

Date : March 28, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 23C22-PTH03

Customer identification : Amyris - Haiti - AH0108R

Type : Essential oil

Source : *Amyris balsamifera*

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 : March 23, 2023

Checked and approved by :

Alexis St-Gelais, Ph. D., Chimiste 2013-174

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This report is an update from the first version, issued on March 27, 2023, to correct a coelution issue on an eudesmol isomer which lead to a miscalculation.

PHYSICOCHEMICAL DATA

Physical aspect: Viscous yellow liquid

Refractive index: 1.5065 ± 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
Furfural	tr	Furan
1,8-Cineole	0.01	Monoterpenic ether
α -Terpineol	0.01	Monoterpenic alcohol
Unknown	0.07	Apocarotenoid
Unknown	0.01	Sesquiterpene
Cyclosativene II	0.01	Sesquiterpene
Neryl acetate	0.01	Monoterpenic ester
Unknown	0.03	Sesquiterpene
β -Elemene	0.08	Sesquiterpene
7-epi-Sesquithujene	0.03	Sesquiterpene
Isocaryophyllene	0.01	Sesquiterpene
α -Gurjunene	0.01	Sesquiterpene
Sesquithujene	0.04	Sesquiterpene
β -Caryophyllene	0.09	Sesquiterpene
<i>cis</i> - α -Bergamotene	0.06	Sesquiterpene
α -Santalene	0.06	Sesquiterpene
β -Copaene	0.01	Sesquiterpene
γ -Elemene	0.02	Sesquiterpene
<i>trans</i> - α -Bergamotene	0.07	Sesquiterpene
Unknown	0.01	Sesquiterpene
Sesquisabinene A	0.03	Sesquiterpene
epi- β -Santalene	0.06	Sesquiterpene
α -Humulene	0.08	Sesquiterpene
Unknown	0.02	Sesquiterpenic ether
Cadina-4,11-diene	0.39	Sesquiterpene
allo-Aromadendrene	0.11	Sesquiterpene
Amorpha-4,11-diene	0.14	Sesquiterpene
Muurolo-4,11-diene	0.75	Sesquiterpene
Unknown	0.07	Sesquiterpenic ether
Selina-4,11-diene	0.21	Sesquiterpene
Unknown	0.76*	Sesquiterpene
β -Selinene	0.76*	Sesquiterpene
γ -Curcumene	0.48	Sesquiterpene
α -Curcumene	0.76	Sesquiterpene
Valencene	0.71	Sesquiterpene
Unknown	0.20	Oxygenated sesquiterpene
Unknown	0.23	Oxygenated sesquiterpene
α -Zingiberene	1.38	Sesquiterpene
4-epi- <i>cis</i> -Dihydroagarofuran	0.61	Sesquiterpenic ether
α -Muurolo-4,11-diene	0.04	Sesquiterpene
(<i>Z</i>)- α -Bisabolene	0.06	Sesquiterpene
β -Bisabolene	0.49	Sesquiterpene
β -Dihydroagarofuran	0.12	Sesquiterpenic ether
Unknown	0.29	Oxygenated sesquiterpene
Liguloxide analog III	0.04	Sesquiterpenic ether

7-epi- α -Selinene	0.05	Sesquiterpene
<i>trans</i> -Calamenene	0.02	Sesquiterpene
β -Sesquiphellandrene	2.71	Sesquiterpene
Unknown	0.07	Oxygenated sesquiterpene
Unknown	0.13	Unknown
Selina-3,7(11)-diene	0.80	Sesquiterpene
α -Agarofuran	0.80	Sesquiterpenic ether
(<i>E</i>)- α -Bisabolene	0.05	Sesquiterpene
α -Elemol	9.83	Sesquiterpenic alcohol
Unknown	0.13	Unknown
(<i>E</i>)-Nerolidol	0.49	Sesquiterpenic alcohol
Spathulenol	0.19	Sesquiterpenic alcohol
Caryophyllene oxide	0.03	Sesquiterpenic ether
Caryophyllene oxide isomer	0.05	Sesquiterpenic ether
Eudesm-5-en-11-ol	0.06	Sesquiterpenic alcohol
Eudesm-5-en-11-ol analog	0.61	Sesquiterpenic alcohol
Humulene epoxide II	0.13	Sesquiterpenic ether
Unknown	0.99	Oxygenated sesquiterpene
Unknown	0.12	Oxygenated sesquiterpene
10-epi- γ -Eudesmol	8.30	Sesquiterpenic alcohol
Unknown	1.35	Oxygenated sesquiterpene
Eremoligenol?	0.49	Sesquiterpenic alcohol
Unknown	0.26	Oxygenated sesquiterpene
Eremoligenol	0.23	Sesquiterpenic alcohol
γ -Eudesmol	5.88	Sesquiterpenic alcohol
Hinesol	0.47	Sesquiterpenic alcohol
Agarospinol?	0.85	Sesquiterpenic alcohol
Unknown	0.27	Oxygenated sesquiterpene
β -Eudesmol	3.21	Sesquiterpenic alcohol
7-epi- α -Eudesmol	14.96	Sesquiterpenic alcohol
Selin-11-en-4 α -ol	0.17	Sesquiterpenic alcohol
α -Eudesmol	3.80	Sesquiterpenic alcohol
Valerianol	23.30	Sesquiterpenic alcohol
4 α -Hydroxydihydroagarofuran	0.19	Sesquiterpenic alcohol
<i>trans</i> -Calamenen-10-ol	0.16	Sesquiterpenic alcohol
Dehydrojinkoh-eremol	0.58	Sesquiterpenic alcohol
Unknown	0.90	Oxygenated sesquiterpene
Unknown	0.12	Oxygenated sesquiterpene
Unknown	0.25	Oxygenated sesquiterpene
Caryophyllene acetate	0.17	Sesquiterpenic ester
Unknown	0.11	Oxygenated sesquiterpene
Unknown	0.49	Oxygenated sesquiterpene
(2 <i>E</i> ,6 <i>Z</i>)-Farnesol	0.06	Sesquiterpenic alcohol
(2 <i>Z</i> ,6 <i>E</i>)-Farnesol	0.07	Sesquiterpenic alcohol
3 β ,4 β -Oxidoagarofuran?	0.08	Sesquiterpenic ether
(2 <i>E</i> ,6 <i>E</i>)-Farnesol	0.29	Sesquiterpenic alcohol
(6 <i>R</i> ,7 <i>R</i>)-Bisabolone	0.54	Sesquiterpenic ketone
Unknown	0.06	Oxygenated sesquiterpene
(6 <i>S</i> ,7 <i>R</i>)-Bisabolone	0.65	Sesquiterpenic ketone
Drimenol	1.76	Sesquiterpenic alcohol
Cryptomeridiol analog	0.09	Sesquiterpenic alcohol
Cryptomeridiol analog	0.03	Sesquiterpenic alcohol

Unknown	0.04	Oxygenated sesquiterpene
Cryptomeridiol	0.07	Sesquiterpenic alcohol
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.02	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.05	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Unknown	0.01	Oxygenated sesquiterpene
Carissone analog II	0.02	Sesquiterpenic alcohol
Carissone analog I	0.02	Sesquiterpenic alcohol
Unknown	0.02	Oxygenated sesquiterpene
Consolidated total	96.34%	

*: 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.

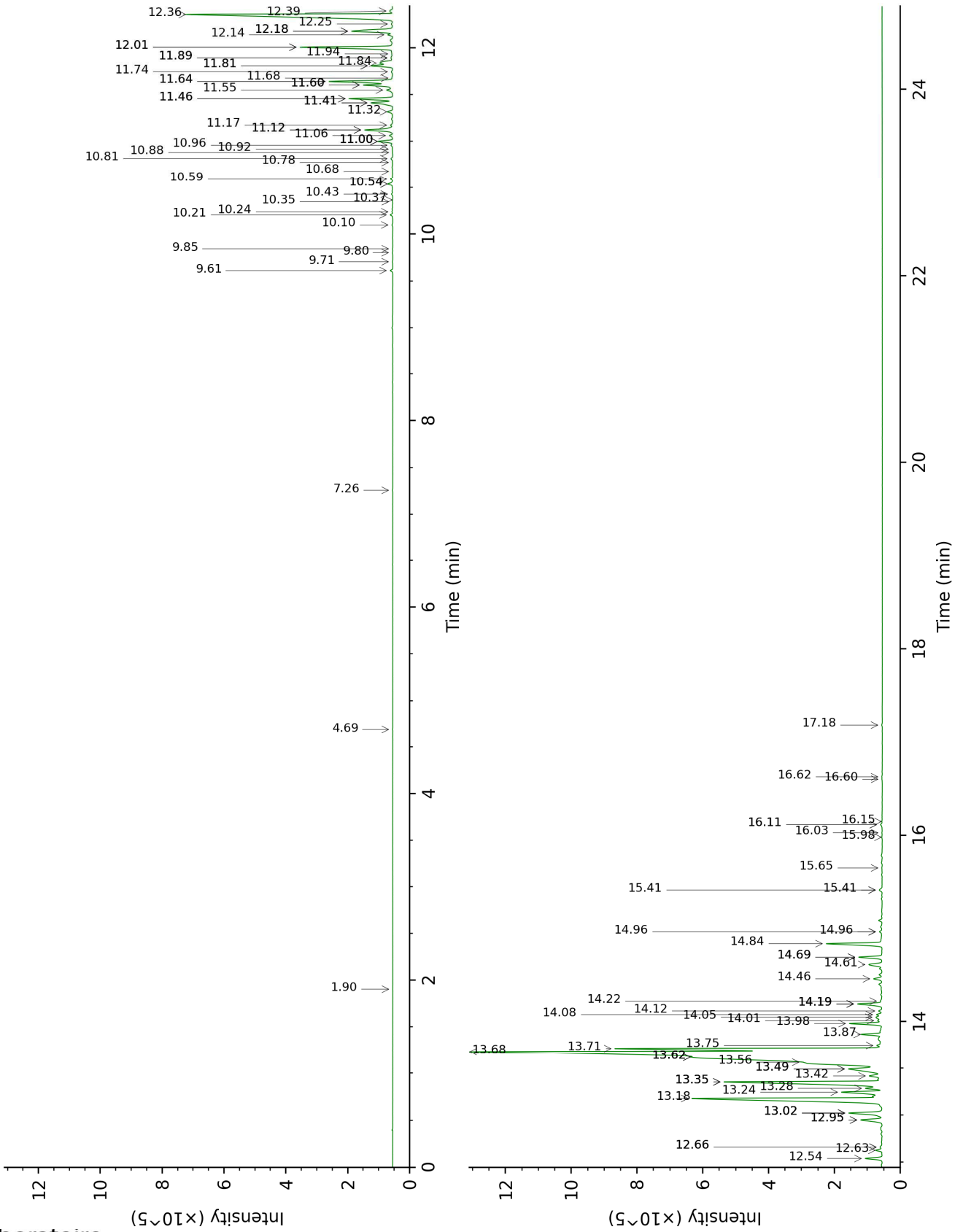
Note: no correction factor was applied

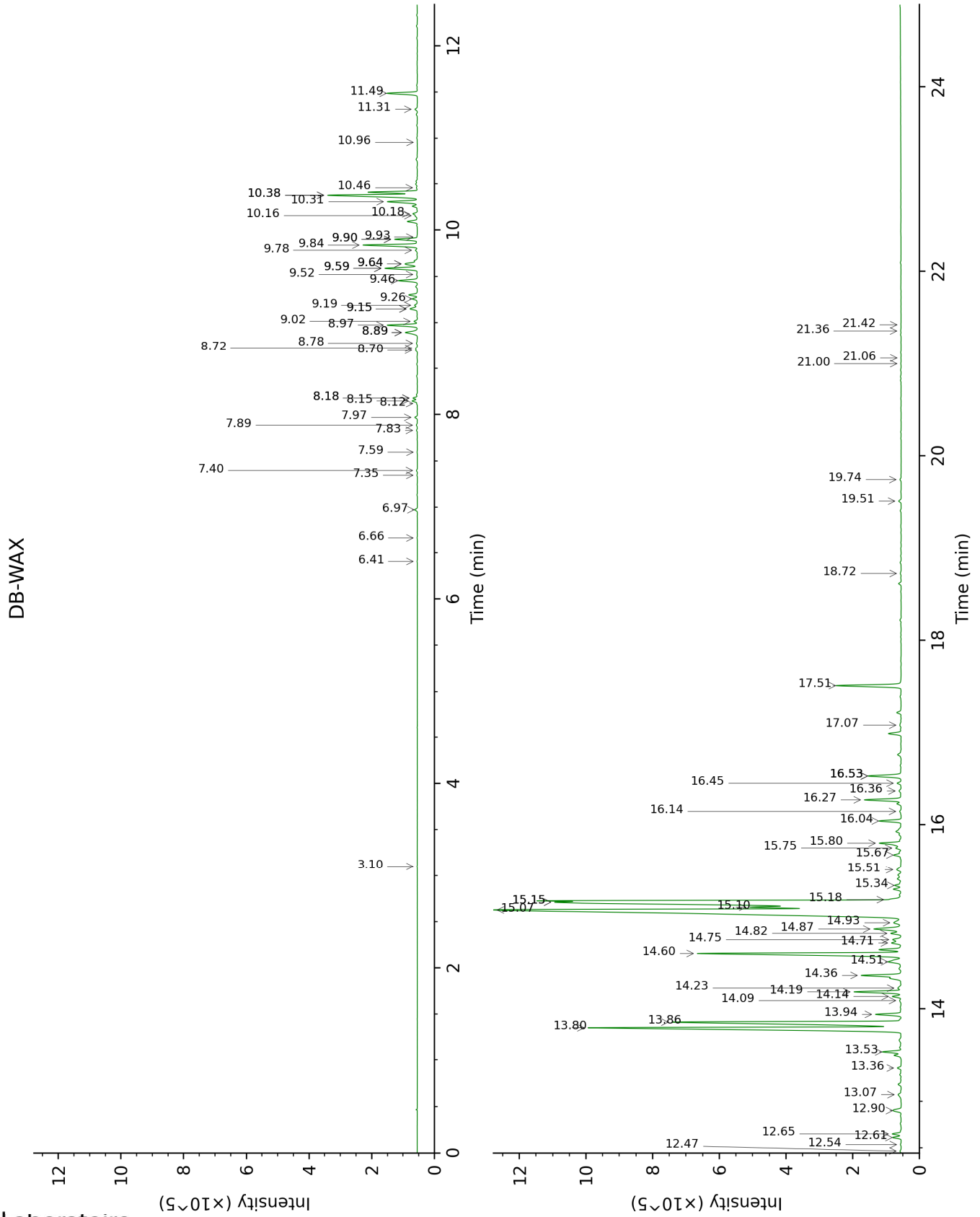
About "consolidated" data: The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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.

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DB-5





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Furfural	1.90	831	tr	6.41	1410	0.01
1,8-Cineole	4.69	1027	0.01	3.10	1167	0.01
α -Terpineol	7.26	1189	0.01	9.52	1652	0.03
Unknown [m/z 177, 107 (57), 81 (55), 95 (50), 41 (34), 93 (34), 123 (32)... 192 (23)]	9.61	1348	0.07	6.97	1453	0.07
Unknown [m/z 123, 81 (45), 107 (30), 79 (28), 41 (28)... 204 (5)]	9.71	1354	0.01			
Cyclosativene II	9.80	1361	0.01	6.66	1429	0.01
Neryl acetate	9.84	1364	0.01	9.93	1686	0.01
Unknown [m/z 189, 105 (79), 91 (73), 107 (67), 93 (65), 133 (65)... 204 (38)]	10.10	1382	0.03	7.40	1485	0.02
β -Elemene	10.21	1390	0.08	8.18*†	1545	[0.24]
7-epi-Sesquithujene	10.24	1392	0.03	7.60	1500	0.01
Isocaryophyllene	10.35	1400	0.01	7.89	1522	0.03
α -Gurjunene	10.37	1401	0.01	7.35	1481	0.01
Sesquithujene	10.43	1405	0.04	7.83	1518	0.02
β -Caryophyllene	10.54*	1413	0.16	8.15†	1543	0.24
<i>cis</i> - α -Bergamotene	10.54*	1413	[0.16]	7.97	1529	0.06
α -Santalene	10.59	1418	0.06			
β -Copaene	10.68	1424	0.01	8.12	1541	0.01
γ -Elemene	10.78	1431	0.02	8.78	1592	0.03
<i>trans</i> - α -Bergamotene	10.82	1434	0.07	8.18*†	1545	[0.24]
Unknown [m/z 121, 93 (80), 91 (25), 79 (20), 77 (16), 119 (15)... 202 (3)]	10.88	1439	0.01			
Sesquisabinene A	10.92	1442	0.03	8.90*	1601	0.42
epi- β -Santalene	10.96	1445	0.06	8.72	1588	0.04
α -Humulene	11.00*	1448	0.44	9.02	1611	0.08
Unknown [m/z 109, 81 (84), 207 (73), 43 (55), 41 (52), 69 (48), 55 (47), 124 (39)]	11.00*	1448	[0.44]	9.15*	1622	0.22
Cadina-4,11-diene	11.00*	1448	[0.44]	8.90*	1601	[0.42]
allo-Aromadendrene	11.06	1452	0.11	8.70	1586	0.04
Amorpha-4,11-diene	11.12*	1457	0.93	9.26	1631	0.14
Muurolo-4,11-diene	11.12*	1457	[0.93]	8.98	1608	0.75
Unknown [m/z 109, 207 (91), 81 (91), 43 (79), 41 (71), 69 (57), 55 (54), 124 (47)]	11.17	1461	0.07	9.19	1625	0.07
Selina-4,11-diene	11.32	1471	0.21	9.15*	1622	[0.22]
Unknown [m/z 189, 91 (95), 105 (93), 133 (84), 119	11.41*	1478	0.76	9.59*†	1658	1.39

(75), 41 (59), 93 (46)... 204 (33)]						
β-Selinene	11.41*	1478	[0.76]	9.59*†	1658	[1.39]
γ-Curcumene	11.46*	1482	1.24	9.46	1647	0.48
α-Curcumene	11.46*	1482	[1.24]	10.38*†	1724	3.81
Valencene	11.55†	1489	1.15	9.64*†	1662	[1.39]
Unknown [m/z 71, 93 (86), 109 (84), 69 (77), 41 (75), 43 (72), 81 (63), 55 (54), 79 (51)... 189 (36), 204 (3), 207 (2)]	11.60*†	1493	[1.15]	12.61	1920	0.20
Unknown [m/z 71, 69 (84), 93 (82), 109 (82), 41 (72), 43 (69), 81 (66), 55 (56), 79 (49)... 189 (37), 204 (3), 207 (3)]	11.60*†	1493	[1.15]	12.65	1924	0.23
α-Zingiberene	11.64*	1495	1.98	9.84	1678	1.38
4-epi-cis-Dihydroagarofuran	11.64*	1495	[1.98]	9.64*†	1662	[1.39]
α-Muurolene	11.68	1498	0.04	9.78	1674	0.06
(Z)-α-Bisabolene	11.74	1503	0.06	9.90*	1684	0.54
β-Bisabolene	11.81*†	1508	1.23	9.90*	1684	[0.54]
β-Dihydroagarofuran	11.81*†	1508	[1.23]	10.18	1706	0.12
Unknown [m/z 136, 121, (59), 93 (55), 80 (51), 81 (50), 71 (44), 123 (40)... 204 (3), 207 (1)]	11.84†	1510	[1.23]	12.90	1947	0.29
Liguloxide analog III	11.89*	1515	0.09			
7-epi-α-Selinene	11.89*	1515	[0.09]	10.16	1705	0.05
trans-Calamenene	11.94	1518	0.02	10.96	1773	0.01
β-Sesquiphellandrene	12.01*	1524	2.78	10.38*†	1724	[3.81]
Unknown [m/z 124, 109 (77), 123 (62), 105 (56), 91 (56), 41 (55), 43 (51), 205 (50)... 220 (21)]	12.01*	1524	[2.78]	11.32	1804	0.07
Unknown [m/z 109, 105 (63), 43 (58), 67 (57), 93 (55), 41 (945), 205 (44)...]	12.14	1534	0.13			
Selina-3,7(11)-diene	12.18*	1537	1.63	10.31	1718	0.80
α-Agarofuran	12.18*	1537	[1.63]	11.49	1819	0.80
(E)-α-Bisabolene	12.25	1543	0.05	10.46	1730	0.03
α-Elemol	12.36	1551	9.83	13.80	2032	9.99
Unknown [m/z 123, 81 (30), 93 (19), 121 (17), 43 (16), 95 (14)...]	12.40	1554	0.13			
(E)-Nerolidol	12.54	1566	0.49	13.53	2006	0.46
Spathulenol	12.63	1572	0.19	14.14	2064	0.22
Caryophyllene oxide	12.66*	1575	0.09	12.54	1913	0.03
Caryophyllene oxide isomer	12.66*	1575	[0.09]	12.47	1906	0.05
Eudesm-5-en-11-ol	12.95*	1598	0.78	14.09	2060	0.06
Eudesm-5-en-11-ol analog	12.95*	1598	[0.78]	13.94	2046	0.61

Humulene epoxide II	13.02*	1603	1.19	13.07	1963	0.13
Unknown [m/z 59, 91 (59), 105 (53), 93 (48), 161 (46), 79 (39), 123 (37)... 204 (12), 222 (1)]	13.02*	1603	[1.19]	14.36	2086	0.99
Unknown [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	13.02*	1603	[1.19]	14.23	2073	0.12
10-epi-γ-Eudesmol	13.18	1616	8.30	13.86	2037	7.77
Unknown [m/z 161, 59 (59), 81 (50), 204 (49), 93 (36), 189 (34)... 220 (t)]	13.24	1621	1.35	14.19	2069	1.15
Eremoligenol?	13.28	1625	0.49	14.51	2100	0.50
Unknown [m/z 105, 161 (51), 91 (36), 59 (30), 147 (29), 189 (24), 204 (23)... 218 (t)]	13.35*†	1630	6.26	14.82	2131	0.26
Eremoligenol	13.35*†	1630	[6.26]	14.75	2125	0.23
γ-Eudesmol	13.35*†	1630	[6.26]	14.60	2110	5.88
Hinesol	13.42	1636	0.47	14.72	2121	0.26
Agarospinol?	13.49*	1642	1.79	14.86	2136	0.85
Unknown [m/z 105, 59 (72), 161 (65), 147 (64), 91 (54), 43 (34), 189 (34)... 204 (30), 220 (1)]	13.49*	1642	[1.79]	14.93	2143	0.27
β-Eudesmol	13.56	1648	3.21	15.16*†	2165	18.74
7-epi-α-Eudesmol	13.62*†	1652	42.41	15.16*†	2165	[18.74]
Selin-11-en-4α-ol	13.62*†	1652	[42.41]	15.34	2184	0.17
α-Eudesmol	13.62*†	1652	[42.41]	15.10	2160	3.80
Valerianol	13.68†	1657	[42.41]	15.07	2157	23.30
4α-Hydroxydihydroagarofuran	13.71†	1660	[42.41]	15.18	2168	0.19
trans-Calamenen-10-ol	13.75	1663	0.16	16.53*	2308	0.94
Dehydrojinkoh-eremol	13.86	1673	0.58	16.04	2257	0.54
Unknown [m/z 109, 81 (67), 69 (64), 41 (63), 95 (46), 67 (35)... 207 (15)...]	13.98	1682	0.90	16.27	2280	0.92
Unknown [m/z 137, 119 (70), 84 (69), 41 (68), 69 (53), 55 (45), 109 (38)... 222 (2)]	14.01	1685	0.12			
Unknown [m/z 69, 41 (90), 123 (74), 122 (51)... 206 (14), 218 (2)]	14.05	1688	0.25	15.51	2201	0.18
Caryophyllene acetate	14.08	1690	0.17	13.36	1989	0.10
Unknown [m/z 69, 41 (59), 118 (33), 43 (32), 55 (31)... 234? (t)]	14.12	1693	0.11	16.45	2299	0.12
Unknown [m/z 81, 136 (77), 109 (68), 121 (61), 41 (48), 93 (41), 79 (35), 107 (34), 123 (30)... 222 (1)]	14.19*	1700	0.82	16.53*	2308	[0.94]

(2E,6Z)-Farnesol	14.19*	1700	[0.82]	16.14	2267	0.06
(2Z,6E)-Farnesol	14.19*	1700	[0.82]	16.36	2290	0.07
3β,4β-Oxidoagarofuran?	14.22	1702	0.08	15.75	2226	0.16
(2E,6E)-Farnesol	14.46	1723	0.29	16.53*	2308	[0.94]
(6R,7R)-Bisabolone	14.61	1736	0.54	15.67	2218	0.21
Unknown [m/z 137, 81 (78), 41 (74), 95 (74), 69 (55), 91 (51)... 222 (8)]	14.69*	1743	0.70	17.08	2367	0.06
(6S,7R)-Bisabolone	14.69*	1743	[0.70]	15.80	2232	0.65
Drimenol	14.84	1755	1.76	17.51	2415	1.74
Cryptomeridiol analog	14.96*	1766	0.12			
Cryptomeridiol analog	14.96*	1766	[0.12]	18.72	2553	0.03
Unknown [m/z 69, 43 (95), 41 (84), 109 (78), 95 (54), 93 (49)... 177 (36), 220 (2)...]	15.41*	1805	0.11	19.74	2674	0.04
Cryptomeridiol	15.41*	1805	[0.11]	19.51	2646	0.07
Unknown [m/z 177, 43 (51), 138 (40), 59 (40), 205 (32)... 238 (5)]	15.65	1827	0.01			
Unknown [m/z 59, 43 (75), 121 (73), 105 (68), 107 (57), 177 (55), 123 (46)... 220 (39), 236 (1)]	15.98	1857	0.02	21.00	2830	0.01
Unknown [m/z 43, 109 (77), 69 (65), 41 (60), 55 (51), 95 (44), 135 (43)... 207 (19)...]	16.03	1861	0.01			
Unknown [m/z 59, 45 (92), 43 (70), 177 (58), 121 (58), 220 (57)... 236 (3)]	16.11*	1869	0.06			
Unknown [m/z 59, 45 (92), 43 (70), 177 (58), 121 (58), 220 (57)... 236 (3)]	16.11*	1869	[0.06]	21.36	2876	0.01
Unknown [m/z 43, 59 (60), 123 (45), 176 (40)... 208 (10)...]	16.15	1872	0.01			
Carissone analog II	16.60	1913	0.02	21.42	2884	0.01
Carissone analog I	16.62	1916	0.02	21.06	2838	0.01
Unknown [m/z 59, 121 (66), 218 (27), 136 (26), 178 (26), 43 (24), 91 (24), 123 (23)... 238 (t)]	17.18	1968	0.02			
Total identified		94.25%			89.45%	
Total reported		97.53%			94.53%	

*: 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