

**Date :** October 23, 2018

## CERTIFICATE OF ANALYSIS – GC PROFILING

### SAMPLE IDENTIFICATION

**Internal code :** 18J15-PTH13-1-CC

**Customer identification :** Lemongrass - India - L8010586R

**Type :** Essential oil

**Source :** *Cymbopogon flexuosus*

**Customer :** Plant Therapy

### ANALYSIS

**Method:** PC-PA-014-17J19 - Analysis of the composition of an essential oil, or other volatile liquid, by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Benoit Roger, Ph. D.

**Analysis date :** October 18, 2018

Checked and approved by :

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Sylvain Mercier, M. Sc., chimiste 2014-005

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#### *P*HYSICO*C*HEMICAL *D*ATA

**Physical aspect:** Light yellow liquid

**Refractive index:**  $1.4838 \pm 0.0003$  (20 °C)

#### *C*ONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

## ANALYSIS SUMMARY

Identification	DB-5 (%)	DB-WAX (%)	Classe
2-Methyl-3-buten-2-ol	0.04	0.04	Aliphatic alcohol
Isovaleral	0.01	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	0.01	Aliphatic aldehyde
2-Methylbutanol	0.01	tr	Aliphatic alcohol
Hexanal	tr	tr	Aliphatic aldehyde
(3Z)-Hexenol	tr		Aliphatic alcohol
Furfuryl alcohol	0.01	0.01	Furan
4-Heptanone	0.01	0.01	Aliphatic ketone
Tricyclene	0.08	0.07	Monoterpene
$\alpha$ -Pinene	0.11	0.11	Monoterpene
Camphene	0.61	0.62	Monoterpene
Sabinene	0.01	0.01	Monoterpene
Dehydro-1,8-cineole	1.09*	0.03	Monoterpenic ether
6-Methyl-5-hepten-2-one	[1.09]*	1.09	Aliphatic ketone
Myrcene	0.06	0.04	Monoterpene
Unknown	0.04*	0.03	Aliphatic ester
6-Methyl-5-hepten-2-ol	[0.04]*	0.23*	Aliphatic alcohol
Octanal	0.06	0.06	Aliphatic aldehyde
para-Cymene	0.01	tr	Monoterpene
Limonene	0.18*	0.17	Monoterpene
1,8-Cineole	[0.18]*	0.02	Monoterpenic ether
(Z)- $\beta$ -Ocimene	0.24	0.23	Monoterpene
(E)- $\beta$ -Ocimene	0.14	0.14	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.02	0.02	Aliphatic aldehyde
cis-Linalool oxide (fur.)	0.01	0.01	Monoterpenic alcohol
4-Nonanone	0.73	0.73	Aliphatic ketone
Terpinolene	0.04*	0.03	Monoterpene
trans-Linalool oxide (fur.)	[0.04]*	0.01	Monoterpenic alcohol
4-Nonanol	0.22*		Aliphatic alcohol
Rosefuran	[0.22]*	0.20*	Monoterpenic ether
Perillene	0.07	0.03	Monoterpenic ether
Linalool	1.01*	0.95	Monoterpenic alcohol
cis-Chrysanthemal?	[1.01]*	[0.20]*	Monoterpenic aldehyde
(Z)-6-Methyl-3,5-heptadien-2-one	0.01	1.10*	Aliphatic ketone
trans-para-Mentha-2,8-dien-1-ol	0.02	0.03	Monoterpenic alcohol
Unknown	0.02	0.08	Unknown
Unknown	0.14	[0.23]*	Unknown
Unknown	0.01	0.01	Unknown
trans-Chrysanthemal	0.34*	0.25*	Monoterpenic aldehyde
exo-Isocitral	[0.34]*	0.09	Monoterpenic aldehyde
Citronellal	0.32	0.34	Monoterpenic aldehyde
Borneol	0.91*	0.31*	Monoterpenic alcohol
Isoneral	[0.91]*	0.67	Monoterpenic aldehyde
$\alpha$ -Phellandren-8-ol	0.02	38.63*	Monoterpenic alcohol
Rosefuran oxide	0.20	0.22	Monoterpenic ether
Terpinen-4-ol	0.05	0.03	Monoterpenic alcohol
Unknown	0.07	0.07	Oxygenated monoterpene
Isogeranial	1.21*	[1.10]*	Monoterpenic aldehyde

Unknown	[1.21]*		Unknown
α-Terpineol	0.13	[0.31]*	Monoterpenic alcohol
trans-Isopiperitenol	0.03	1.53*	Monoterpenic alcohol
Decanal	0.18*	[0.25]*	Aliphatic aldehyde
Unknown	[0.18]*		Oxygenated monoterpane
cis-Isopiperitenol	0.04	[1.53]*	Monoterpenic alcohol
2,3-Epoxyneral?	0.04		Monoterpenic aldehyde
Nerol	0.21	0.24	Monoterpenic alcohol
Neral	30.40*	29.88*	Monoterpenic aldehyde
Citronellol	[30.40]*	0.13	Monoterpenic alcohol
Piperitone	0.07	0.12*	Monoterpenic ketone
Geraniol	7.83	8.23	Monoterpenic alcohol
Geranial	39.24	[38.63]*	Monoterpenic aldehyde
Unknown	0.14	0.11	Oxygenated monoterpane
Geranyl formate	0.04	[0.12]*	Monoterpenic ester
Unknown	0.04	0.14*	Unknown
α-Cubebene	0.01	0.02	Sesquiterpene
Citronellyl acetate	0.06	[29.88]*	Monoterpenic ester
Cyclosativene I	0.12	0.12	Sesquiterpene
Cyclosativene II	0.15	[0.23]*	Sesquiterpene
Neryl acetate	0.07	0.09	Monoterpenic ester
α-Copaene	0.03	0.04	Sesquiterpene
Geranic acid	0.07		Aliphatic acid
β-Bourbonene	0.03	0.02	Sesquiterpene
Geranyl acetate	4.74*	4.40	Monoterpenic ester
β-Cubebene	[4.74]*	0.07	Sesquiterpene
β-Elemene	0.15	2.08*	Sesquiterpene
Longifolene	0.02	0.01	Sesquiterpene
β-Caryophyllene	2.06	[2.08]*	Sesquiterpene
β-Copaene	0.03	[2.08]*	Sesquiterpene
trans-α-Bergamotene	0.02	0.02	Sesquiterpene
α-Humulene	0.23	0.22	Sesquiterpene
(E)-Isoeugenol	0.47	0.44	Phenylpropanoid
cis-Muurola-4(15),5-diene	0.03	0.03	Sesquiterpene
trans-Cadina-1(6),4-diene	0.04	0.07	Sesquiterpene
Germacrene D	0.30	0.29	Sesquiterpene
γ-Amorphene	0.03	0.02	Sesquiterpene
epi-Cubebol	0.16	0.14	Sesquiterpenic alcohol
α-Muurolene	0.06	0.06	Sesquiterpene
δ-Amorphene	0.04	[0.12]*	Sesquiterpene
γ-Cadinene	1.49*	[1.53]*	Sesquiterpene
Cubebol	[1.49]*	0.38	Sesquiterpenic alcohol
δ-Cadinene	0.38	[1.53]*	Sesquiterpene
10-epi-Cubebol?	0.19*	0.04*	Sesquiterpenic alcohol
(E)-γ-Bisabolene	[0.19]*	[1.53]*	Sesquiterpene
α-Cadinene	0.05	0.04	Sesquiterpene
Neryl butyrate	0.09		Monoterpenic ester
α-Elemol	0.10*	0.06	Sesquiterpenic alcohol
Germacrene B	[0.10]*	0.02	Sesquiterpene
Geranyl butyrate	0.05	0.07	Monoterpenic ester
Caryophyllene oxide	0.63*	0.52	Sesquiterpenic ether
Caryophyllene oxide isomer	[0.63]*	0.02	Sesquiterpenic ether

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Humulene epoxide II	0.07	0.09	Sesquiterpenic ether
Selin-6-en-4 $\alpha$ -ol?	0.03	0.01	Sesquiterpenic alcohol
1-epi-Cubenol	0.04	[0.04]*	Sesquiterpenic alcohol
Cubenol	0.01	0.02	Sesquiterpenic alcohol
Farnesal isomer	0.02		Sesquiterpenic aldehyde
(2E,6E)-Farnesal	0.02	0.04	Sesquiterpenic aldehyde
Neophytadiene	0.02	[0.14]*	Diterpene
Unknown	0.02		Unknown
Dicitral	0.09	0.03	Aliphatic alcohol
Unknown	0.01		Unknown
<b>Total identified</b>	<b>98.29%</b>	<b>96.31%</b>	

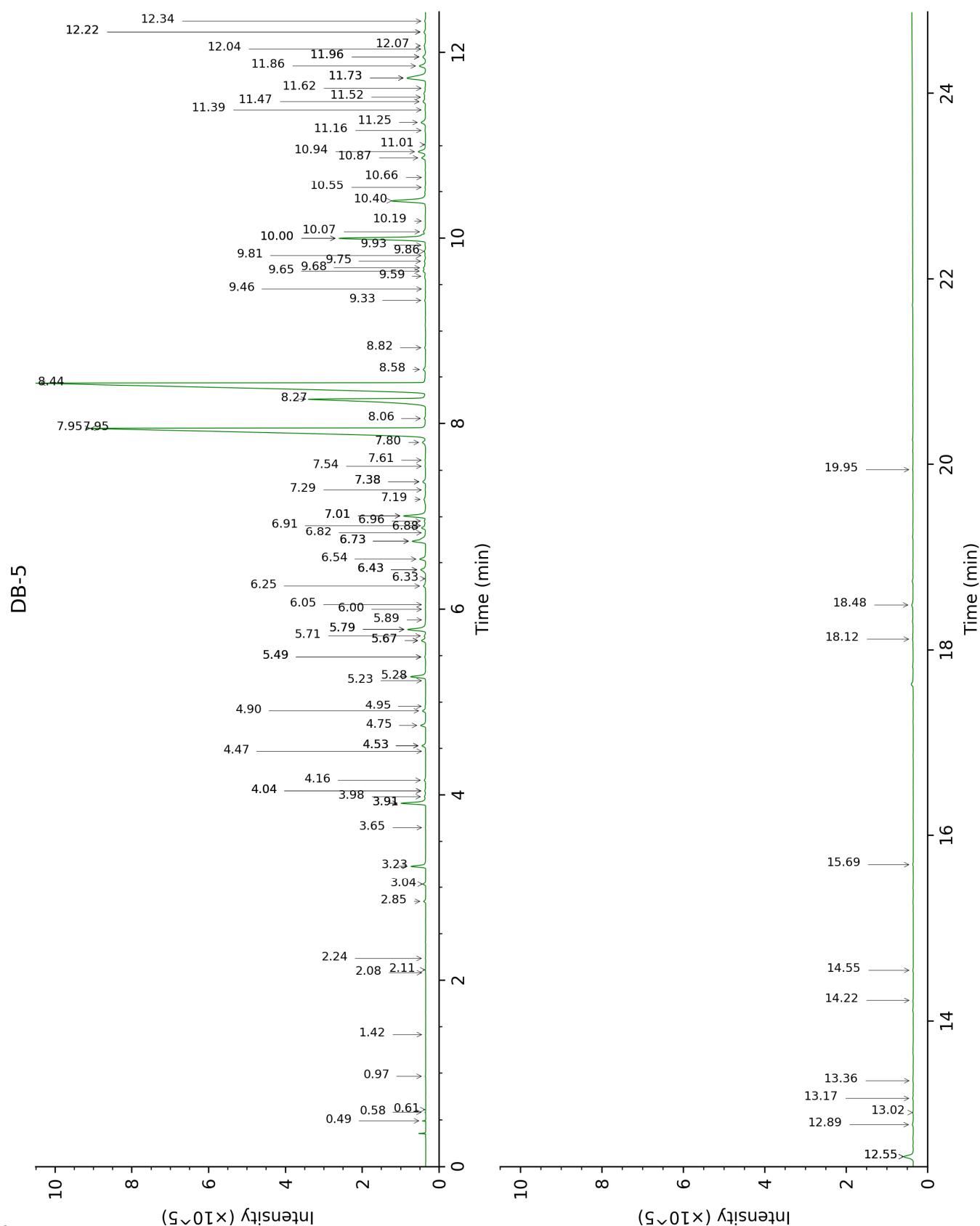
\*: Two or more compounds are coeluting on this column

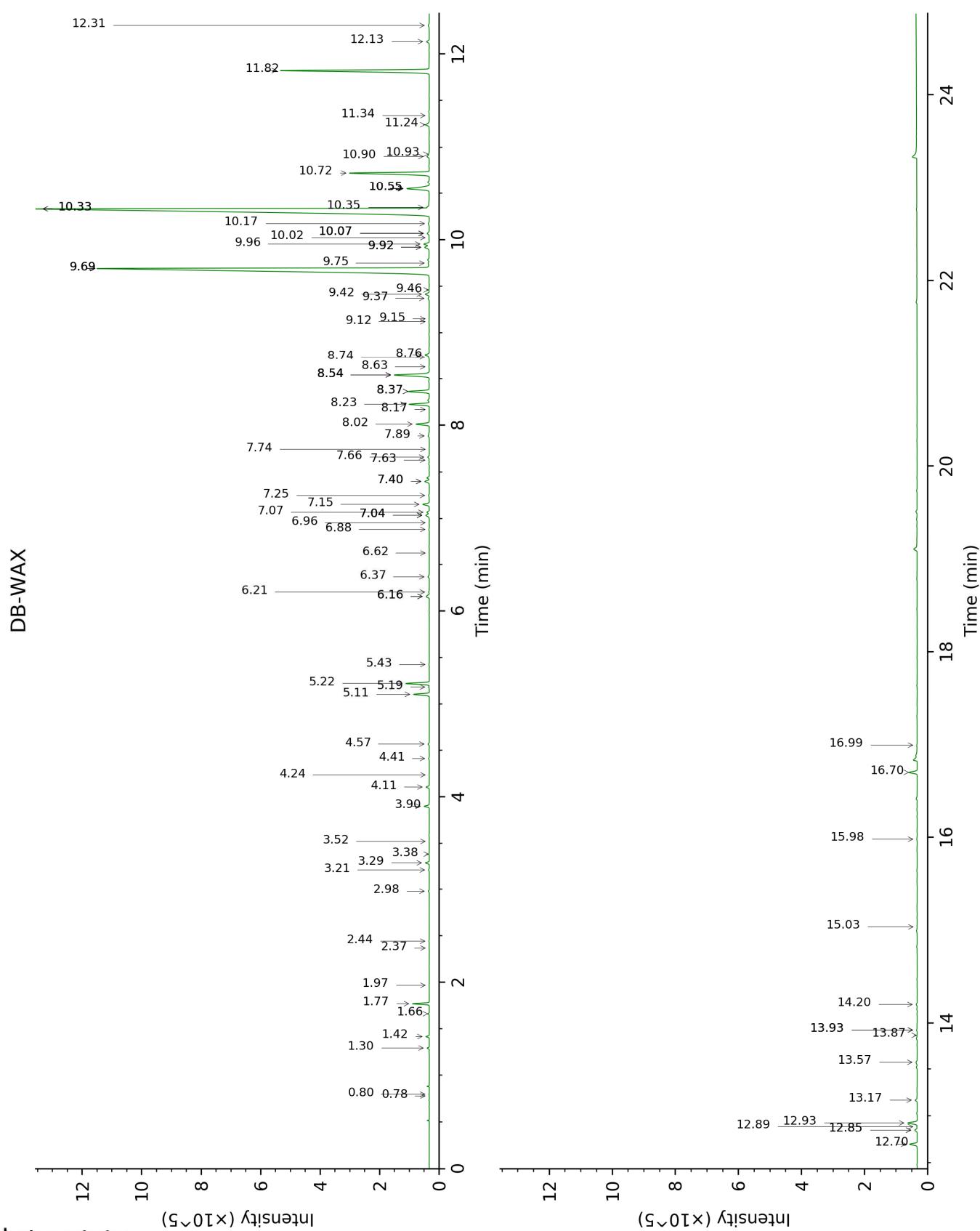
[xx]: Duplicate percentage due to coelutions, not taken account in the identified total

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

Note: no correction factor was applied

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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	603	0.04	1.66	1018	0.04
Isovaleral	0.58	638	0.01	0.80	890	0.01
2-Methylbutyral	0.61	647	tr	0.78	884	0.01
2-Methylbutanol	0.97	733	0.01	3.52	1176	tr
Hexanal	1.42	798	tr	1.97	1046	tr
(3Z)-Hexenol	2.08	857	tr			
Furfuryl alcohol	2.11	859	0.01	9.15	1590	0.01
4-Heptanone	2.24	870	0.01	2.44	1092	0.01
Tricyclene	2.85	917	0.08	1.30	973	0.07
$\alpha$ -Pinene	3.04	929	0.11	1.42	991	0.11
Camphene	3.23	942	0.61	1.77	1028	0.62
Sabinene	3.65	969	0.01	2.37	1084	0.01
Dehydro-1,8-cineole	3.91*	986	1.09	3.22	1152	0.03
6-Methyl-5-hepten-2-one	3.91*	986	[1.09]	5.22	1300	1.09
Myrcene	3.98	991	0.06	2.98	1134	0.04
Unknown [m/z 67, 82 (50), 41 (47), 55 (31), 98 (14)]	4.04*	995	0.04	5.19	1297	0.03
6-Methyl-5-hepten-2-ol	4.04*	995	[0.04]	7.04*	1430	0.23
Octanal	4.16	1003	0.06	4.57	1256	0.06
para-Cymene	4.47	1022	0.01	4.24	1231	tr
Limonene	4.53*	1026	0.18	3.29	1158	0.17
1,8-Cineole	4.53*	1026	[0.18]	3.38	1166	0.02
(Z)- $\beta$ -Ocimene	4.75	1039	0.24	3.90	1206	0.23
(E)- $\beta$ -Ocimene	4.90	1049	0.14	4.10	1221	0.14
2,6-Dimethyl-5-heptenal (melonal)	4.95	1052	0.02	5.43	1314	0.02
cis-Linalool oxide (fur.)	5.23	1069	0.01	6.62	1400	0.01
4-Nonanone	5.28	1072	0.73	5.11	1296	0.73
Terpinolene	5.49*	1085	0.04	4.41	1244	0.03
trans-Linalool oxide (fur.)	5.49*	1085	[0.04]	6.96	1424	0.01
4-Nonanol	5.66*	1096	0.22			
Rosefuran	5.66*	1096	[0.22]	6.16*	1366	0.20
Perillene	5.72	1099	0.07	6.20	1370	0.03
Linalool	5.78*	1103	1.01	8.23	1519	0.95
cis-Chrysanthemal?	5.78*	1103	[1.01]	6.16*	1366	[0.20]
(Z)-6-Methyl-3,5-heptadien-	5.89	1110	0.01	8.37*	1529	1.10

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2-one						
<i>trans</i> -para-Mentha-2,8-dien-1-ol	6.00	1117	0.02	9.12	1588	0.03
Unknown [m/z 81, 79 (19), 41 (12), 92 (8), 77 (8) ...]	6.05	1120	0.02	6.37	1381	0.08
Unknown [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43) ...]	6.25	1132	0.14	7.04*	1430	[0.23]
Unknown [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62) ...]	6.33	1137	0.01	7.74	1482	0.01
<i>trans</i> -Chrysanthemal	6.43*	1144	0.34	7.40*	1457	0.25
exo-Isocitral	6.43*	1144	[0.34]	7.66	1476	0.09
Citronellal	6.54	1151	0.32	7.15	1439	0.34
Borneol	6.73*	1163	0.91	9.92*	1651	0.31
Isoneral	6.73*	1163	[0.91]	8.02	1502	0.67
$\alpha$ -Phellandren-8-ol	6.82	1168	0.02	10.33*	1685	38.63
Rosefuran oxide	6.88	1172	0.20	8.76	1560	0.22
Terpinen-4-ol	6.91	1174	0.05	8.74	1558	0.03
Unknown [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40) ... 152 (2)]	6.96	1177	0.07	9.75	1638	0.07
Isogeranial	7.01*	1180	1.21	8.37*	1529	[1.10]
Unknown [m/z 69, 41 (65), 109 (36), 67 (16), 84 (11), 43 (10), 55 (9) ...]	7.01*	1180	[1.21]			
$\alpha$ -Terpineol	7.19	1192	0.13	9.92*	1651	[0.31]
<i>trans</i> -Isopiperitenol	7.29	1198	0.03	10.55*	1702	1.53
Decanal	7.38*	1204	0.18	7.40*	1457	[0.25]
Unknown [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54) ... 152 (4)]	7.38*	1204	[0.18]			
<i>cis</i> -Isopiperitenol	7.54	1215	0.04	10.55*	1702	[1.53]
2,3-Epoxyneral?	7.61	1219	0.04			

Nerol	7.80	1232	0.21	11.24	1761	0.24
Neral	7.95*	1242	30.40	9.69*	1633	29.88
Citronellol	7.95*	1242	[30.40]	10.90	1732	0.13
Piperitone	8.06	1249	0.07	10.07*	1663	0.12
Geraniol	8.26	1262	7.83	11.82	1810	8.23
Geranal	8.44	1274	39.24	10.33*	1685	[38.63]
Unknown [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]	8.58	1283	0.14	13.17	1930	0.11
Geranyl formate	8.82	1300	0.04	10.07*	1663	[0.12]
Unknown [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	9.33	1336	0.04	12.85*	1901	0.14
$\alpha$ -Cubebene	9.46	1345	0.01	6.88	1419	0.02
Citronellyl acetate	9.59	1354	0.06	9.69*	1633	[29.88]
Cyclosativene I	9.65	1358	0.12	7.07	1432	0.12
Cyclosativene II	9.68	1360	0.15	7.04*	1430	[0.23]
Neryl acetate	9.75	1365	0.07	10.35	1686	0.09
$\alpha$ -Copaene	9.81	1370	0.03	7.25	1446	0.04
Geranic acid	9.86	1373	0.07			
$\beta$ -Bourbonene	9.93	1377	0.03	7.63	1474	0.02
Geranyl acetate	10.00*	1382	4.74	10.72	1717	4.40
$\beta$ -Cubebene	10.00*	1382	[4.74]	7.89	1493	0.07
$\beta$ -Elemene	10.07	1387	0.15	8.54*	1543	2.08
Longifolene	10.18	1395	0.02	8.17	1514	0.01
$\beta$ -Caryophyllene	10.40	1411	2.06	8.54*	1543	[2.08]
$\beta$ -Copaene	10.55	1421	0.03	8.54*	1543	[2.08]
<i>trans-a</i> -Bergamotene	10.66	1430	0.02	8.63	1550	0.02
$\alpha$ -Humulene	10.87	1445	0.23	9.42	1611	0.22
(E)-Isoeugenol	10.94	1450	0.47	16.70	2276	0.44
<i>cis</i> -Muurola-4(15),5-diene	11.01	1455	0.03	9.46	1615	0.03
<i>trans</i> -Cadina-1(6),4-diene	11.16	1467	0.04	9.37	1607	0.07
Germacrene D	11.25	1473	0.30	9.96	1654	0.29
$\gamma$ -Amorphene	11.39	1483	0.03	10.02	1660	0.02
epi-Cubebol	11.48	1489	0.16	12.14	1838	0.14
$\alpha$ -Muurolene	11.52	1493	0.06	10.17	1672	0.06
$\delta$ -Amorphene	11.62	1500	0.04	10.07*	1663	[0.12]
$\gamma$ -Cadinene	11.73*	1508	1.49	10.55*	1702	[1.53]
Cubebol	11.73*	1508	[1.49]	12.70	1888	0.38
$\delta$ -Cadinene	11.86	1518	0.38	10.55*	1702	[1.53]
10- <i>epi</i> -Cubebol?	11.96*	1526	0.19	13.93*	2000	0.04
(E)- $\gamma$ -Bisabolene	11.96*	1526	[0.19]	10.55*	1702	[1.53]
$\alpha$ -Cadinene	12.04	1532	0.05	10.93	1734	0.04

Neryl butyrate	12.07	1535	0.09			
α-Elemol	12.22*	1546	0.10	14.20	2027	0.06
Germacrene B	12.22*	1546	[0.10]	11.34	1769	0.02
Geranyl butyrate	12.34	1555	0.05	12.31	1853	0.07
Caryophyllene oxide	12.55*	1572	0.63	12.93	1908	0.52
Caryophyllene oxide isomer	12.55*	1572	[0.63]	12.89	1904	0.02
Humulene epoxide II	12.89	1598	0.07	13.57	1968	0.09
Selin-6-en-4α-ol?	13.02	1608	0.03	15.03	2107	0.01
1-epi-Cubenol	13.17	1621	0.04	13.93*	2000	[0.04]
Cubenol	13.36	1636	0.01	13.87	1995	0.02
Farnesal isomer	14.22	1707	0.02			
(2E,6E)-Farnesal	14.55	1735	0.02	15.98	2202	0.04
Neophytadiene	15.69	1835	0.02	12.85*	1901	[0.14]
Unknown [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53), 109 (50)... 235 (10)...]	18.12	2064	0.02			
Dicitral	18.48	2101	0.09	16.99	2307	0.03
Unknown [m/z 123, 94 (100), 43 (86), 69 (75), 95 (47), 41 (47), 93 (45)...]	19.94	2254	0.01			
<b>Total identified</b>	<b>98.29%</b>			<b>96.31%</b>		
<b>Total reported</b>	<b>98.73%</b>			<b>96.61%</b>		

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken account in the identified 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