiterpene
Isogermacrene D	0.03	Sesquiterpene
9-epi-Isocaryophyllene	0.03	Sesquiterpene
(E)-Cinnamyl acetate	2.03	Phenylpropanoid ester
(E)-Isoeugenol	0.92	Phenylpropanoid
α-Humulene	1.60	Sesquiterpene
cis-Cadina-1(6),4-diene	0.23	Sesquiterpene
cis-Muurolo-4(15),5-diene	0.24	Sesquiterpene
trans-Cadina-1(6),4-diene	0.29	Sesquiterpene
γ-Muurolo-1	1.95	Sesquiterpene
Germacrene D	16.58	Sesquiterpene
γ-Amorphene	0.51	Sesquiterpene
Prenyl benzoate	0.17	Phenolic ester
epi-Cubebol	0.04	Sesquiterpenic alcohol
Bicyclogermacrene	0.87	Sesquiterpene
α-Muurolo-1	0.45	Sesquiterpene
(3Z,6E)-α-Farnesene	0.07	Sesquiterpene
Unknown	0.73	Sesquiterpene
δ-Amorphene	0.45	Sesquiterpene
γ-Cadinene	0.54	Sesquiterpene
Cubebol	0.04	Sesquiterpenic alcohol
(3E,6E)-α-Farnesene	18.42	Sesquiterpene
(Z)-γ-Bisabolene	0.48	Sesquiterpene
δ-Cadinene	3.17	Sesquiterpene
trans-Calamenene	0.02	Sesquiterpene
Zonarene	0.19	Sesquiterpene
trans-Cadina-1,4-diene	0.23	Sesquiterpene
α-Cadinene	0.25	Sesquiterpene
α-Calacorene	0.06	Sesquiterpene
cis-Dracunculifolol	0.03	Sesquiterpenic alcohol
α-Elemol	0.04	Sesquiterpenic alcohol
Germacrene B	0.11	Sesquiterpene
(E)-Nerolidol	0.14	Sesquiterpenic alcohol
(3Z)-Hexenyl benzoate	0.11	Phenolic ester

Caryophyllene oxide	0.10	Sesquiterpenic ether
10-epi-Junenol	0.08	Sesquiterpenic alcohol
Unknown	0.06	Sesquiterpenic alcohol
Unknown	0.11	Oxygenated sesquiterpene
Viridiflorol	0.03	Sesquiterpenic alcohol
Guaiol	0.10	Sesquiterpenic alcohol
Copaborneol	0.07	Sesquiterpenic alcohol
Humulene epoxide II	0.07	Sesquiterpenic ether
Junenol	0.35	Sesquiterpenic alcohol
(E)-Isoeugenyl acetate	0.08	Phenylpropanoid ester
10-epi-Cubenol	0.14	Sesquiterpenic alcohol
1-epi-Cubenol	0.35	Sesquiterpenic alcohol
γ-Eudesmol	0.14	Sesquiterpenic alcohol
Cubenol	0.11	Sesquiterpenic alcohol
τ-Cadinol	0.38	Sesquiterpenic alcohol
τ-Muurolol	0.93	Sesquiterpenic alcohol
α-Muurolol	0.40	Sesquiterpenic alcohol
Unknown	0.27	Sesquiterpenic alcohol
α-Cadinol	1.72	Sesquiterpenic alcohol
<i>trans</i> -Calamene-10-ol	0.05	Sesquiterpenic alcohol
Bulnesol	0.02	Sesquiterpenic alcohol
Unknown	0.19	Oxygenated sesquiterpene
Eudesma-4(15),7-dien-1β-ol	0.01	Sesquiterpenic alcohol
(2E,6Z)-Farnesol	0.03	Sesquiterpenic alcohol
(2E,6E)-Farnesol	1.58	Sesquiterpenic alcohol
(2E,6E)-Farnesal	0.02	Sesquiterpenic aldehyde
Benzyl benzoate	6.13	Phenolic ester
(2E,6E)-Farnesyl acetate	3.46	Sesquiterpenic ester
Benzyl salicylate	3.70	Phenolic ester
Geranyl benzoate	0.01	Phenolic ester
Unknown	0.04	Unknown
Unknown	0.09	Unknown
Consolidated total	95.40%	

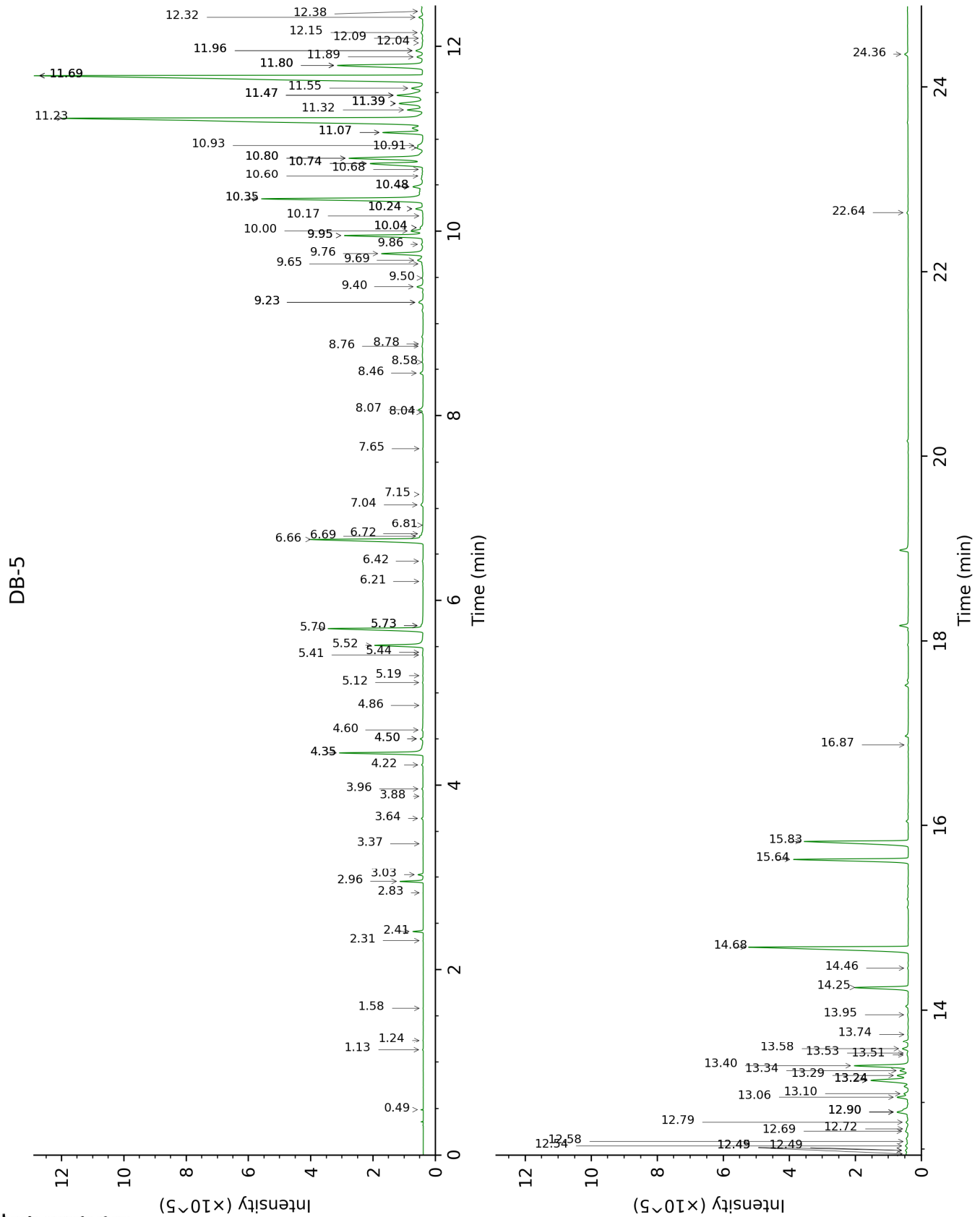
tr: The compound has been detected below 0.005% of total signal.

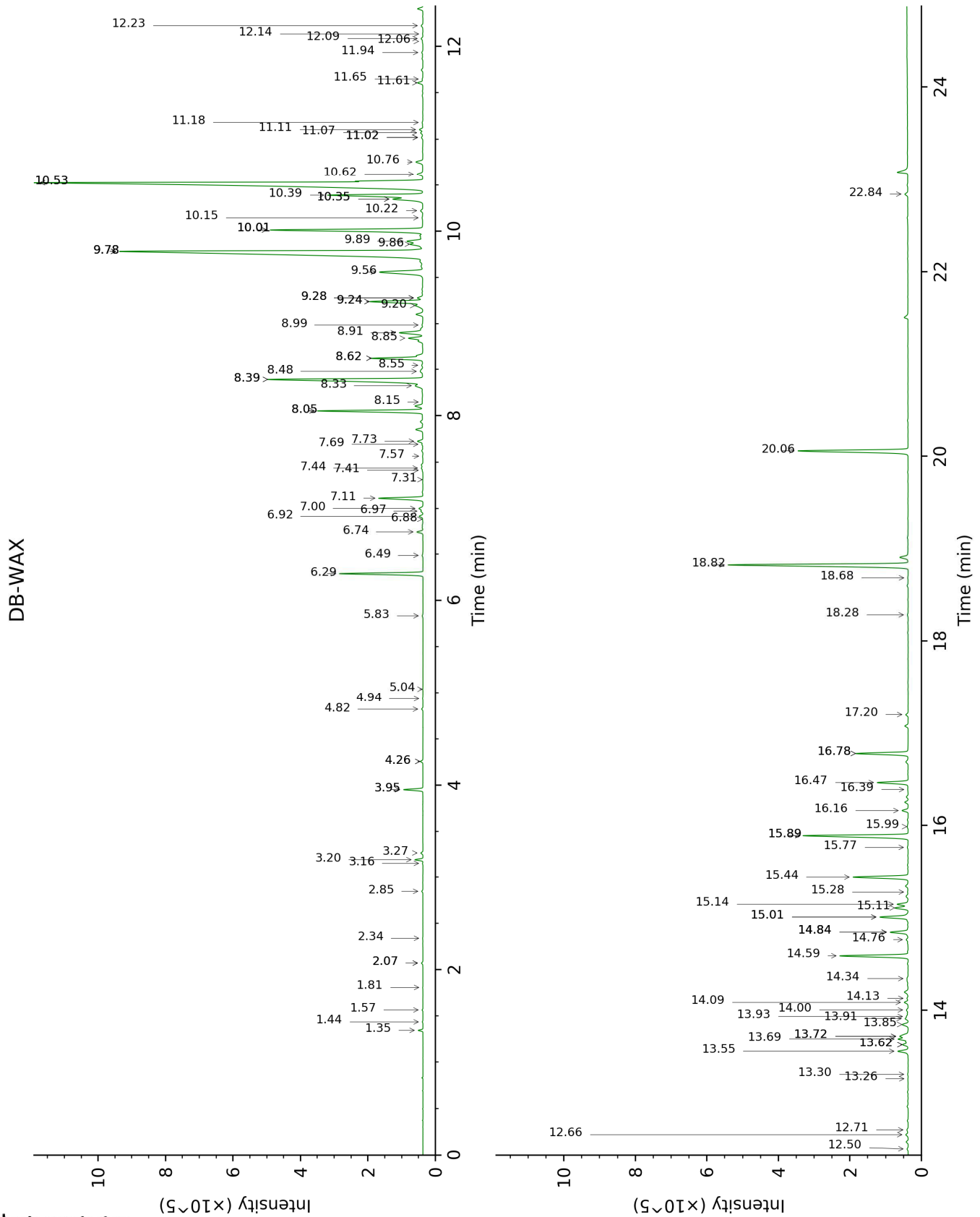
Note: no correction factor was applied

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	%
2-Methyl-3-buten-2-ol	0.49	599	0.02	1.57	1016	0.02
Toluene	1.13	759	0.01	1.44	1004	0.02
Prenol	1.24	774	tr	4.94	1289	0.01
Butyl acetate	1.58	816	tr	1.81	1040	0.01
2-Methylbutyl acetate	2.32	877	tr	2.34	1093	0.01
3-Methyl-3-butenyl acetate	2.41	885	0.18	3.20	1161	0.19
Isobutyl isobutyrate	2.83	917	tr	2.07*	1066	0.04
Prenyl acetate	2.96	925	0.45	3.95*	1218	0.48
α -Pinene	3.03	930	0.10	1.35	992	0.10
Benzaldehyde	3.37	952	0.01	7.31	1463	0.01
β -Pinene	3.64	971	0.04	2.07*	1066	[0.04]
6-Methyl-5-hepten-2-one	3.88	986	0.01	5.04	1297	0.01
Myrcene	3.96	992	0.03	2.85	1134	0.03
(3Z)-Hexenyl acetate	4.22	1009	0.03	4.82	1281	0.04
Hexyl acetate	4.35*	1017	2.29	4.26*	1240	0.07
para-Methylanisole	4.35*	1017	[2.29]	6.29	1387	2.28
Limonene	4.50*	1026	0.07	3.16	1158	0.01
1,8-Cineole	4.50*	1026	[0.07]	3.27	1166	0.06
Benzyl alcohol	4.60	1032	0.03	11.65	1814	0.02
(E)- β -Ocimene	4.86	1049	0.01	3.95*	1218	[0.48]
cis-Sabinene hydrate	5.12	1065	0.01	6.88	1431	0.01
cis-Linalool oxide (fur.)	5.19	1070	0.01	6.49	1401	0.04
para-Cresol	5.41	1084	0.02	13.85	2015	0.20
Terpinolene	5.44	1086	0.01	4.26*	1240	[0.07]
Methyl benzoate	5.52	1091	1.42	8.62*	1563	1.53
Linalool	5.70†	1102	2.96	8.06*	1519	3.03
Nonanal	5.73*†	1104	[2.96]	5.84	1354	0.03
2-Nonanol	5.73*†	1104	[2.96]	7.69	1492	0.03
Benzeneacetonitrile	6.21	1135	0.01	12.14	1857	0.01
ortho-Dimethoxybenzene	6.42	1149	0.03			
Benzyl acetate	6.66	1164	3.82	10.01*	1675	5.14
para-Cresyl acetate	6.69	1166	0.10			
Ethyl benzoate	6.72	1168	0.07	9.28*†	1615	[1.91]
Terpinen-4-ol	6.81	1174	0.02	8.55	1558	0.04
α -Terpineol	7.04	1189	0.07	9.78*	1656	17.17
Methylchavicol	7.15	1196	0.01	9.28*†	1615	[1.91]
Nerol	7.65	1229	0.01	11.02*	1759	0.05
Phenylethyl acetate	8.04	1256	0.03	11.02*	1759	[0.05]
Geraniol	8.07	1258	0.14	11.61	1810	0.16
(E)-Anethole	8.46	1285	0.10	11.10	1767	0.10

1-Nitro-2-phenylethane	8.58	1293	0.02	14.13	2042	0.04
(E)-Cinnamyl alcohol	8.76	1305	0.02	15.89*	2216	3.46
4-Vinylguaiaicol	8.78	1307	0.01	15.01*	2127	0.94
Bicycloelemene	9.23*	1334	0.19	7.00	1440	0.14
δ-Elemene	9.23*	1334	[0.19]	6.97	1438	0.06
α-Cubebene	9.40	1346	0.21	6.74	1420	0.18
Eugenol	9.50	1353	0.04	14.76	2102	0.07
Neryl acetate	9.65	1364	0.04	10.15	1686	0.03
α-Ylangene	9.69	1366	0.26	6.92	1434	0.12
α-Copaene	9.76	1371	1.38	7.11	1448	1.35
β-Bourbonene	9.86	1378	0.07	7.44	1472	0.06
β-Cubebene	9.95*	1385	2.37	7.73	1494	0.17
Geranyl acetate	9.95*	1385	[2.37]	10.52*	1717	20.62
β-Elemene	10.00	1389	0.41	8.39*	1546	6.14
Cyperene	10.04*	1391	0.11	7.41	1470	0.02
Vanillin	10.04*	1391	[0.11]	18.28	2473	0.03
Isocaryophyllene	10.17	1400	0.01	8.15	1527	0.02
Methyleugenol	10.24*	1406	0.25	13.26	1960	0.01
α-Gurjunene	10.24*	1406	[0.25]	7.57	1482	0.02
β-Caryophyllene	10.35*	1414	6.01	8.39*	1546	[6.14]
β-Ylangene	10.35*	1414	[6.01]	8.06*	1519	[3.03]
β-Copaene	10.48*	1423	0.41	8.33	1540	0.31
Caryophylla-4(12),8(13)-diene	10.48*	1423	[0.41]	8.62*	1563	[1.53]
Aromadendrene	10.60	1432	0.04	8.48	1552	0.15
Isogermacrene D	10.68	1438	0.03	8.85	1581	0.46
9-epi-Isocaryophyllene	10.74*	1442	2.07	8.99	1592	0.03
(E)-Cinnamyl acetate	10.74*	1442	[2.07]	14.59	2086	2.03
(E)-Isoeugenol	10.80*	1447	2.95	16.47	2275	0.92
α-Humulene	10.80*	1447	[2.95]	9.24*†	1612	1.91
cis-Cadina-1(6),4-diene	10.91	1455	0.23	8.91	1586	0.87
cis-Muurolo-4(15),5-diene	10.93	1457	0.24	9.24*†	1612	[1.91]
trans-Cadina-1(6),4-diene	11.07*†	1467	20.80	9.20	1609	0.29
γ-Muurolole	11.07*†	1467	[20.80]	9.56	1638	1.95
Germacrene D	11.23†	1479	[20.80]	9.78*	1656	[17.17]
γ-Amorphene	11.32	1486	0.51	9.78*	1656	[17.17]
Prenyl benzoate	11.39*	1491	1.08	13.69†	2000	0.66
epi-Cubebol	11.39*	1491	[1.08]	11.94	1839	0.04
Bicyclgermacrene	11.39*	1491	[1.08]	10.01*	1675	[5.14]
α-Muurolole	11.48*	1497	1.25	10.01*	1675	[5.14]
(3Z,6E)-α-Farnesene	11.48*	1497	[1.25]	10.22	1692	0.07
Unknown [m/z 119, 41 (95), 123 (53), 80 (49), 161 (44), 105 (42)... 204 (2)]	11.48*	1497	[1.25]			

δ-Amorphene	11.55	1503	0.45	9.89	1665	0.58
γ-Cadinene	11.69*	1513	19.49	10.35*	1702	1.07
Cubebol	11.69*	1513	[19.49]	12.50	1889	0.04
(3E,6E)-α-Farnesene	11.69*	1513	[19.49]	10.52*	1717	[20.62]
(Z)-γ-Bisabolene	11.69*	1513	[19.49]	9.86	1662	0.48
δ-Cadinene	11.80*	1522	3.38	10.39	1706	3.17
trans-Calamenene	11.80*	1522	[3.38]	11.18	1773	0.02
Zonarene	11.80*	1522	[3.38]	10.35*	1702	[1.07]
trans-Cadina-1,4-diene	11.89	1529	0.23	10.62	1725	0.20
α-Cadinene	11.96*	1535	0.33	10.76	1737	0.25
α-Calacorene	11.96*	1535	[0.33]	12.09	1852	0.06
cis-Dracunculifolol	12.04	1541	0.03	12.06	1850	0.02
α-Elemol	12.09	1545	0.04	14.00	2030	0.06
Germacrene B	12.15	1550	0.11	11.07	1764	0.07
(E)-Nerolidol	12.32	1563	0.14	13.72*†	2003	[0.66]
(3Z)-Hexenyl benzoate	12.38	1568	0.11	14.34	2062	0.08
Caryophyllene oxide	12.45	1573	0.10	12.71	1910	0.06
10-epi-Junenol	12.49*	1576	0.11	12.66	1906	0.08
Unknown cadinol or muurolol analog [m/z 161, 119 (77), 120 (76), 105 (73), 93 (57)... 204 (36)]	12.49*	1576	[0.11]	12.23	1865	0.06
Unknown [m/z 161, 105 (84), 43 (80), 119 (72), 93 (62), 121 (54)... 204 (38), 222 (2)]	12.54	1580	0.11	13.91	2021	0.10
Viridiflorol	12.58	1584	0.03	13.93	2023	0.04
Guaiol	12.69	1592	0.10	14.09	2038	0.12
Copaborneol	12.72	1594	0.07	14.84*	2111	0.59
Humulene epoxide II	12.79	1600	0.07	13.30	1965	0.02
Junenol	12.90*†	1609	0.57	13.55	1987	0.35
(E)-Isoeugenyl acetate	12.90*†	1609	[0.57]	17.20	2353	0.08
10-epi-Cubebol	12.90*†	1609	[0.57]	13.62*†	1994	0.25
1-epi-Cubebol	13.06	1622	0.35	13.72*†	2003	[0.66]
γ-Eudesmol	13.10	1625	0.14	14.84*	2111	[0.59]
Cubebol	13.24*	1637	1.49	13.62*†	1994	[0.25]
τ-Cadinol	13.24*	1637	[1.49]	14.84*	2111	[0.59]
τ-Muurolol	13.24*	1637	[1.49]	15.01*	2127	[0.94]
α-Muurolol	13.29	1641	0.40	15.10	2137	0.43
Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)]	13.34	1646	0.27	15.14	2141	0.34

α -Cadinol	13.40	1650	1.72	15.44	2170	1.72
<i>trans</i> -Calamennen-10-ol	13.51	1659	0.05	16.78*	2308	1.54
Bulnesol	13.53	1661	0.02	15.28	2154	0.02
Unknown [m/z 123, 95 (31), 81 (29), 105 (27)... 222 (5)]	13.58	1665	0.19	16.16	2244	0.18
Eudesma-4(15),7-dien-1 β -ol	13.74	1678	0.01	15.99	2226	0.04
(2E,6Z)-Farnesol	13.95	1696	0.03	16.39	2267	0.02
(2E,6E)-Farnesol	14.25	1721	1.58	16.78*	2308	[1.54]
(2E,6E)-Farnesal	14.46	1739	0.02	15.77	2203	0.03
Benzyl benzoate	14.68	1758	6.13	18.82	2534	6.09
(2E,6E)-Farnesyl acetate	15.64	1843	3.46	15.89*	2216	[3.46]
Benzyl salicylate	15.83	1860	3.70	20.06	2681	3.68
Geranyl benzoate	16.87	1957	0.01	18.68	2518	0.02
Unknown [m/z 326, 311 (47), 327 (22), 202 (16), 137 (15)...]	22.64	2576	0.04			
Unknown [m/z 69, 81 (42), 147 (26), 119 (25), 93 (25), 41 (24)...]	24.36	2792	0.09	22.84	3040	0.10
Total identified		97.60%			95.38%	
Total reported		98.31%			96.16%	

*: 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