

Date : 2024-09-25

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 24111-PTH02

**Customer Identification :** Lemongrass - India - L80117R

**Type :** Essential Oil

**Source :** *Cymbopogon flexuosus*

**Customer :** Plant Therapy

Checked and approved by:

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

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

**Date :** 2024-09-25

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.4862 \pm 0.0003$  (20 °C)

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

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

**Date :** 2024-09-17

## 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
Isobutyral	tr	Aliphatic aldehyde
2-Methyl-3-buten-2-ol	0.03	Aliphatic alcohol
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	tr	Aliphatic aldehyde
Isoamyl alcohol	0.01	Aliphatic alcohol
Hexanal	0.01	Aliphatic aldehyde
Unknown	0.01	Unknown
(2E)-Hexenal	tr	Aliphatic aldehyde
(3Z)-Hexenal	0.01	Aliphatic alcohol
4-Heptanone	0.02	Aliphatic ketone
Unknown	tr	Unknown
Nonane	0.01	Alkane
Tricyclene	0.14	Monoterpene
$\alpha$ -Pinene	0.20	Monoterpene
Camphene	1.12	Monoterpene
Benzaldehyde	0.01	Simple phenolic
Sabinene	0.01	Monoterpene
$\beta$ -Pinene	0.01	Monoterpene
6-Methyl-5-hepten-2-one	1.08	Aliphatic ketone
Myrcene	0.07	Monoterpene
6-Methyl-5-hepten-2-ol	0.07	Aliphatic alcohol
$\alpha$ -Phellandrene	0.01	Monoterpene
Octanal	0.08	Aliphatic aldehyde
$\alpha$ -Terpinene	tr	Monoterpene
<i>para</i> -Cymene	0.01	Monoterpene
1,8-Cineole	0.04	Monoterpenic ether
Limonene	0.26	Monoterpene
Benzeneacetaldehyde	0.01	Simple phenolic
(Z)- $\beta$ -Ocimene	0.35	Monoterpene
(E)- $\beta$ -Ocimene	0.22	Monoterpene
2,6-Dimethyl-5-heptenal (melonal)	0.02	Aliphatic aldehyde
$\gamma$ -Terpinene	0.01	Monoterpene
<i>cis</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
4-Nonanone	0.86	Aliphatic ketone
Octanol	0.01	Aliphatic alcohol
Camphenilone	0.01	Normonoterpenic ketone
<i>trans</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
Terpinolene	0.05	Monoterpene
4-Nonanol	0.02	Aliphatic alcohol
Rosefuran	0.21	Monoterpenic ether

Linalool	1.00	Monoterpenic alcohol
<i>cis</i> -Chrysanthemal?	0.02	Monoterpenic aldehyde
( <i>Z</i> )-6-Methyl-3,5-heptadien-2-one	0.03	Aliphatic ketone
<i>trans-para</i> -Mentha-2,8-dien-1-ol	0.03	Monoterpenic alcohol
Unknown	0.15	Unknown
Unknown	0.01	Unknown
<i>exo</i> -Isocitral	0.04	Monoterpenic aldehyde
<i>trans</i> -Chrysanthemal	0.32	Monoterpenic aldehyde
Citronellal	0.20	Monoterpenic aldehyde
Borneol	0.18	Monoterpenic alcohol
Isoneral	0.51	Monoterpenic aldehyde
$\alpha$ -Phellandren-8-ol	0.13	Monoterpenic alcohol
Unknown	0.10	Oxygenated monoterpene
Rosefuran oxide	0.12	Monoterpenic ether
Terpinen-4-ol	0.08	Monoterpenic alcohol
Unknown	0.05	Unknown
Isogeranial	0.95	Monoterpenic aldehyde
$\alpha$ -Terpineol	0.16	Monoterpenic alcohol
Myrtenal	0.01	Monoterpenic aldehyde
Unknown	0.06	Unknown
Myrtenol	0.04	Monoterpenic alcohol
<i>trans</i> -Isopiperitenol	0.06	Monoterpenic alcohol
Unknown	0.05	Oxygenated monoterpene
Decanal	0.19	Aliphatic aldehyde
<i>cis</i> -Isopiperitenol	0.04	Monoterpenic alcohol
2,3-Epoxyneral?	0.04	Monoterpenic aldehyde
Nerol	0.02	Monoterpenic alcohol
Citronellol	0.14	Monoterpenic alcohol
Neral	32.62	Monoterpenic aldehyde
Piperitone	0.05	Monoterpenic ketone
Geraniol	4.53	Monoterpenic alcohol
Geranial	42.65	Monoterpenic aldehyde
Unknown	0.13	Oxygenated monoterpene
Geranyl formate	0.03	Monoterpenic ester
Methyl geranate	0.02	Monoterpenic ester
Unknown	0.01	Unknown
$\alpha$ -Cubebene	0.02	Sesquiterpene
Citronellyl acetate	0.04	Monoterpenic ester
Cyclosativene I	0.08	Sesquiterpene
Cyclosativene II	0.08	Sesquiterpene
$\alpha$ -Ylangene	0.05	Sesquiterpene
Geranic acid	0.15	Aliphatic acid
$\alpha$ -Copaene	0.02	Sesquiterpene
$\beta$ -Bourbonene	0.03	Sesquiterpene
Geranyl acetate	2.16	Monoterpenic ester

β-Cubebene	0.06	Sesquiterpene
β-Elemene	0.11	Sesquiterpene
Longifolene	0.02	Sesquiterpene
β-Caryophyllene	1.55	Sesquiterpene
β-Ylangene	0.04	Sesquiterpene
β-Copaene	0.03	Sesquiterpene
<i>trans</i> -α-Bergamotene	0.02	Sesquiterpene
6,9-Guaiadiene	0.02	Sesquiterpene
( <i>E</i> )-Isoeugenol	0.54	Phenylpropanoid
α-Humulene	0.14	Sesquiterpene
<i>cis</i> -Muurolo-4(15),5-diene	0.04	Sesquiterpene
<i>trans</i> -Cadina-1(6),4-diene	0.04	Sesquiterpene
Germacrene D	0.23	Sesquiterpene
γ-Amorphene	0.03	Sesquiterpene
epi-Cubebol	0.11	Sesquiterpenic alcohol
α-Muurolole	0.05	Sesquiterpene
δ-Amorphene	0.03	Sesquiterpene
γ-Cadinene	1.21	Sesquiterpene
Cubebol	0.23	Sesquiterpenic alcohol
δ-Cadinene	0.28	Sesquiterpene
( <i>E</i> )-γ-Bisabolene	0.17	Sesquiterpene
α-Cadinene	0.07	Sesquiterpene
Neryl butyrate	0.04	Monoterpenic ester
( <i>E</i> )-α-Bisabolene	0.01	Sesquiterpene
α-Elemol	0.07	Sesquiterpenic alcohol
Germacrene B	0.05	Sesquiterpene
Geranyl butyrate	0.15	Monoterpenic ester
Caryophyllene oxide isomer	0.06	Sesquiterpenic ether
Caryophyllene oxide	0.39	Sesquiterpenic ether
Humulene epoxide II	0.04	Sesquiterpenic ether
Selin-6-en-4α-ol isomer	0.02	Sesquiterpenic alcohol
1-epi-Cubebol	0.03	Sesquiterpenic alcohol
Cubebol	0.03	Sesquiterpenic alcohol
α-Eudesmol	0.01	Sesquiterpenic alcohol
(2 <i>Z</i> ,6 <i>Z</i> )-Farnesol	0.01	Sesquiterpenic alcohol
Farnesal isomer	0.02	Sesquiterpenic aldehyde
(2 <i>E</i> ,6 <i>E</i> )-Farnesal	0.02	Sesquiterpenic aldehyde
Phytone	0.02	Terpenic ketone
Geranyl caprylate	0.01	Monoterpenic ester
Unknown	0.02	Unknown
Unknown	0.04	Unknown
Unknown	0.04	Unknown
Dicitral	0.04	Diterpenic aldehyde
Phytol isomer I	0.01	Diterpenic alcohol
Unknown	0.03	Unknown

<b>Consolidated total</b>	<b>98.60</b>
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tr: The compound has been detected below 0.005% of the total signal

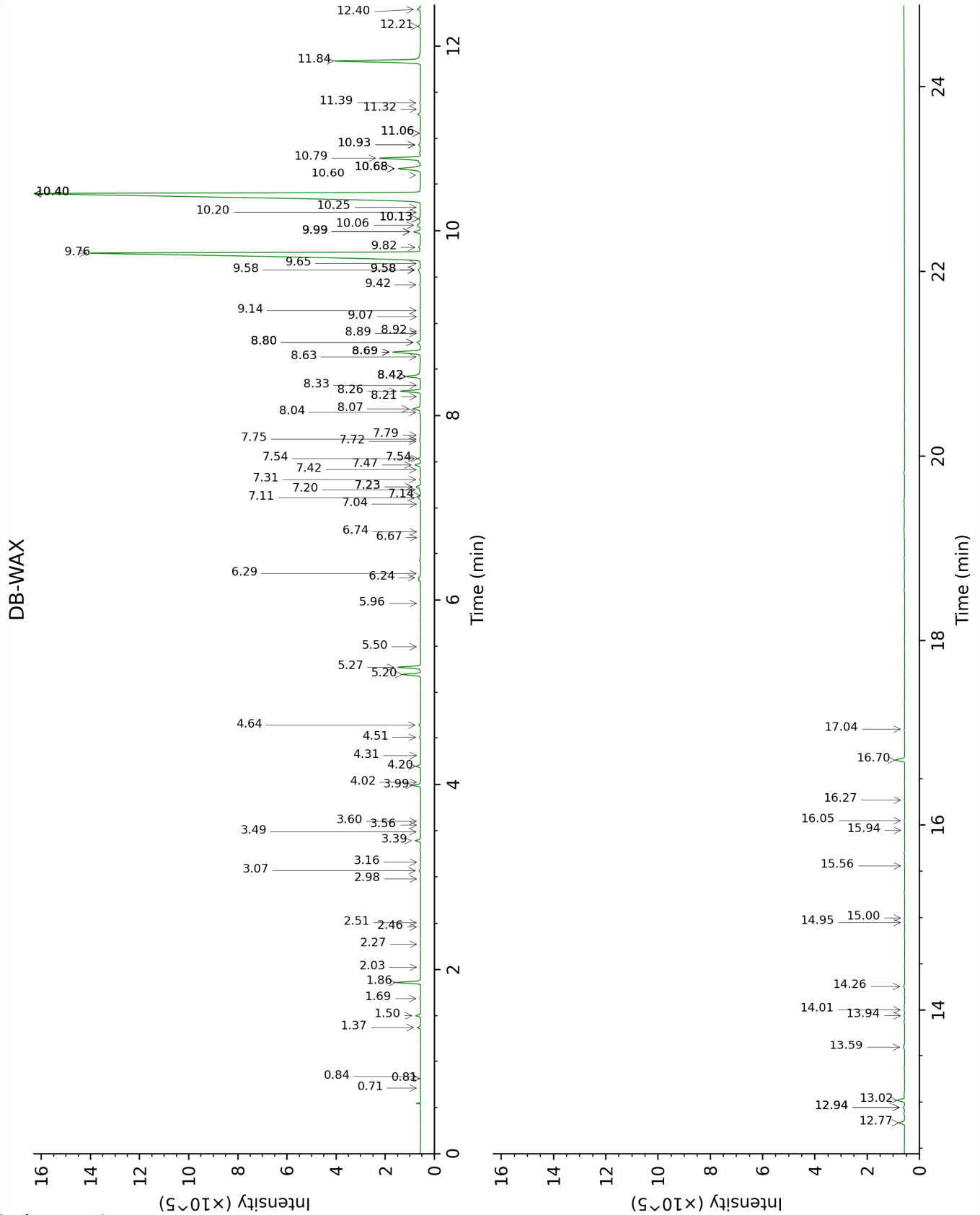
Note: no correction factor was applied

**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.

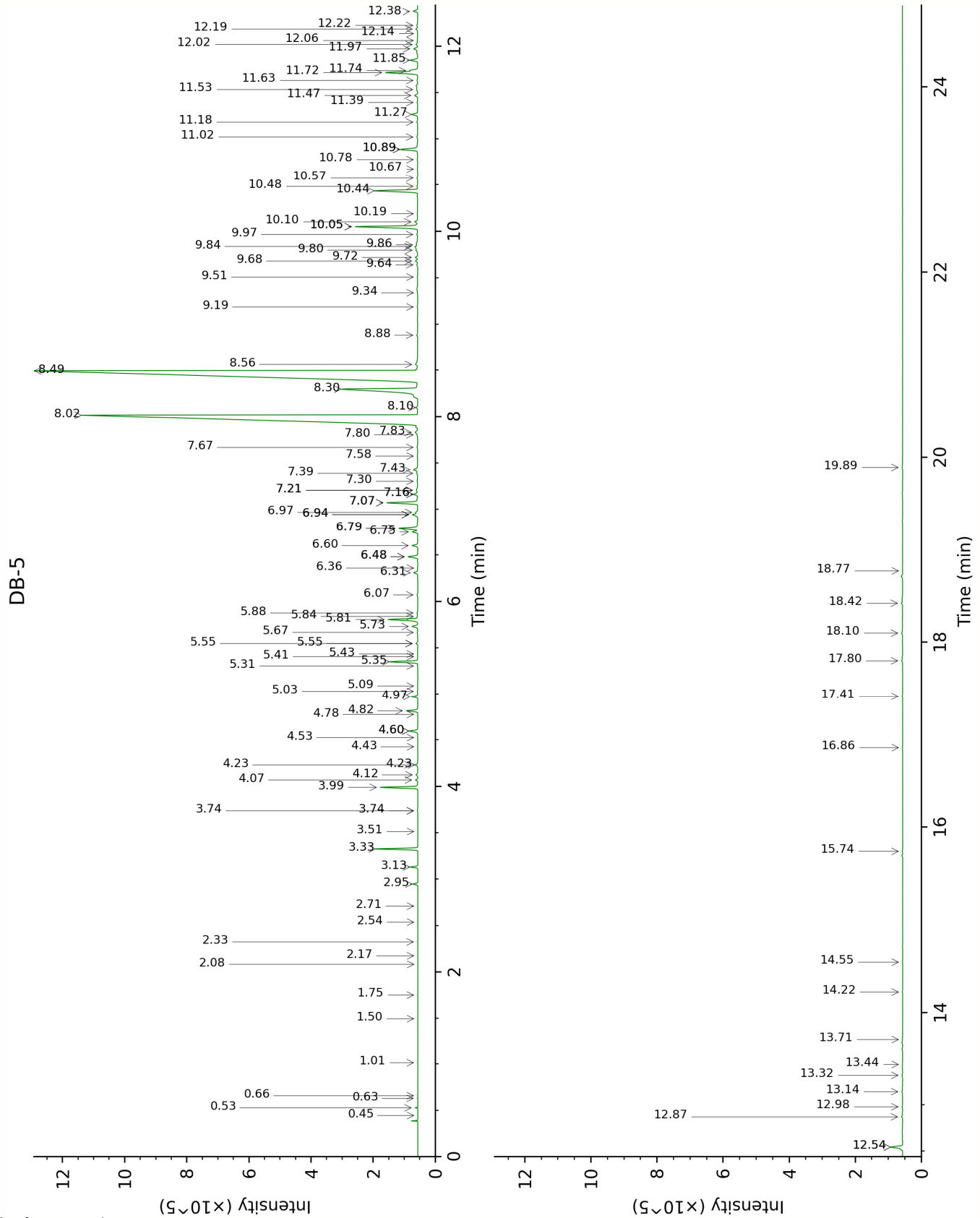
**Unknowns:** Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

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

This page was intentionally left blank. The following pages present the complete data of the analysis.







FULL ANALYSIS DATA

Isobutyral	Column DB-WAX			Column DB-5		
				0.44	536.6	tr
2-Methyl-3-buten-2-ol	1.69	1012.7	0.03	0.53	605.3	0.03
Isovaleral	0.84	885.1	0.01	0.63	640.6	0.01
2-Methylbutyral	0.82	877.6	tr	0.66	650.7	tr
Isoamyl alcohol	3.60	1174.7	0.02	1.02	732.2	0.01
Hexanal	2.03	1045.0	0.01	1.50	799.8	0.01
Unknown PEGR III [m/z 81, 69 (80), 41 (65), 83 (52), 109 (48), 55 (47)...]	0.71	842.2	0.01	1.75	822.5	0.01
(2E)-Hexenal	3.56	1171.7	tr	2.08	850.0	tr
(3Z)-Hexenol	5.96	1344.9	0.01	2.18	857.6	0.01
4-Heptanone	2.51	1090.7	0.02	2.32	870.1	0.02
Unknown CULE I [m/z 69, 41 (57), 81 (57), 80 (18), 79 (18), 67 (17)...]				2.54	887.7	tr
Nonane				2.71	902.0	0.01
Tricyclene	1.37	974.2	0.14	2.95	918.0	0.14
$\alpha$ -Pinene	1.50	993.9	0.20	3.13	930.2	0.20
Camphene	1.86	1029.2	1.13	3.33	943.1	1.12
Benzaldehyde	7.54*	1459.5	[0.12]	3.51	955.5	0.01
Sabinene	2.46	1086.3	0.01	3.74*	970.3	[0.02]
$\beta$ -Pinene	2.27	1068.5	0.01	3.74*	970.3	[0.02]
6-Methyl-5-hepten-2-one	5.27	1293.0	1.10	3.99	987.0	1.08
Myrcene	3.07	1134.5	0.07	4.07	992.2	0.07
6-Methyl-5-hepten-2-ol	7.20	1434.7	0.07	4.12	995.9	0.07
$\alpha$ -Phellandrene	2.98	1127.7	0.01	4.23*	1003.0	[0.10]
Octanal	4.64	1249.0	0.08	4.23*	1003.0	[0.10]
$\alpha$ -Terpinene	3.16	1141.4	tr	4.43	1015.3	tr
<i>para</i> -Cymene	4.31	1225.9	0.01	4.53	1021.5	0.01
1,8-Cineole	3.49	1166.1	0.04	4.60*	1025.9	[0.29]
Limonene	3.39	1158.9	0.26	4.60*	1025.9	[0.29]
Benzeneacetaldehyde	9.08	1576.9	0.01	4.78	1037.2	0.01
(Z)- $\beta$ -Ocimene	3.99	1203.4	0.35	4.82	1039.6	0.35
(E)- $\beta$ -Ocimene	4.20	1217.8	0.22	4.97	1049.4	0.22
2,6-Dimethyl-5-heptenal (melonal)	5.50	1311.4	0.02	5.03	1053.1	0.02
$\gamma$ -Terpinene	4.02	1205.7	0.01	5.09	1056.7	0.01
<i>cis</i> -Linalool oxide (fur.)	6.74	1400.4	0.02	5.31	1070.3	0.01

4-Nonanone	5.20	1287.6	0.89	5.35	1073.2	0.86
Octanol	8.42*	1526.5	[0.99]	5.41	1076.6	0.01
Camphenilone	6.67	1395.7	0.01	5.44	1078.4	0.01
<i>trans</i> -Linalool oxide (fur.)	7.14	1430.2	0.01	5.55*	1085.5	[0.06]
Terpinolene	4.51	1239.7	0.05	5.55*	1085.5	[0.06]
4-Nonanol				5.67	1093.0	0.02
Rosefuran	6.24†	1364.8	0.11	5.73	1097.0	0.21
Linalool	8.26	1514.2	1.00	5.81	1101.7	1.00
<i>cis</i> -Chrysanthemal?	6.29	1368.0	0.03	5.84	1103.8	0.02
( <i>Z</i> )-6-Methyl-3,5-heptadien-2-one	8.42*	1526.5	[0.99]	5.88	1106.2	0.03
<i>trans-para</i> -Mentha-2,8-dien-1-ol	9.14	1582.0	0.03	6.07	1118.7	0.03
Unknown CYFL III [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	7.11	1428.2	0.15	6.31	1133.8	0.15
Unknown CYFL IV [m/z 95, 67 (86), 41 (68), 82 (64), 123 (62)...]	7.79	1478.3	0.03	6.36	1137.1	0.01
exo-Isocitral	7.75	1475.1	0.04	6.48*	1144.9	[0.35]
<i>trans</i> -Chrysanthemal	7.47	1454.5	0.32	6.48*	1144.9	[0.35]
Citronellal	7.23*	1436.9	[0.25]	6.60	1152.6	0.20
Borneol	9.99*	1650.0	[0.37]	6.75	1162.1	0.18
Isoneral	8.07	1499.4	0.51	6.79*	1164.5	[0.63]
$\alpha$ -Phellandren-8-ol	10.40*	1683.2	[42.96]	6.79*	1164.5	[0.63]
Unknown CYFL V [m/z 84, 83 (74), 137 (56), 41 (47), 93 (43), 108 (40)... 152 (2)]	9.82	1636.4	0.10	6.94*	1174.4	[0.22]
Rosefuran oxide	8.80*	1555.6	[0.22]	6.94*	1174.4	[0.22]
Terpinen-4-ol	8.80*	1555.6	[0.22]	6.97	1175.9	0.08
Unknown CYFL XIV [m/z 69, 41 (65), 109 (36), 67 (16), 84 (11), 43 (10), 55 (9)...]				7.07*	1182.6	[1.01]
Isogeranial	8.42*	1526.5	[0.99]	7.07*	1182.6	[1.01]
$\alpha$ -Terpineol	9.99*	1650.0	[0.37]	7.16*	1188.4	[0.17]
Myrtenal	8.92	1564.9	0.01	7.16*	1188.4	[0.17]
Unknown DRMO III [m/z 43, 81 (47), 67 (45), 69 944), 41 (42), 59 (40), 55 (39)...]	9.42	1603.8	0.06	7.21*	1191.1	[0.10]

Myrtenol	11.06*	1738.4	[0.04]	7.21*	1191.1	[0.10]
<i>trans</i> -Isopiperitenol	10.60	1699.8	0.02	7.30	1197.3	0.06
Unknown CYFL VI [m/z 84, 41 (83), 83 (79), 91 (76), 93 (67), 119 (64), 137 (63), 109 (54), 108 (54)... 152 (4)]	10.40*	1683.2	[42.96]	7.39	1202.9	0.05
Decanal	7.54*	1459.5	[0.12]	7.43	1205.5	0.19
<i>cis</i> -Isopiperitenol				7.58	1215.2	0.04
2,3-Epoxyneral?				7.67	1221.5	0.04
Nerol	11.32	1760.2	0.02	7.80	1230.6	0.02
Citronellol	10.93*	1727.8	[0.11]	7.83	1232.4	0.14
Neral	9.76	1631.4	32.76	8.02	1244.7	32.62
Piperitone	10.13*	1661.2	[0.10]	8.10	1250.2	0.05
Geraniol	11.84	1804.8	4.99	8.30	1263.5	4.53
Geranial	10.40*	1683.2	[42.96]	8.49	1276.7	42.65
Unknown CYFL VII [m/z 43, 69 (77), 41 (70), 109 (54)... 152 (6)]				8.56	1281.4	0.13
Geranyl formate	10.13*	1661.2	[0.10]	8.88	1302.9	0.03
Methyl geranate	9.99*	1650.0	[0.37]	9.19	1324.3	0.02
Unknown CYFL VIII [m/z 82, 59 (44), 41 (43), 95 (31), 43 (29), 81 (24)...]	12.94*	1902.6	[0.07]	9.34	1335.0	0.01
$\alpha$ -Cubebene	7.04	1423.1	0.01	9.51	1346.9	0.02
Citronellyl acetate	9.65	1622.3	0.03	9.64	1356.2	0.04
Cyclosativene I				9.68	1359.1	0.08
Cyclosativene II	7.23*	1436.9	[0.25]	9.72	1361.8	0.08
$\alpha$ -Ylangene	7.31	1442.8	0.05	9.80*†	1367.2	[0.06]
Geranic acid				9.84*†	1370.1	[0.14]
$\alpha$ -Copaene	7.42	1450.7	0.02	9.86	1371.3	0.02
$\beta$ -Bourbonene	7.72	1473.3	0.04	9.97	1379.1	0.03
Geranyl acetate	10.79	1715.6	2.16	10.05*	1385.1	[2.16]
$\beta$ -Cubebene	8.04	1496.7	0.06	10.05*	1385.1	[2.16]
$\beta$ -Elemene	8.69*	1546.9	[1.64]	10.10	1388.7	0.11
Longifolene	8.21	1509.7	0.01	10.19	1394.8	0.02
$\beta$ -Caryophyllene	8.69*	1546.9	[1.64]	10.44	1412.7	1.55
$\beta$ -Ylangene	8.33	1519.1	0.03	10.48	1416.3	0.04
$\beta$ -Copaene	8.63	1542.8	0.05	10.57	1423.1	0.03
<i>trans</i> - $\alpha$ -Bergamotene	8.69*	1546.9	[1.64]	10.67	1430.5	0.02
6,9-Guaiadiene	8.90	1563.0	0.02	10.78	1438.2	0.02
( <i>E</i> )-Isoeugenol	16.70	2269.5	0.54	10.89*	1446.4	[0.68]

$\alpha$ -Humulene	9.58*	1616.7	[0.20]	10.89*	1446.4	[0.68]
<i>cis</i> -Muurolo-4(15),5-diene	9.58*	1616.7	[0.20]	11.02	1456.4	0.04
<i>trans</i> -Cadina-1(6),4-diene	9.58*	1616.7	[0.20]	11.18	1468.3	0.04
Germacrene D	10.06	1655.6	0.24	11.26	1474.5	0.23
$\gamma$ -Amorphene				11.39	1484.1	0.03
epi-Cubebol	12.21	1837.9	0.11	11.47	1489.7	0.11
$\alpha$ -Muurolole	10.25	1671.1	0.03	11.53	1494.5	0.05
$\delta$ -Amorphene	10.20	1666.8	0.02	11.63	1501.8	0.03
$\gamma$ -Cadinene	10.68*	1706.0	[1.46]	11.72	1508.4	1.21
Cubebol	12.77	1887.4	0.29	11.74	1510.0	0.23
$\delta$ -Cadinene	10.68*	1706.0	[1.46]	11.85	1518.8	0.28
( <i>E</i> )- $\gamma$ -Bisabolene	10.68*	1706.0	[1.46]	11.97	1528.5	0.17
$\alpha$ -Cadinene	11.06*	1738.4	[0.04]	12.02	1532.1	0.07
Neryl butyrate				12.06	1535.5	0.04
( <i>E</i> )- $\alpha$ -Bisabolene	10.93*	1727.8	[0.11]	12.14	1541.3	0.01
$\alpha$ -Elemol	14.26	2025.2	0.07	12.18	1545.2	0.07
Germacrene B	11.39	1766.1	0.07	12.22	1548.3	0.05
Geranyl butyrate	12.40	1854.2	0.18	12.38	1560.4	0.15
Caryophyllene oxide isomer	12.94*	1902.6	[0.07]	12.54*	1573.3	[0.45]
Caryophyllene oxide	13.02	1909.8	0.39	12.54*	1573.3	[0.45]
Humulene epoxide II	13.59	1962.6	0.09	12.87	1599.0	0.04
Selin-6-en-4 $\alpha$ -ol isomer	15.00	2096.5	0.01	12.98	1607.7	0.02
1-epi-Cubebol	14.00	2000.9	0.04	13.14	1621.2	0.03
Cubebol	13.94	1994.8	0.03	13.32	1635.8	0.03
$\alpha$ -Eudesmol	15.56	2152.5	0.01	13.44	1645.4	0.01
(2 <i>Z</i> ,6 <i>Z</i> )-Farnesol	16.27	2224.8	0.01	13.71	1668.3	0.01
Farnesal isomer				14.22	1711.0	0.02
(2 <i>E</i> ,6 <i>E</i> )-Farnesal	16.05	2201.7	0.02	14.55	1738.9	0.02
Phytone	14.95	2091.5	0.02	15.74	1844.4	0.02
Geranyl caprylate	15.94	2190.8	0.01	16.86	1947.9	0.01
Unknown LICU V [m/z 41, 69 (95), 109 (41), 95 (39), 55 (36), 121 (36)...]				17.41	2000.8	0.02
Unknown LICU VII [m/z 69, 41 (94), 81 (42), 109 (39), 107 (33), 43 (31)...]				17.80	2039.2	0.04
Unknown CYFL IX [m/z 93, 69 (95), 135 (76), 107 (53), 41 (53),				18.10	2068.8	0.04

109 (50)... 235 (10)...						
Dicitral	17.04	2304.8	0.02	18.42	2100.8	0.04
Phytol isomer I				18.77	2136.9	0.01
Unknown CYFL XII [m/z 123, 94 (100), 43 (86), 69 (75), 95 (47), 41 (47), 93 (45)...				19.89	2255.2	0.03
Total reported	98.32%			98.52%		

\*: 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