

**Date :** February 10, 2020

**CERTIFICATE OF ANALYSIS – GC PROFILING**

*SAMPLE IDENTIFICATION*

**Internal code :** 19H28-INT10-1-SCC

**Customer identification :** EW 281096

**Type :** Essential oil

**Source :** *Aniba sp.*

**Customer :** Interne

*ANALYSIS*

**Method:** PC-MAT-007 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Alexis St-Gelais, M. Sc., chimiste

**Analysis date :** January 27, 2020

Checked and approved by :

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

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## ANALYSIS SUMMARY – CONSOLIDATED CONTENTS

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

Identification	%	Classe
3-Methyl-1-penten-3-ol	tr	Aliphatic alcohol
(3Z)-Hexenol	0.01	Aliphatic alcohol
Hexanol	0.02	Aliphatic alcohol
$\alpha$ -Thujene	0.01	Monoterpene
$\alpha$ -Pinene	0.73	Monoterpene
Camphene	0.02	Monoterpene
$\alpha$ -Fenchene	tr	Monoterpene
Geranic oxide	tr	Monoterpenic ether
$\beta$ -Pinene	0.75	Monoterpene
Sabinene	0.05	Monoterpene
6-Methyl-5-hepten-2-one	0.02	Aliphatic ketone
Myrcene	0.10	Monoterpene
$\Delta^3$ -Carene	0.15	Monoterpene
ortho-Cymene	0.02	Monoterpene
para-Cymene	0.07	Monoterpene
1,8-Cineole	0.41	Monoterpenic ether
Limonene	0.39	Monoterpene
Lavender lactone	0.01	Aliphatic lactone
Benzyl alcohol	0.13	Simple phenolic
<i>cis</i> -Linalool oxide (fur.)	0.57	Monoterpenic alcohol
para-Cymenene	0.04	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.63	Monoterpenic alcohol
$\alpha$ -Pinene oxide	0.04	Monoterpenic ether
Linalool	85.02	Monoterpenic alcohol
<i>trans</i> -Pinocarveol	0.03	Monoterpenic alcohol
Epoxyterpinolene	0.05	Monoterpenic ether
Pinocarvone	0.01	Monoterpenic ketone
<i>cis</i> -Linalool oxide (pyr.)	0.04	Monoterpenic alcohol
<i>trans</i> -Linalool oxide (pyr.)	0.05	Monoterpenic alcohol
Terpinen-4-ol	0.03	Monoterpenic alcohol
meta-Cymen-8-ol	0.02	Monoterpenic alcohol
para-Cymen-8-ol	0.07	Monoterpenic alcohol
$\alpha$ -Terpineol	0.18	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
Hodiendiol	0.14	Monoterpenic alcohol
Unknown	0.47	Unknown
Unknown	0.02	Oxygenated monoterpene
Unknown	0.35	Unknown
Unknown	0.02	Oxygenated monoterpene
Nerol	0.04	Monoterpenic alcohol
Unknown	0.01	Unknown
Neral	0.01	Monoterpenic aldehyde
2,6-Dimethyl-3,7-octadiene-2,6-diol analog?	0.01	Monoterpenic alcohol
Unknown	0.01	Unknown

Geraniol	0.09	Monoterpenic alcohol
3,7-Dimethyl-octa-1,7-diene-3,6-diol	0.01	Monoterpenic alcohol
Geranial	0.02	Monoterpenic aldehyde
Unknown	0.01	Oxygenated monoterpene
Unknown	0.28	Unknown
$\alpha$ -Cubebene	0.06	Sesquiterpene
Cyclosativene II	0.02	Sesquiterpene
Hodiendiol derivative III	1.52	Oxygenated monoterpene
Methyl para-anisate	0.06	Phenolic ester
Unknown	0.04	Unknown
$\alpha$ -Copaene	0.87	Sesquiterpene
$\beta$ -Elemene	0.35	Sesquiterpene
Unknown	0.27	Unknown
Isocaryophyllene	0.03	Sesquiterpene
$\alpha$ -Gurjunene	0.22	Sesquiterpene
<i>cis</i> - $\alpha$ -Bergamotene	tr	Sesquiterpene
$\beta$ -Caryophyllene	0.16	Sesquiterpene
$\alpha$ -Guaiene	0.03	Sesquiterpene
$\alpha$ -Humulene	0.07	Sesquiterpene
allo-Aromadendrene	0.10	Sesquiterpene
4,5-diepi-Aristolochene	0.04	Sesquiterpene
5-epi-Aristolochene?	0.03	Sesquiterpene
Selina-4,11-diene	0.12	Sesquiterpene
Unknown	0.04	Unknown
$\beta$ -Selinene	0.64	Sesquiterpene
<i>trans</i> - $\beta$ -Bergamotene	0.05	Sesquiterpene
allo-Aromadendr-9-ene	0.06	Sesquiterpene
Viridiflorene	0.02	Sesquiterpene
Valencene	0.02	Sesquiterpene
$\alpha$ -Selinene	0.40	Sesquiterpene
$\alpha$ -Muurolene	0.08	Sesquiterpene
$\delta$ -Guaiene	0.02	Sesquiterpene
7-epi- $\alpha$ -Selinene	0.03	Sesquiterpene
$\gamma$ -Cadinene	0.14	Sesquiterpene
<i>trans</i> -Calamenene	0.04	Sesquiterpene
$\delta$ -Cadinene	0.04	Sesquiterpene
$\alpha$ -Cadinene	0.03	Sesquiterpene
$\alpha$ -Calacorene	0.02	Sesquiterpene
Isocaryophyllene epoxide B	0.01	Sesquiterpenic ether
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Palustrol	0.01	Sesquiterpenic alcohol
( <i>E</i> )-Nerolidol	0.04	Sesquiterpenic alcohol
Spathulenol	0.07	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.04	Sesquiterpenic ether
Caryophyllene oxide	0.25	Sesquiterpenic ether
Ledol	0.04	Sesquiterpenic alcohol
Humulene epoxide II	0.05	Sesquiterpenic ether
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Caryophylladienol I	0.04	Sesquiterpenic alcohol
$\tau$ -Cadinol	0.03	Sesquiterpenic alcohol

τ-Muurolol	0.01	Sesquiterpenic alcohol
α-Muurolol	0.03	Sesquiterpenic alcohol
α-Cadinol	0.06	Sesquiterpenic alcohol
Selin-11-en-4α-ol	0.06	Sesquiterpenic alcohol
cis-Calamenen-10-ol	0.03	Sesquiterpenic alcohol
trans-Calamenen-10-ol	0.05	Sesquiterpenic alcohol
Unknown	0.03	Oxygenated sesquiterpene
Unknown	0.07	Unknown
Unknown	0.01	Oxygenated sesquiterpene
Isocyperol	0.03	Sesquiterpenic alcohol
Cyperol	0.02	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.11	Lignan
Unknown	0.13	Oxygenated sesquiterpene
Unknown	0.18	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Patchoulone	0.03	Sesquiterpenic ketone
Benzyl benzoate	0.24	Phenolic ester
Unknown	0.02	Oxygenated sesquiterpene
Hotrienol	0.04	Monoterpenic alcohol
<b>Consolidated total</b>	<b>98.70%</b>	

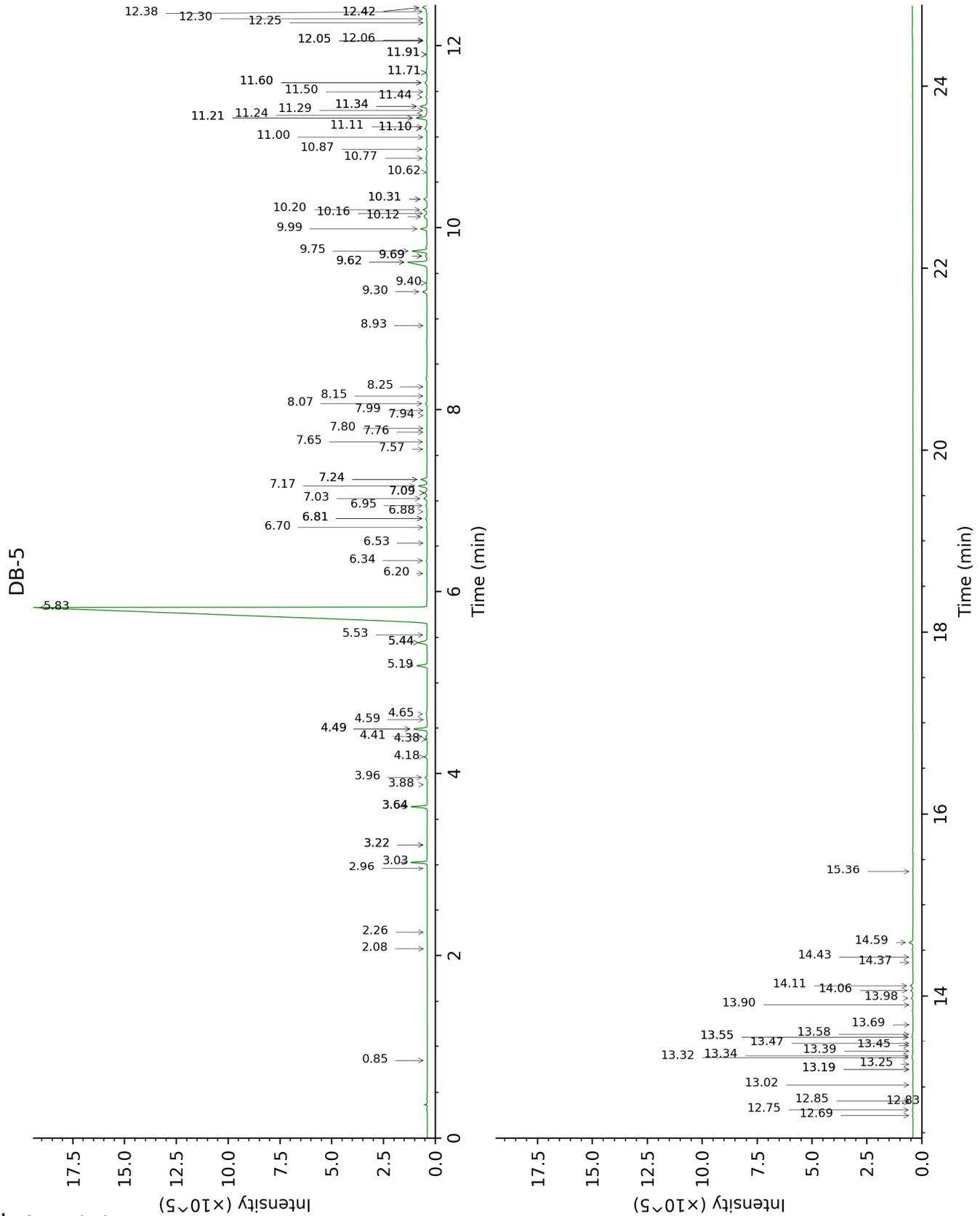
tr: The compound has been detected below 0.005% of total signal.

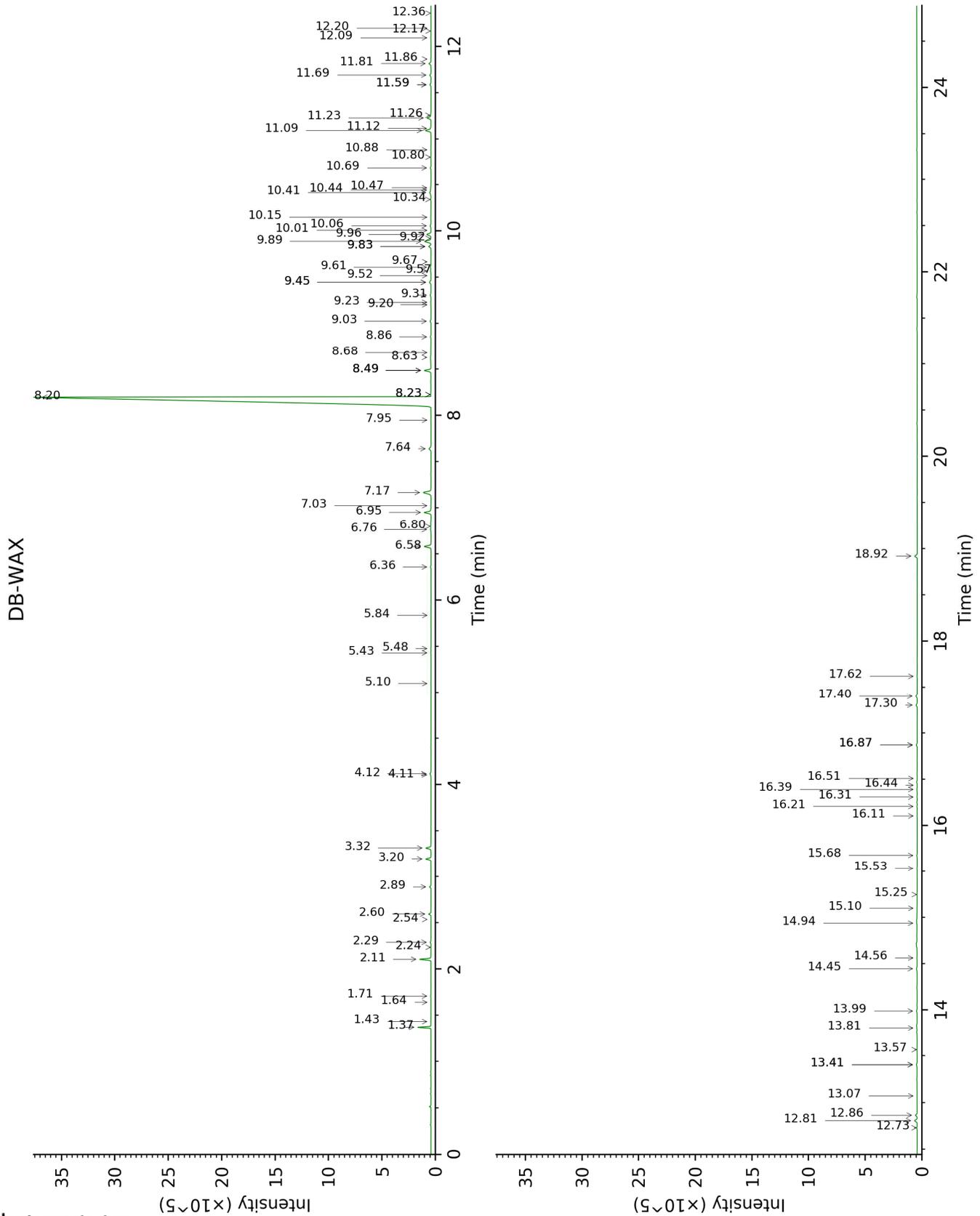
Note: no correction factor was applied

**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-Methyl-1-penten-3-ol	0.85	721	tr	2.54	1107	0.01
(3Z)-Hexenol	2.08	857	0.01	5.84	1351	0.01
Hexanol	2.26	872	0.02	5.48	1325	0.02
$\alpha$ -Thujene	2.96	925	0.01	1.43	1000	0.01
$\alpha$ -Pinene	3.03	930	0.73	1.37	992	0.71
Camphene	3.22*	942	0.03	1.71	1027	0.02
$\alpha$ -Fenchene	3.22*	942	[0.03]	1.64	1021	tr
Geranic oxide	3.64*	970	0.77	2.24	1080	tr
$\beta$ -Pinene	3.64*	970	[0.77]	2.11	1067	0.75
Sabinene	3.64*	970	[0.77]	2.29	1085	0.05
6-Methyl-5-hepten-2-one	3.88	986	0.02	5.10	1298	0.01
Myrcene	3.96	991	0.10	2.89	1134	0.10
$\Delta$ 3-Carene	4.18	1006	0.15	2.60	1111	0.16
ortho-Cymene	4.38	1018	0.02	4.10	1226	0.02
para-Cymene	4.41	1020	0.07	4.12	1227	0.08
1,8-Cineole	4.49*	1025	0.77	3.32	1167	0.41
Limonene	4.49*	1025	[0.77]	3.20	1158	0.39
Lavender lactone	4.59	1032	0.01	9.20	1604	0.02
Benzyl alcohol	4.65	1036	0.13	11.82	1821	0.18
<i>cis</i> -Linalool oxide (fur.)	5.19	1070	0.57	6.58	1404	0.59
para-Cymenene	5.44*	1086	0.62	6.36	1388	0.04
<i>trans</i> -Linalool oxide (fur.)	5.44*	1086	[0.62]	6.95	1432	0.63
$\alpha$ -Pinene oxide	5.53	1091	0.04	5.43	1322	0.02
Linalool	5.83	1110	85.02	8.20	1526	86.96
<i>trans</i> -Pinocarveol	6.20	1135	0.03	9.23	1606	0.02
Epoxyterpinolene	6.34	1144	0.05	6.76	1418	0.05
Pinocarpone	6.53	1156	0.01	7.95	1506	0.01
<i>cis</i> -Linalool oxide (pyr.)	6.70	1168	0.04	10.34	1695	0.03
<i>trans</i> -Linalool oxide (pyr.)	6.81*	1175	0.07	10.69	1725	0.05
Terpinen-4-ol	6.81*	1175	[0.07]	8.63	1559	0.03
meta-Cymen-8-ol	6.88	1180	0.02	11.59*	1801	0.10
para-Cymen-8-ol	6.95	1184	0.07	11.59*	1801	[0.10]
$\alpha$ -Terpineol	7.03	1189	0.18	9.83*	1654	0.21
Myrtenal	7.09*	1193	0.15	8.68	1563	0.01
Hodiendiol	7.09*	1193	[0.15]	12.86	1914	0.14
Unknown [m/z 43, 71 (80), 67 (55), 59 (51), 68 (44), 41 (43)...]	7.17	1198	0.47	11.09	1759	0.49
Unknown [m/z 109, 91 (100), 81 (88), 94 (75), 119]	7.24*	1203	0.33	10.88	1741	0.02

(74), 96 (73), 41 (63)... 150 (2)] Unknown [m/z 43, 71 (66), 59 (52), 41 (47), 68 (46)...]	7.24*	1203	[0.33]	11.23	1770	0.35
Unknown [m/z 71, 43 (72), 84 (51), 69 (49), 55 (19), 41 (17), 83 (8)...]	7.57	1225	0.02	13.57	1979	0.01
Nerol	7.65	1231	0.04	11.12	1761	0.03
Unknown [m/z 69, 41 (67), 82 (29), 110 (24), 68 (22), 109 (20)...]	7.76	1238	0.01			
Neral	7.80	1241	0.01	9.52	1629	0.01
2,6-Dimethyl-3,7- octadiene-2,6-diol analog?	7.94	1251	0.01			
Unknown [m/z 95, 43 (42), 109 (32), 67 (29), 126 (22)... 168 (3)]	7.99	1255	0.01			
Geraniol	8.07	1260	0.09	11.69	1810	0.10
3,7-Dimethyl- octa-1,7-diene- 3,6-diol	8.15	1266	0.01			
Geranial	8.25	1273	0.02	10.15	1680	0.04
Unknown [m/z 150, 107 (98), 91 (79), 108 (61)]	8.93	1314	0.01	12.09	1846	0.03
Unknown [m/z 133, 105 (45), 91 (38), 119 (36)... 150 (3)]	9.30	1341	0.28			
$\alpha$ -Cubebene	9.40	1348	0.06	6.80	1421	0.05
Cyclosativene II	9.62*	1364	1.54	7.03	1438	0.02
Hodiendiol derivative III	9.62*	1364	[1.54]			
Methyl para- anisate	9.69*	1368	0.10	13.99	2019	0.06
Unknown [m/z 93, 43 (59), 41 (40), 91 (40), 69 (33), 77 (22)...]	9.69*	1368	[0.10]			
$\alpha$ -Copaene	9.75	1372	0.87	7.17	1448	0.86
$\beta$ -Elemene	9.99	1390	0.35	8.49*	1548	0.54
Unknown [m/z 71, 43 (71), 67 (51), 55 (38), 41 (35), 69 (25), 81	10.12	1399	0.27			

(21), 93 (20), 82 (18)...						
Isocaryophyllene	10.16	1401	0.03	8.23*	1528	0.04
$\alpha$ -Gurjunene	10.20	1404	0.22	7.64	1483	0.22
<i>cis</i> - $\alpha$ -Bergamotene	10.31*	1413	0.21	8.23*	1528	[0.04]
$\beta$ -Caryophyllene	10.31*	1413	[0.21]	8.49*	1548	[0.54]
$\alpha$ -Guaiene	10.62	1435	0.03	8.49*	1548	[0.54]
$\alpha$ -Humulene	10.77	1447	0.07	9.31	1612	0.09
allo-Aromadendrene	10.87	1454	0.10	9.03	1589	0.08
4,5-diepi-Aristolochene	11.00	1464	0.04	9.45*	1623	0.15
5-epi-Aristolochene?	11.10*	1471	0.16	9.83*	1654	[0.21]
Selina-4,11-diene	11.10*	1471	[0.16]	9.45*	1623	[0.15]
Unknown [m/z 43, 67 (65), 71 (56), 68 (34), 55 (33), 82 (30)...	11.11	1473	0.04			
$\beta$ -Selinene	11.21*	1480	0.67	9.89	1659	0.64
<i>trans</i> - $\beta$ -Bergamotene	11.21*	1480	[0.67]	9.57	1633	0.05
allo-Aromadendr-9-ene	11.24	1482	0.06	9.61	1636	0.06
Viridiflorene	11.29	1486	0.02	9.67	1641	0.02
Valencene	11.34*	1489	0.44	9.92	1661	0.02
$\alpha$ -Selinene	11.34*	1489	[0.44]	9.96	1665	0.40
$\alpha$ -Muurolene	11.44	1497	0.08	10.06	1672	0.08
$\delta$ -Guaiene	11.50	1501	0.02	10.01	1668	0.02
7-epi- $\alpha$ -Selinene	11.60*	1509	0.14	10.47	1706	0.03
$\gamma$ -Cadinene	11.60*	1509	[0.14]	10.42	1702	0.14
<i>trans</i> -Calamenene	11.71*†	1518	0.11	11.26	1773	0.04
$\delta$ -Cadinene	11.71*†	1518	[0.11]	10.44	1704	0.04
$\alpha$ -Cadinene	11.91*	1533	0.04	10.80	1735	0.03
$\alpha$ -Calacorene	11.91*	1533	[0.04]	12.17	1852	0.02
Isocaryophyllene epoxide B	12.05*	1545	0.03	12.20	1855	0.01
Unknown [m/z 83, 82 (46), 43 (34), 95 (29), 81 (26)... 220 (8)]	12.05*	1545	[0.03]			
Unknown [m/z 107, 43 (92), 93 (91), 79 (87), 91 (73), 41 (63), 121 (62)... 205 (20), 220 (4)]	12.06	1546	0.02	11.86	1825	0.02
Palustrol	12.25	1560	0.01	12.36	1869	0.01
( <i>E</i> )-Nerolidol	12.30	1564	0.04	13.81	2001	0.03
Spathulenol	12.38	1570	0.07	14.45	2063	0.08
Caryophyllene	12.42*	1574	0.30	12.73	1902	0.04

oxide isomer						
Caryophyllene oxide	12.42*	1574	[0.30]	12.81	1909	0.25
Ledol	12.69	1595	0.04	13.41*	1964	0.07
Humulene epoxide II	12.75	1600	0.05	13.41*	1964	[0.07]
Unknown [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	12.83	1606	0.02	14.56	2074	0.02
Unknown [m/z 162, 119 (73), 79 (69), 107 (60), 43 (51), 159 (40)...]	12.85	1607	0.02			
Caryophylladienol I	13.02	1622	0.04	16.10	2228	0.02
τ-Cadinol	13.19*	1636	0.04	14.94	2111	0.03
τ-Muurolol	13.19*	1636	[0.04]	15.10	2127	0.01
α-Muurolol	13.25	1640	0.03	15.25	2141	0.02
α-Cadinol	13.32	1646	0.06	15.53	2170	0.04
Selin-11-en-4α-ol	13.34	1648	0.06	15.68	2184	0.05
cis-Calamenen-10-ol	13.39	1652	0.03	16.51	2270	0.02
trans-Calamenen-10-ol	13.45	1657	0.05	16.87*	2308	0.09
Unknown [m/z 205, 93 (93), 43 (58), 79 (510, 91 (48), 119 (45)... 220 (3)]	13.48	1659	0.03	16.21	2238	0.03
Unknown [m/z 203, 105 (61), 119 (60), 91 (52), 147 (49), 159 (43)...]	13.55*	1665	0.08			
Unknown [m/z 93, 43 (82), 119 (62), 162 (51), 91 (50), 147 (42)... 220 (2)]	13.55*	1665	[0.08]	13.07	1933	0.01
Isocyperol	13.58	1668	0.03	16.31	2249	0.03
Cyperol	13.69	1676	0.02	16.44	2262	0.02
Unknown [m/z 124, 97 (91), 67 (78), 137 (77), 107 (66), 136 (59), 177 (57), 81 (55)... 220 (20)...]	13.90	1694	0.02			
Unknown [m/z 133, 93 (97), 131 (85), 145 (83), 107 (69)...220]	13.98	1700	0.11	16.87*	2308	[0.09]

Unknown [m/z 93, 81 (90), 107 (83), 95 (75), 91 (71), 71 (70), 121 (68), 105 (68)... 220 (47)]	14.06	1708	0.13	17.30	2354	0.12
Unknown [m/z 159, 93 (87), 105 (84), 91 (81), 107 (71), 131 (69), 79 (65), 119 (63), 145 (62), 41 (61), 220 (61)]	14.11	1712	0.18	17.40	2364	0.13
Unknown [m/z 177, 123 (74), 159 (55), 91 (72), 43 (41), 93 (40)... 220 (17)]	14.37	1734	0.02	17.62	2388	0.03
Patchoulenone	14.43	1739	0.03	16.39	2258	0.05
Benzyl benzoate	14.59	1753	0.24	18.92	2534	0.24
Unknown [m/z 203, 95 (88), 138 (81), 105 (74), 107 (74), 109 (72), 81 (71), 91 (68)... 220 (23)]	15.36	1821	0.02			
Hotrienol				8.86	1576	0.04
<b>Total identified</b>		<b>96.88%</b>			<b>96.88%</b>	
<b>Total reported</b>		<b>98.58%</b>			<b>98.14%</b>	

\*: 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