

Date : 2024-02-13

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 24B02-PTH01

**Customer Identification :** Egyptian Geranium - Egypt - G30111R

**Type :** Essential Oil

**Source :** *Pelargonium graveolens* ct. Egyptian

**Customer :** Plant Therapy

Checked and approved by:

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

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## GAS CHROMATOGRAPHIC ANALYSIS

**Method :** PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID

**✖ISO**

**Results :** See analysis summary (next page)

**Analyst :** Sylvain Mercier, M. Sc., Chimiste 2014-005

**Date :** 2024-02-06

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.4684 \pm 0.0003$  (20 °C)

**Method :** PC-MAT-016 - Measure of the refractive index of a liquid.

**Analyst :** Cindy Caron B. Sc.

**Date :** 2024-02-06

## 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
2-Methyl-3-buten-2-ol	tr	Aliphatic alcohol
Isovaleral	tr	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
Prenal	0.01	Aliphatic aldehyde
Hexanal	tr	Aliphatic aldehyde
Unknown	0.01	Unknown
3-Methylpentanol	0.04	Aliphatic alcohol
5-Methyl-2-hexanone	tr	Aliphatic ketone
(3Z)-Hexenol	0.02	Aliphatic alcohol
3-Acetyl-3-methylcyclopentene	0.01	Aliphatic ketone
3-Methylpentyl formate?	0.02	Aliphatic ester
$\alpha$ -Pinene	0.40	Monoterpene
Unknown	0.02	Unknown
Camphene	0.02	Monoterpene
Benzaldehyde	0.01	Simple phenolic
Geranic oxide	0.04	Monoterpenic ether
$\beta$ -Pinene	0.01	Monoterpene
Sabinene	0.01	Monoterpene
Octen-3-ol	0.02	Aliphatic alcohol
6-Methyl-5-hepten-2-one	0.06	Aliphatic ketone
<i>trans</i> -Dehydroxylinalool oxide	0.03	Monoterpenic ether
6-Methyl-5-hepten-2-ol	0.01	Aliphatic alcohol
Myrcene	0.09	Monoterpene
$\alpha$ -Phellandrene	0.07	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.03	Monoterpenic ether
$\alpha$ -Terpinene	tr	Monoterpene
<i>para</i> -Cymene	0.08	Monoterpene
Unknown	0.04	Unknown
Limonene	0.14	Monoterpene
Unknown	0.04	Unknown
1,8-Cineole	0.01	Monoterpenic ether
$\beta$ -Phellandrene	0.06	Monoterpene
Benzeneacetaldehyde	tr	Simple phenolic
(Z)- $\beta$ -Ocimene	0.09	Monoterpene
(E)- $\beta$ -Ocimene	0.10	Monoterpene
Unknown	0.02	Unknown
2,6-Dimethyl-5-heptenal (melonal)	0.02	Aliphatic aldehyde
$\gamma$ -Terpinene	0.01	Monoterpene
<i>cis</i> -Sabinene hydrate	0.01	Monoterpenic alcohol

Unknown	0.02	Oxygenated monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.20	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
Fenchone	0.02	Monoterpenic ketone
<i>trans</i> -Linalool oxide (fur.)	0.11	Monoterpenic alcohol
Terpinolene	0.03	Monoterpene
<i>trans</i> -Sabinene hydrate	0.02	Monoterpenic alcohol
Linalool	4.17	Monoterpenic alcohol
<i>cis</i> -Rose oxide	1.14	Monoterpenic ether
Phenylethyl alcohol	0.02	Simple phenolic
Myrcenol	0.01	Monoterpenic alcohol
<i>trans</i> -Rose oxide	0.48	Monoterpenic ether
Unknown	0.04	Unknown
Unknown	0.08	Oxygenated normonoterpene
Isopulegol	0.04	Monoterpenic alcohol
Menthone	0.72	Monoterpenic ketone
Citronellal	0.05	Monoterpenic aldehyde
iso-Isopulegol	0.17	Monoterpenic alcohol
Isomenthone	5.93	Monoterpenic ketone
Borneol	0.04	Monoterpenic alcohol
neo-Menthol	0.07	Monoterpenic alcohol
Menthol	0.02	Monoterpenic alcohol
Terpinen-4-ol	0.05	Monoterpenic alcohol
Isomenthol	0.17	Monoterpenic alcohol
<i>para</i> -Cymen-8-ol	0.02	Monoterpenic alcohol
$\alpha$ -Terpineol	0.30	Monoterpenic alcohol
Unknown	0.02	Unknown
Unknown	0.03	Oxygenated monoterpene
$\beta$ -Cyclocitral	0.03	Monoterpenic aldehyde
Nerol	0.22	Monoterpenic alcohol
Citronellol	31.77	Monoterpenic alcohol
Neral	0.58	Monoterpenic aldehyde
Piperitone	0.09	Monoterpenic ketone
Geraniol	13.22	Monoterpenic alcohol
Geranial	0.80	Monoterpenic aldehyde
Citronellyl formate	7.21	Monoterpenic ester
Neryl formate	0.08	Monoterpenic ester
Geranyl formate	2.75	Monoterpenic ester
(3 <i>Z</i> )-Hexenyl tiglate	0.02	Aliphatic ester
Methyl geranate	0.03	Monoterpenic ester
Citronellic acid	0.07	Monoterpenic acid
$\alpha$ -Cubebene	0.23	Sesquiterpene
Phenylethyl propionate	0.03	Phenolic ester
Citronellyl acetate	0.25	Monoterpenic ester
Neryl acetate	0.05	Monoterpenic ester

$\alpha$ -Ylangene	0.05	Sesquiterpene
Geranic acid	0.06	Aliphatic acid
$\alpha$ -Copaene	0.54	Sesquiterpene
$\beta$ -Bourbonene	1.10	Sesquiterpene
1,5-diepi- $\beta$ -Bourbonene	0.08	Sesquiterpene
Geranyl acetate	0.47	Monoterpenic ester
$\beta$ -Elemene	0.08	Sesquiterpene
Phenylethyl isobutyrate	0.05	Phenolic ester
Isocaryophyllene	0.03	Sesquiterpene
$\alpha$ -Gurjunene	0.09	Sesquiterpene
$\beta$ -Caryophyllene	1.37	Sesquiterpene
Thymohydroquinone dimethyl ether	0.01	Monoterpenic ether
$\beta$ -Copaene	0.15	Sesquiterpene
Heptyl tiglate	0.01	Aliphatic ester
Aromadendrene	0.04	Sesquiterpene
6,9-Guaiadiene	0.40	Sesquiterpene
Isogermacrene D	0.03	Sesquiterpene
Citronellyl propionate	0.45	Monoterpenic ester
Unknown	0.40	Sesquiterpene
$\alpha$ -Humulene	0.31	Sesquiterpene
allo-Aromadendrene	0.20	Sesquiterpene
Unknown	0.07	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.26	Sesquiterpene
$\gamma$ -Murolene	0.10	Sesquiterpene
Germacrene D	1.48	Sesquiterpene
Geranyl propionate	0.66	Monoterpenic ester
$\alpha$ -Amorphene	0.21	Sesquiterpene
$\beta$ -Selinene	0.17	Sesquiterpene
Phenylethyl isovalerate	0.05	Phenolic ester
$\gamma$ -Amorphene	0.15	Sesquiterpene
Bicyclogermacrene	0.49	Sesquiterpene
$\alpha$ -Selinene	0.08	Sesquiterpene
Viridiflorene	0.26	Sesquiterpene
$\alpha$ -Murolene	0.17	Sesquiterpene
4-epi- <i>cis</i> -Dihydroagarofuran	0.17	Sesquiterpenic ether
$\gamma$ -Cadinene	0.39	Sesquiterpene
7-epi- $\alpha$ -Selinene	0.09	Sesquiterpene
Geranyl isobutyrate	0.20	Monoterpenic ester
Zonarene	0.06	Sesquiterpene
$\delta$ -Cadinene	0.81	Sesquiterpene
<i>trans</i> -Calamenene	0.13	Sesquiterpene
Citronellyl butyrate	0.54	Monoterpenic ester
<i>trans</i> -Cadina-1,4-diene	0.10	Sesquiterpene
Phenylethyl angelate?	0.14	Phenolic ester
$\alpha$ -Agarofuran	0.35	Sesquiterpenic ether

1-nor-Bourbonanone	0.04	Norsesquiterpenic ketone
Geranyl butyrate	1.00	Monoterpenic ester
Spathulenol	0.24	Sesquiterpenic alcohol
Caryophyllene oxide	0.15	Sesquiterpenic ether
Globulol	0.09	Sesquiterpenic alcohol
Phenylethyl tiglate	0.76	Phenolic ester
Viridiflorol	0.07	Sesquiterpenic alcohol
Eudesm-5-en-11-ol analog	0.06	Sesquiterpenic alcohol
Geranyl 2-methylbutyrate?	0.09	Monoterpenic ester
Geranyl isovalerate	0.08	Monoterpenic ester
10-epi- $\gamma$ -Eudesmol	4.52	Sesquiterpenic alcohol
1-epi-Cubenol	0.13	Sesquiterpenic alcohol
$\gamma$ -Eudesmol	0.21	Sesquiterpenic alcohol
Unknown	0.19	Oxygenated sesquiterpene
Citronellyl valerate?	0.04	Monoterpenic ester
Agarospinol?	0.05	Sesquiterpenic alcohol
$\tau$ -Muurolool	0.06	Sesquiterpenic alcohol
Cubenol	0.17	Sesquiterpenic alcohol
$\tau$ -Cadinol	tr	Sesquiterpenic alcohol
$\beta$ -Eudesmol	0.27	Sesquiterpenic alcohol
$\alpha$ -Eudesmol	0.28	Sesquiterpenic alcohol
$\alpha$ -Cadinol	0.15	Sesquiterpenic alcohol
Geranyl valerate	0.19	Monoterpenic ester
Citronellyl tiglate	0.34	Monoterpenic ester
Citronellyl 4-methylvalerate	0.10	Monoterpenic ester
Geranyl tiglate	1.09	Monoterpenic ester
3 $\beta$ ,4 $\beta$ -Oxidoagarofuran?	tr	Sesquiterpenic ether
Geranyl 4-methylvalerate?	0.17	Monoterpenic ester
Citronellyl caproate	0.05	Monoterpenic ester
Geranyl caproate	0.10	Monoterpenic ester
Citronellyl heptanoate	0.07	Monoterpenic ester
Phytone	0.04	Terpenic ketone
Geranyl heptanoate	0.11	Monoterpenic ester
Unknown	0.02	Unknown
Citronellyl caprylate	0.04	Monoterpenic ester
Geranyl caprylate	0.05	Monoterpenic ester
Unknown	0.06	Unknown
Unknown	0.04	Unknown
<b>Consolidated total</b>	<b>97.19</b>	

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

Note: no correction factor was applied

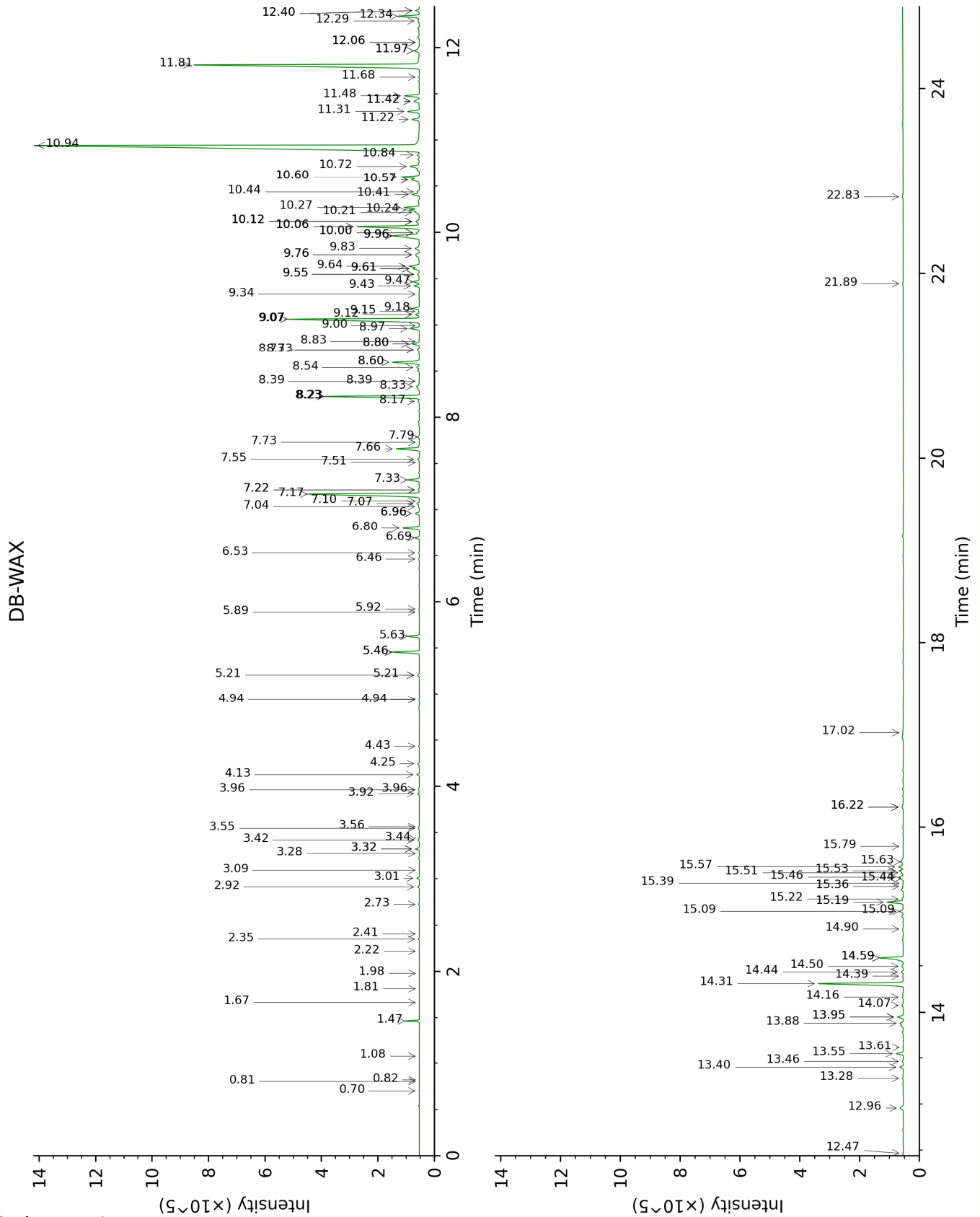
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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

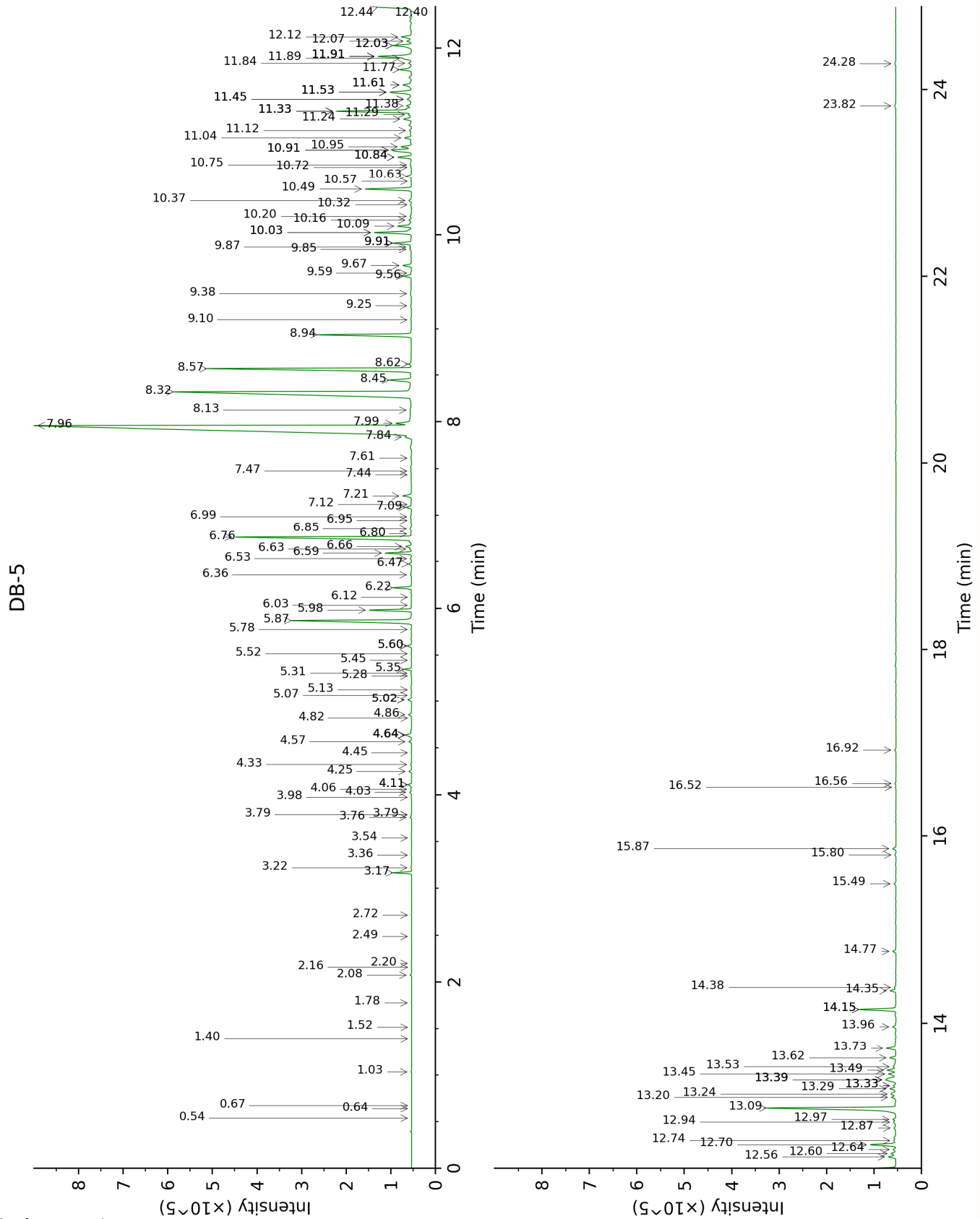
**Unknowns:** Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

**Bracketed value ([xx]):** A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

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## FULL ANALYSIS DATA

2-Methyl-3-buten-2-ol	Column DB-WAX			Column DB-5		
	1.67	1012.0	0.01	0.54	606.0	tr
Isovaleral	0.82	882.1	tr	0.64	640.5	tr
2-Methylbutyral	0.80	876.3	tr	0.67	651.1	tr
Isoamyl alcohol	3.56	1173.2	0.02	1.03	732.5	0.01
Prenal	3.32*	1154.9	[0.15]	1.40	782.4	0.01
Hexanal	1.98	1041.8	tr	1.52	799.2	tr
Unknown PEGR III [m/z 81, 69 (80), 41 (65), 83 (52), 109 (48), 55 (47)...]	0.70	842.1	0.01	1.78	823.0	0.01
3-Methylpentanol	5.21*	1291.6	[0.10]	2.08	847.3	0.04
5-Methyl-2-hexanone	2.73	1109.6	0.03	2.16	854.1	tr
(3Z)-Hexenol	5.92	1344.2	0.02	2.20	857.6	0.02
3-Acetyl-3-methylcyclopentene	1.08	930.8	0.01	2.49	881.1	0.01
3-Methylpentyl formate?	3.28	1151.3	0.01	2.72	899.8	0.02
$\alpha$ -Pinene	1.47	989.4	0.39	3.17	930.6	0.40
Unknown PEGR IV [m/z 122, 107 (38), 121 (35), 79 (28), 77 (27), 43 (26)...]				3.22	934.1	0.02
Camphene	1.82	1026.1	tr	3.36	943.0	0.02
Benzaldehyde	7.51	1459.8	0.01	3.54	955.1	0.01
Geranic oxide	2.35	1076.7	0.03	3.76	969.5	0.04
$\beta$ -Pinene	2.22	1064.2	0.01	3.79*	971.4	[0.02]
Sabinene	2.41	1082.0	0.01	3.79*	971.4	[0.02]
Octen-3-ol	6.96*	1419.1	[0.21]	3.98	983.7	0.02
6-Methyl-5-hepten-2-one	5.21*	1291.6	[0.10]	4.03	987.2	0.06
<i>trans</i> -Dehydroxylinalool oxide	3.55	1171.8	0.04	4.06	989.3	0.03
6-Methyl-5-hepten-2-ol	7.10	1429.0	0.01	4.11*	992.5	[0.12]
Myrcene	3.01	1130.9	0.09	4.11*	992.5	[0.12]
$\alpha$ -Phellandrene	2.92	1123.9	0.07	4.25	1001.9	0.07
<i>cis</i> -Dehydroxylinalool oxide	3.96*	1203.1	[0.06]	4.32	1006.6	0.03
$\alpha$ -Terpinene	3.09	1137.4	0.01	4.45	1014.5	tr
<i>para</i> -Cymene	4.24	1223.1	0.08	4.57	1021.9	0.08
Unknown COCI XLIII [m/z 59, 43 (11), 109	6.46	1382.7	0.04	4.64*	1026.3	[0.23]

(10), 41 (10), 127 (8)...						
Limonene	3.32*	1154.9	[0.15]	4.64*	1026.3	[0.23]
Unknown COCI XLIV [m/z 59, 43 (12), 109 (11), 41 (10), 127 (8)...	6.53	1387.5	0.04	4.64*	1026.3	[0.23]
1,8-Cineole	3.44	1163.6	0.01	4.64*	1026.3	[0.23]
$\beta$ -Phellandrene	3.42	1162.2	0.06	4.64*	1026.3	[0.23]
Benzeneacetaldehyde	9.00	1572.6	0.01	4.82	1037.6	tr
(Z)- $\beta$ -Ocimene	3.92	1200.1	0.07	4.86	1040.0	0.09
(E)- $\beta$ -Ocimene	4.13	1214.7	0.10	5.02*	1049.9	[0.12]
Unknown COCI V [m/z 125, 69 (75), 41 (34), 55 (25), 93 (22)... 140 (3)]	4.94*	1272.5	[0.02]	5.02*	1049.9	[0.12]
2,6-Dimethyl-5- heptenal (melonal)	5.46*	1310.9	[1.14]	5.07	1053.3	0.02
$\gamma$ -Terpinene	3.96*	1203.1	[0.06]	5.13	1057.0	0.01
<i>cis</i> -Sabinene hydrate	7.07*†	1426.9	[0.12]	5.28	1066.2	0.01
Unknown PIMA I [m/z 79, 93 (60), 43 (40), 94 (35), 137 (33), 77 (26), 91 (20), 152 (18)]	4.94*	1272.5	[0.02]	5.31	1068.1	0.02
<i>cis</i> -Linalool oxide (fur.)	6.69	1399.1	0.19	5.35	1070.7	0.20
Octanol	8.39*	1525.8	[0.02]	5.45	1076.7	0.01
Fenchone	5.89	1341.8	0.02	5.52	1081.1	0.02
<i>trans</i> -Linalool oxide (fur.)	7.04*†	1424.6	[0.06]	5.60*	1086.3	[0.14]
Terpinolene	4.43	1236.4	0.03	5.60*	1086.3	[0.14]
<i>trans</i> -Sabinene hydrate	8.17	1509.0	0.07	5.78	1097.3	0.02
Linalool	8.23*	1513.1	[4.04]	5.87	1103.2	4.17
<i>cis</i> -Rose oxide	5.46*	1310.9	[1.14]	5.98	1110.3	1.14
Phenylethyl alcohol	12.29	1845.5	0.10	6.03	1113.6	0.02
Myrcenol	9.07*	1577.9	[7.29]	6.12	1119.1	0.01
<i>trans</i> -Rose oxide	5.63	1323.1	0.47	6.22	1125.5	0.48
Unknown CYFL IV [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...	7.73	1475.9	0.01	6.36	1134.4	0.04
Unknown COCI VIII [m/z 41, 69 (87), 82 (66), 67 (55), 109 (46)... 142 (18)]	9.55*	1616.0	[0.10]	6.48	1141.8	0.08
Isopulegol	8.33	1521.3	0.17	6.53	1145.4	0.04

Menthone	6.80	1407.0	0.72	6.59	1149.1	0.72
Citronellal	7.22*	1437.9	[0.06]	6.64	1152.0	0.05
iso-Isopulegol	8.23*	1513.1	[4.04]	6.66	1153.6	0.17
Isomenthone	7.17	1434.6	6.04	6.76	1160.1	5.93
Borneol	9.96*†	1649.3	[1.88]	6.80	1162.3	0.04
neo-Menthol	8.80*	1557.5	[0.34]	6.85	1165.8	0.07
Menthol	9.34	1598.7	0.03	6.94	1171.7	0.02
Terpinen-4-ol	8.74*	1552.3	[0.13]	6.99	1174.3	0.05
Isomenthol	9.12	1581.7	0.17	7.09	1180.8	0.17
<i>para</i> -Cymen-8-ol	11.68	1792.2	0.02	7.12	1182.7	0.02
$\alpha$ -Terpineol	9.96*†	1649.3	[1.88]	7.21	1188.6	0.30
Unknown MEPI V [m/z 43, 99 (84), 81 (46), 986 (43), 126 (36), 71 (28)... 170 (12)]				7.44	1203.0	0.02
Unknown DRMO II [m/z 123, 81 (40), 67 (29), 79 (29), 93 (26), 121 (25), 41 (24), 55 (18), 69 (15)...]				7.48	1205.5	0.03
$\beta$ -Cyclocitral	8.83	1559.3	0.01	7.61	1214.7	0.03
Nerol	11.22	1753.6	0.32	7.84	1229.8	0.22
Citronellol	10.94	1729.9	31.84	7.96	1238.0	31.77
Neral	9.64	1623.0	0.51	7.98	1239.6	0.58
Piperitone	10.12*	1661.8	[0.22]	8.13	1249.0	0.09
Geraniol	11.81	1803.7	13.08	8.32	1262.1	13.22
Geranial	10.27	1674.0	0.67	8.45	1270.5	0.80
Citronellyl formate	9.07*	1577.9	[7.29]	8.57	1278.7	7.21
Neryl formate	9.61*	1620.8	[0.31]	8.62	1281.9	0.08
Geranyl formate	10.06*	1657.3	[3.02]	8.94	1303.3	2.75
(3Z)-Hexenyl tiglate	9.55*	1616.0	[0.10]	9.10	1314.3	0.02
Methyl geranate	9.96*†	1649.3	[1.88]	9.25	1325.0	0.03
Citronellic acid	16.22*	2219.5	[0.14]	9.38	1334.0	0.07
$\alpha$ -Cubebene	6.96*	1419.1	[0.21]	9.56	1347.1	0.23
Phenylethyl propionate	12.06*	1825.1	[0.02]	9.59	1349.4	0.03
Citronellyl acetate	9.61*	1620.8	[0.31]	9.67	1355.1	0.25
Neryl acetate	10.41*†	1685.3	[0.34]	9.85	1367.2	0.05
$\alpha$ -Ylangene	7.22*	1437.9	[0.06]	9.87	1369.0	0.05
Geranic acid	17.02	2303.3	0.06	9.91*	1371.9	[0.55]
$\alpha$ -Copaene	7.32	1445.9	0.54	9.91*	1371.9	[0.55]
$\beta$ -Bourbonene	7.66	1470.7	1.10	10.02*	1379.8	[1.18]
1,5-diepi- $\beta$ - Bourbonene	7.55	1462.3	0.08	10.02*	1379.8	[1.18]
Geranyl acetate	10.72	1710.8	0.51	10.09	1384.6	0.47

β-Elemene	8.60*	1541.6	[1.32]	10.16	1389.2	0.08
Phenylethyl isobutyrate	11.97*	1817.1	[0.38]	10.20	1391.9	0.05
Isocaryophyllene	8.39*	1525.8	[0.02]	10.32	1400.7	0.03
α-Gurjunene	7.79	1480.2	0.08	10.37	1403.8	0.09
β-Caryophyllene	8.60*	1541.6	[1.32]	10.49	1412.9	1.37
Thymohydroquinone dimethyl ether	12.06*	1825.1	[0.02]	10.57	1419.1	0.01
β-Copaene	8.54	1537.2	0.13	10.63	1423.4	0.15
Heptyl tiglate				10.72	1430.5	0.01
Aromadendrene	8.74*	1552.3	[0.13]	10.75	1432.5	0.04
6,9-Guaiadiene	8.80*	1557.5	[0.34]	10.84*	1438.7	[0.42]
Isogermacrene D	9.15	1584.4	0.03	10.84*	1438.7	[0.42]
Citronellyl propionate	10.44*†	1687.6	[0.10]	10.91*	1444.2	[0.86]
Unknown BOCA IV [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]	8.97	1570.1	0.40	10.91*	1444.2	[0.86]
α-Humulene	9.47	1609.4	0.30	10.95	1447.0	0.31
allo-Aromadendrene	9.18	1586.9	0.32	11.04	1454.0	0.20
Unknown AMBA XXIX [m/z 161, 105 (68), 119 (54), 91 (52), 93 (41), 79 (39)... 204 (6)]				11.12	1459.9	0.07
<i>trans</i> -Cadina-1(6),4-diene	9.42	1605.9	0.24	11.24	1469.0	0.26
γ-Murolene	9.76*	1632.9	[0.31]	11.29	1472.5	0.10
Germacrene D	10.00*†	1652.0	[0.12]	11.33*	1475.2	[2.31]
Geranyl propionate	11.48	1775.2	0.66	11.33*	1475.2	[2.31]
α-Amorphene	9.76*	1632.9	[0.31]	11.33*	1475.2	[2.31]
β-Selinene	10.06*	1657.3	[3.02]	11.38	1479.5	0.17
Phenylethyl isovalerate	13.28	1934.5	0.05	11.45*	1484.7	[0.21]
γ-Amorphene	10.00*†	1652.0	[0.12]	11.45*	1484.7	[0.21]
Bicyclogermacrene	10.24	1671.6	0.49	11.53*	1490.3	[0.83]
α-Selinene	10.12*	1661.8	[0.22]	11.53*	1490.3	[0.83]
Viridiflorene	9.83	1638.4	0.26	11.53*	1490.3	[0.83]
α-Murolene	10.21	1669.6	0.17	11.61*	1496.0	[0.34]
4-epi- <i>cis</i> -Dihydroagarofuran	10.12*	1661.8	[0.22]	11.61*	1496.0	[0.34]
γ-Cadinene	10.57*	1698.2	[0.46]	11.77	1508.4	0.39
7-epi-α-Selinene	10.60*	1700.9	[0.90]	11.84	1513.7	0.09
Geranyl isobutyrate	11.42*	1770.2	[0.33]	11.89	1517.9	0.20
Zonarene	10.57*	1698.2	[0.46]	11.91*	1519.5	[1.13]
δ-Cadinene	10.60*	1700.9	[0.90]	11.91*	1519.5	[1.13]

<i>trans</i> -Calamenene	11.42*	1770.2	[0.33]	11.91*	1519.5	[1.13]
Citronellyl butyrate	11.31	1760.9	0.54	12.03*	1528.6	[0.64]
<i>trans</i> -Cadina-1,4-diene	10.84	1721.3	0.10	12.03*	1528.6	[0.64]
Phenylethyl angelate?	14.44	2042.8	0.11	12.08	1532.3	0.14
$\alpha$ -Agarofuran	11.97*	1817.1	[0.38]	12.12	1535.8	0.35
1-nor-Bourbonanone	13.61	1965.3	0.02	12.40	1558.2	0.04
Geranyl butyrate	12.34	1850.0	1.00	12.44	1560.8	1.00
Spathulenol	14.59*	2057.5	[1.32]	12.56	1570.6	0.24
Caryophyllene oxide	12.96	1904.9	0.24	12.60	1573.5	0.15
Globulol	14.08	2008.3	0.09	12.64	1576.8	0.09
Phenylethyl tiglate	15.19	2116.0	0.76	12.70	1580.9	0.76
Viridiflorol	14.16	2016.8	0.07	12.74	1584.4	0.07
Eudesm-5-en-11-ol analog	14.39	2038.6	0.04	12.87	1594.9	0.06
Geranyl 2-methylbutyrate?	12.40*	1855.5	[0.19]	12.94	1599.8	0.09
Geranyl isovalerate	12.40*	1855.5	[0.19]	12.97	1602.1	0.08
10-epi- $\gamma$ -Eudesmol	14.31	2030.9	4.27	13.09	1612.0	4.52
1-epi-Cubenol	13.95*	1996.4	[0.31]	13.20	1621.4	0.13
$\gamma$ -Eudesmol	15.09*	2106.1	[0.21]	13.24	1624.3	0.21
Unknown PEGR II [m/z 147, 162 (79), 43 (64), 59 (64), 95 (47), 91 (44), 105 (43)... 238 (13)]	15.46	2143.0	0.22	13.29	1629.0	0.19
Citronellyl valerate?	12.47	1861.1	0.04	13.33*	1631.7	[0.07]
Agarospinol?	15.36	2133.0	0.05	13.33*	1631.7	[0.07]
$\tau$ -Muurolol	15.22	2119.3	0.06	13.39*	1636.9	[0.57]
Cubenol	13.88	1990.0	0.17	13.39*	1636.9	[0.57]
$\tau$ -Cadinol	15.09*	2106.1	[0.21]	13.39*	1636.9	[0.57]
$\beta$ -Eudesmol	15.57	2154.1	0.24	13.45	1642.1	0.27
$\alpha$ -Eudesmol	15.53	2149.9	0.23	13.49	1645.4	0.28
$\alpha$ -Cadinol	15.63	2159.6	0.13	13.53	1648.5	0.15
Geranyl valerate	13.40	1945.7	0.16	13.62	1656.4	0.19
Citronellyl tiglate	13.55	1959.1	0.34	13.73	1664.9	0.34
Citronellyl 4-methylvalerate				13.96	1684.3	0.10
Geranyl tiglate	14.59*	2057.5	[1.32]	14.15*	1699.5	[1.07]
3 $\beta$ ,4 $\beta$ -Oxidoagarofuran?	16.22*	2219.5	[0.14]	14.15*	1699.5	[1.07]
Geranyl 4-methylvalerate?	13.95*	1996.4	[0.31]	14.35	1716.7	0.17
Citronellyl caproate	13.46	1951.4	0.05	14.38	1719.7	0.05
Geranyl caproate	14.50	2048.8	0.08	14.77	1753.1	0.10

Citronellyl heptanoate				15.49	1816.2	0.07
Phytone	14.90	2087.4	0.03	15.80	1844.2	0.04
Geranyl heptanoate	15.44	2141.2	0.09	15.87	1850.3	0.11
Unknown LAAN VII [m/z 69, 81 (44), 41 (28), 95 (26), 93 (26), 71 (24)...]	15.39	2136.4	0.02	16.52	1910.1	0.02
Citronellyl caprylate	15.51	2147.8	0.06	16.56	1914.0	0.04
Geranyl caprylate	15.79	2176.2	0.03	16.92	1947.9	0.05
Unknown COCI L [m/z 69, 83 (59), 81 (56), 137 (48), 41 (29), 139 (28)...]	21.89	2873.8	0.05	23.82	2708.2	0.06
Unknown CYWI III [m/z 69, 81 (84), 137 (53), 83 (30), 95 (27), 41 (19)...]	22.83	2996.7	0.05	24.28	2766.6	0.04
Total reported	96.19%			97.47%		

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

[xx]: Duplicate percentage due to coelutions, only the first one is 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