

Date : 2024-01-30

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 24A23-PTH02

**Customer Identification :** Thyme (Thymol / Red) - Hungary - T40112R

**Type :** Essential Oil

**Source :** *Thymus vulgaris*

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

**Date :** 2024-01-26

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.496 \pm 0.0003$  (20 °C)

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

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

**Date :** 2024-01-24

## 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
Isovaleral	0.01	Aliphatic aldehyde
2-Methylbutyral	0.01	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	tr	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Methyl 2-methylbutyrate	0.06	Aliphatic ester
(3Z)-Hexenol	0.01	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
Hashishene	0.01	Monoterpene
Tricyclene	0.03	Monoterpene
$\alpha$ -Thujene	1.15	Monoterpene
$\alpha$ -Pinene	2.00	Monoterpene
$\beta$ -Fenchene	0.01	Monoterpene
Unknown	0.04	Monoterpene
$\alpha$ -Fenchene	tr	Monoterpene
Camphene	0.64	Monoterpene
Thuja-2,4(10)-diene	0.02	Monoterpene
$\beta$ -Pinene	1.89	Monoterpene
Sabinene	0.04	Monoterpene
Unknown	0.05	Monoterpene
Octen-3-ol	0.31	Aliphatic alcohol
Octan-3-one	0.05	Aliphatic ketone
Myrcene	2.43	Monoterpene
Octan-3-ol	0.04	Aliphatic alcohol
Pseudolimonene	0.10	Monoterpene
$\alpha$ -Phellandrene	0.10	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.01	Monoterpenic ether
$\Delta^3$ -Carene	0.07	Monoterpene
$\alpha$ -Terpinene	1.68	Monoterpene
<i>para</i> -Cymene	23.36	Monoterpene
1,8-Cineole	0.31	Monoterpenic ether
Limonene	1.98	Monoterpene
$\beta$ -Phellandrene	0.11	Monoterpene
(Z)- $\beta$ -Ocimene	0.02	Monoterpene
(E)- $\beta$ -Ocimene	0.14	Monoterpene
$\gamma$ -Terpinene	11.74	Monoterpene
<i>cis</i> -Sabinene hydrate	0.08	Monoterpenic alcohol
3-Methyl-3-butenyl butyrate?	0.06	Aliphatic ester
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol

Octanol	0.01	Aliphatic alcohol
Fenchone	0.03	Monoterpenic ketone
Terpinolene	0.11	Monoterpene
<i>para</i> -Cymenene	0.11	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.03	Monoterpenic alcohol
<i>trans</i> -Sabinene hydrate	0.03	Monoterpenic alcohol
Linalool	4.58	Monoterpenic alcohol
Hotrienol	0.01	Monoterpenic alcohol
Nonanal	0.01	Aliphatic aldehyde
endo-Fenchol	0.04	Monoterpenic alcohol
Unknown	0.03	Unknown
<i>trans</i> -Pinocarveol	0.01	Monoterpenic alcohol
Unknown	0.02	Unknown
<i>trans-para</i> -Menth-2-en-1-ol	0.02	Monoterpenic alcohol
Camphor	0.15	Monoterpenic ketone
Camphene hydrate	0.01	Monoterpenic alcohol
Menthone	0.16	Monoterpenic ketone
Isoborneol	0.02	Monoterpenic alcohol
Unknown	0.03	Unknown
Borneol	1.07	Monoterpenic alcohol
Lavandulol	0.02	Monoterpenic alcohol
Terpinen-4-ol	1.95	Monoterpenic alcohol
<i>meta</i> -Cymen-8-ol	0.01	Monoterpenic alcohol
<i>para</i> -Cymen-8-ol	0.03	Monoterpenic alcohol
Unknown	0.03	Unknown
$\alpha$ -Terpineol	0.08	Monoterpenic alcohol
<i>cis</i> -Dihydrocarvone	0.09	Monoterpenic ketone
<i>cis</i> -Piperitol	0.04	Monoterpenic alcohol
<i>trans</i> -Dihydrocarvone	0.01	Monoterpenic ketone
Bornyl formate	0.01	Monoterpenic ester
Thymol methyl ether	0.26	Monoterpenic ether
Neral	0.01	Monoterpenic aldehyde
Carvacrol methyl ether	0.62	Monoterpenic ether
Geraniol	0.06	Monoterpenic alcohol
Geranial	0.01	Monoterpenic aldehyde
Decanol	0.02	Aliphatic alcohol
Bornyl acetate	0.05	Monoterpenic ester
Thymol analogue I (isothymol?)	0.13	Monoterpenic alcohol
Thymol	32.33	Monoterpenic alcohol
Carvacrol	2.81	Monoterpenic alcohol
$\alpha$ -Terpinyl acetate	0.02	Monoterpenic ester
Thymyl acetate	0.02	Monoterpenic ester
$\alpha$ -Copaene	0.06	Sesquiterpene
$\beta$ -Bourbonene	0.05	Sesquiterpene
Geranyl acetate	0.02	Monoterpenic ester

Unknown	0.01	Unknown
Isocaryophyllene	0.01	Sesquiterpene
$\alpha$ -Gurjunene	0.01	Sesquiterpene
$\beta$ -Caryophyllene	2.45	Sesquiterpene
Aromadendrene	0.08	Sesquiterpene
Unknown	0.01	Unknown
$\alpha$ -Humulene	0.07	Sesquiterpene
allo-Aromadendrene	0.01	Sesquiterpene
Thymohydroquinone isomer?	0.01	Simple phenolic
( <i>E</i> )- $\beta$ -Farnesene	0.14	Sesquiterpene
$\gamma$ -Murolene	0.10	Sesquiterpene
Germacrene D	0.41	Sesquiterpene
allo-Aromadendr-9-ene	0.01	Sesquiterpene
$\beta$ -Selinene	0.03	Sesquiterpene
Viridiflorene	0.01	Sesquiterpene
$\beta$ -Himachalene	0.03	Sesquiterpene
Bicyclogermacrene	0.03	Sesquiterpene
$\alpha$ -Murolene	0.05	Sesquiterpene
$\beta$ -Bisabolene	0.03	Sesquiterpene
$\gamma$ -Cadinene	0.14	Sesquiterpene
Cubebol	0.01	Sesquiterpenic alcohol
$\delta$ -Cadinene	0.19	Sesquiterpene
<i>trans</i> -Calamenene	0.01	Sesquiterpene
<i>trans</i> -Cadina-1,4-diene	0.02	Sesquiterpene
$\alpha$ -Cadinene	0.02	Sesquiterpene
Geranyl butyrate	0.01	Monoterpenic ester
Caryophyllene oxide isomer	0.02	Sesquiterpenic ether
Caryophyllene oxide	0.27	Sesquiterpenic ether
Unknown	0.01	Oxygenated sesquiterpene
Humulene epoxide II	0.01	Sesquiterpenic ether
10-epi- $\gamma$ -Eudesmol	0.03	Sesquiterpenic alcohol
1-epi-Cubebol	0.01	Sesquiterpenic alcohol
Caryophylladienol II	0.02	Sesquiterpenic alcohol
Isospathulenol	0.01	Sesquiterpenic alcohol
$\tau$ -Cadinol	0.08	Sesquiterpenic alcohol
$\alpha$ -Cadinol	0.01	Sesquiterpenic alcohol
(3 <i>Z</i> )-Caryophylla-3,8(13)-dien-5 $\beta$ -ol	0.02	Sesquiterpenic alcohol
Shyobunol	0.01	Sesquiterpenic alcohol
Unknown	0.01	Unknown
Unknown	0.03	Unknown
Unknown	0.04	Unknown
<i>meta</i> -Camphorene	0.06	Diterpene
Unknown	0.02	Unknown
Unknown	0.04	Unknown
Unknown	0.01	Unknown

Unknown	0.01	Unknown
Unknown	0.02	Unknown
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Unknown	0.02	Unknown
Unknown	0.01	Unknown
<b>Consolidated total</b>	<b>98.51</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.

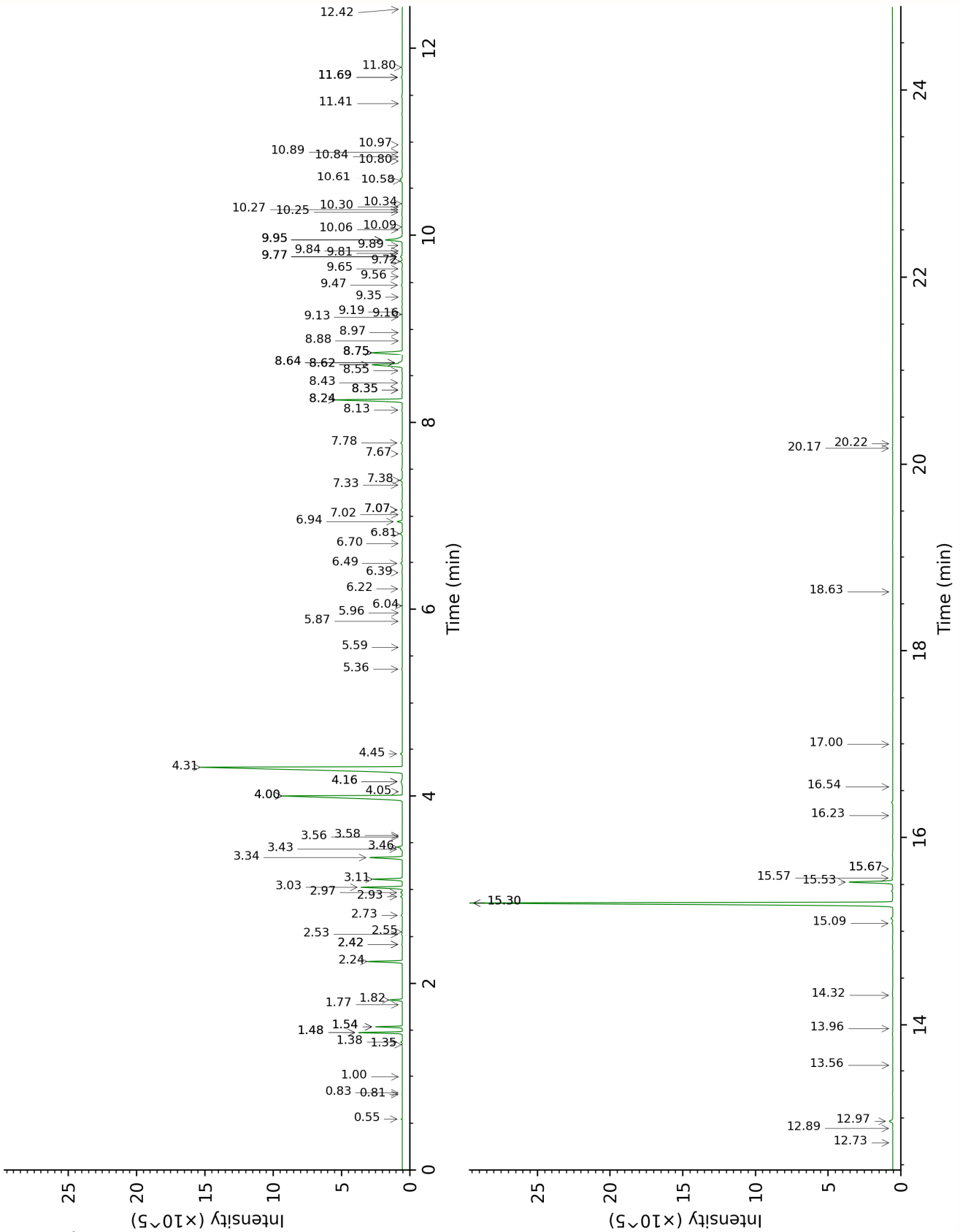
**Unknowns:** Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

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

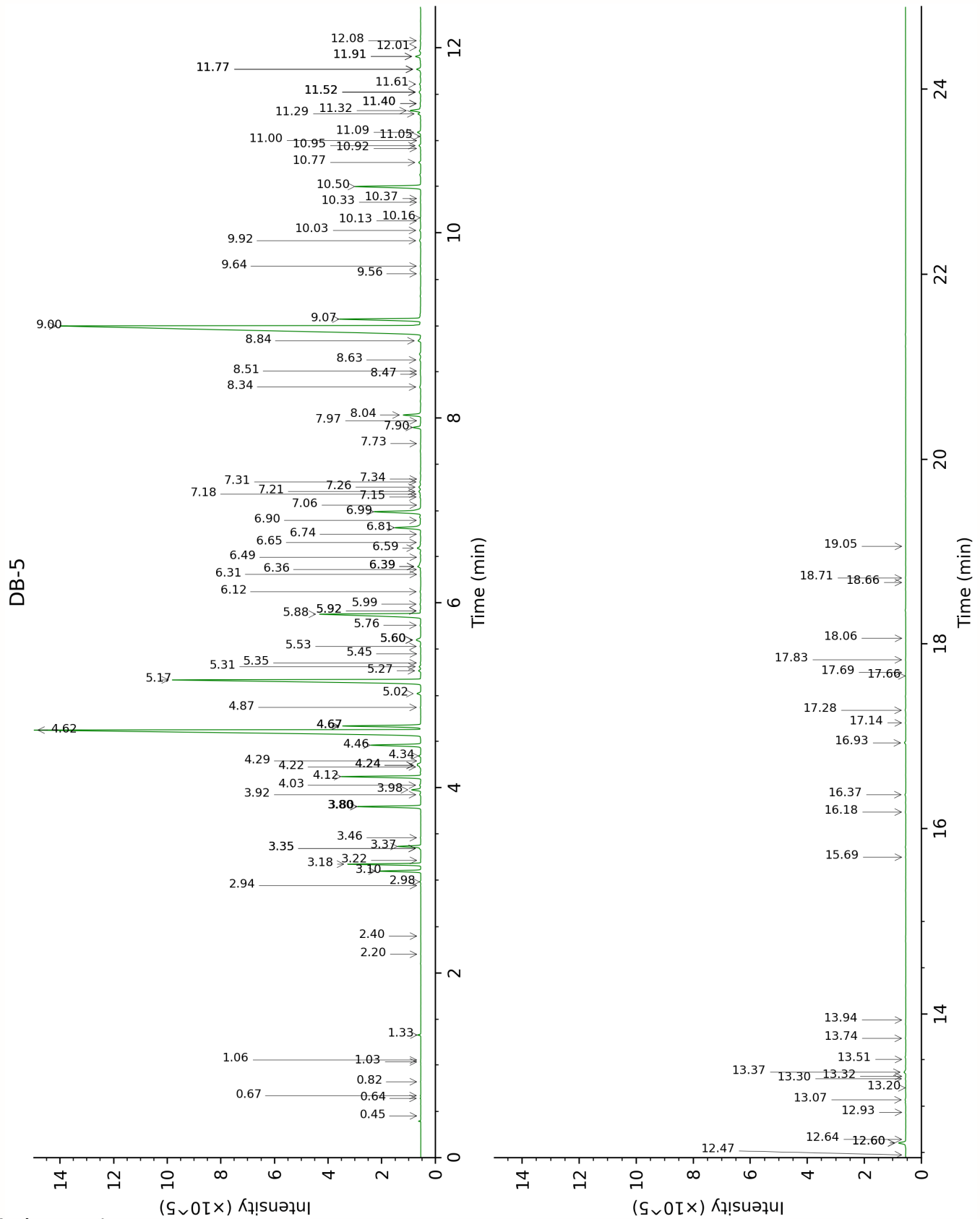
This page was intentionally left blank. The following pages present the complete data of the analysis.

Thyme (Thymol / Red) - Hungary - T40112R

DB-WAX







FULL ANALYSIS DATA

Isobutyral	Column DB-WAX			Column DB-5		
	0.54	774.7	0.03	0.45	536.3	tr
Isovaleral	0.83	883.2	0.01	0.64	640.7	0.01
2-Methylbutyral	0.81	877.1	0.01	0.67	650.8	0.01
2-Ethylfuran	1.00	918.5	tr	0.82	700.9	tr
Isoamyl alcohol	3.58	1174.3	0.01	1.04	732.9	tr
2-Methylbutanol	3.56	1173.0	0.01	1.06	735.7	tr
Methyl 2-methylbutyrate	1.38	975.5	0.06	1.33	773.9	0.06
(3Z)-Hexenol	5.96	1347.0	0.01	2.20	857.9	0.01
Hexanol	5.60	1320.8	0.02	2.40	874.0	0.01
Hashishene	1.48*	991.0	[2.01]	2.94	915.9	0.01
Tricyclene	1.35	971.5	0.02	2.98	918.6	0.03
$\alpha$ -Thujene	1.54*	1000.0	[1.15]	3.10	926.2	1.15
$\alpha$ -Pinene	1.48*	991.0	[2.01]	3.18	931.1	2.00
$\beta$ -Fenchene	1.54*	1000.0	[1.15]	3.22	933.8	0.01
Unknown SAOF I [m/z 91, 92 (47), 65 (11)... 134 (1)]	2.53	1093.2	0.04	3.34*†	942.3	[0.03]
$\alpha$ -Fenchene	1.77	1022.3	tr	3.34*†	942.3	[0.03]
Camphene	1.82	1027.1	0.64	3.37*†	943.7	[0.66]
Thuja-2,4(10)-diene	2.42*	1083.0	[0.04]	3.46	949.9	0.02
$\beta$ -Pinene	2.24	1065.8	1.89	3.80*	972.0	[1.92]
Sabinene	2.42*	1083.0	[0.04]	3.80*	972.0	[1.92]
Unknown ORVU I [m/z 93, 79 (73), 67 (49), 95 (42), 91 (41), 121 (38)...]	2.55	1095.6	0.02	3.92	980.4	0.05
Octen-3-ol	6.94	1417.7	0.32	3.98	983.9	0.31
Octan-3-one	4.16*	1216.7	[0.18]	4.03	987.2	0.05
Myrcene	3.03	1132.4	2.43	4.12	993.3	2.43
Octan-3-ol	6.22	1365.3	0.04	4.22*†	1000.1	[0.03]
Pseudolimonene	2.97	1128.1	0.10	4.24*†	1001.3	[0.11]
$\alpha$ -Phellandrene	2.93	1124.8	0.10	4.24*†	1001.3	[0.11]
<i>cis</i> - Dehydroxylinalool oxide	4.05	1209.1	0.01	4.29	1004.4	0.01
$\Delta^3$ -Carene	2.73	1109.6	0.07	4.34	1007.8	0.07
$\alpha$ -Terpinene	3.11	1138.9	1.67	4.46	1015.0	1.68
<i>para</i> -Cymene	4.31	1227.5	23.34	4.62	1025.2	23.36
1,8-Cineole	3.46	1164.9	0.31	4.67*	1027.9	[2.43]
Limonene	3.34	1156.4	1.98	4.67*	1027.9	[2.43]
$\beta$ -Phellandrene	3.43	1163.2	0.11	4.67*	1027.9	[2.43]
(Z)- $\beta$ -Ocimene	4.00*	1205.8	[11.73]	4.87	1040.5	0.02

(E)-β-Ocimene	4.16*	1216.7	[0.18]	5.02	1050.2	0.14
γ-Terpinene	4.00*	1205.8	[11.73]	5.17	1059.5	11.74
cis-Sabinene hydrate	7.07*	1427.0	[0.10]	5.27	1065.7	0.08
3-Methyl-3-butenyl butyrate?	5.36	1304.1	0.04	5.31	1068.4	0.06
cis-Linalool oxide (fur.)	6.70	1399.9	0.03	5.35	1071.0	0.02
Octanol	8.35*	1522.5	[0.04]	5.45	1077.1	0.01
Fenchone	5.87	1340.6	0.02	5.53	1082.1	0.03
Terpinolene	4.45	1237.7	0.11	5.60*	1086.4	[0.23]
para-Cymenene	6.49	1384.8	0.11	5.60*	1086.4	[0.23]
trans-Linalool oxide (fur.)	7.07*	1427.0	[0.10]	5.60*	1086.4	[0.23]
trans-Sabinene hydrate	8.13	1506.0	0.04	5.76	1096.3	0.03
Linalool	8.24*	1514.4	[4.58]	5.88	1103.8	4.58
Hotrienol	8.97	1570.2	0.01	5.92*	1106.0	[0.03]
Nonanal	6.04	1352.4	0.01	5.92*	1106.0	[0.03]
endo-Fenchol	8.55	1538.4	0.04	5.99	1110.7	0.04
Unknown CYFL II [m/z 81, 79 (19), 41 (12), 92 (8), 77 (8)...]	6.39	1377.7	0.04	6.12	1119.2	0.03
trans-Pinocarveol	9.34	1599.4	0.01	6.31	1131.1	0.01
Unknown CYFL III [m/z 81, 70 (98), 67 (63), 82 (53), 41 (46), 69 (46), 109 (43)...]	7.02	1423.2	0.02	6.36	1134.5	0.02
trans-para-Menth-2-en-1-ol	9.19	1587.1	0.02	6.39*	1136.5	[0.19]
Camphor	7.38	1450.3	0.15	6.39*	1136.5	[0.19]
Camphene hydrate	8.64*	1545.0	[0.20]	6.49	1142.9	0.01
Menthone	6.81	1407.6	0.16	6.59	1149.2	0.16
Isoborneol	9.56	1617.0	0.01	6.65	1153.1	0.02
Unknown RHGR XVIII [m/z 123, 81 (46), 43 (45), 95 (34), 166 (30)]	9.13	1583.0	0.02	6.74	1158.8	0.03
Borneol	9.95*	1648.5	[1.48]	6.81	1163.2	1.07
Lavandulol	9.81	1636.9	0.03	6.90	1168.7	0.02
Terpinen-4-ol	8.75*	1553.7	[2.44]	6.99	1174.7	1.95
meta-Cymen-8-ol	11.69*	1793.1	[0.08]	7.06	1179.3	0.01
para-Cymen-8-ol	11.69*	1793.1	[0.08]	7.15	1184.8	0.03
Unknown UNKN VI [m/z 43, 135 (73), 59 (46), 93 (39), 91 (35),				7.18	1186.8	0.03

81 (32)...						
$\alpha$ -Terpineol	9.95*	1648.5	[1.48]	7.21	1188.6	0.08
<i>cis</i> -Dihydrocarvone	8.64*	1545.0	[0.20]	7.26	1191.6	0.09
<i>cis</i> -Piperitol	9.77*	1634.1	[0.15]	7.31	1195.2	0.04
<i>trans</i> -Dihydrocarvone	8.88	1563.5	0.01	7.34	1197.2	0.01
Bornyl formate	8.24*	1514.4	[4.58]	7.73	1222.4	0.01
Thymol methyl ether	8.62*	1543.3	[2.58]	7.90	1234.0	0.26
Neral	9.65	1623.7	0.04	7.97	1238.8	0.01
Carvacrol methyl ether	8.75*	1553.7	[2.44]	8.04	1243.0	0.62
Geraniol	11.80	1802.4	0.05	8.34	1263.1	0.06
Geranial	10.30	1676.7	0.01	8.47	1272.3	0.01
Decanol	10.89	1725.6	0.03	8.51	1274.6	0.02
Bornyl acetate	8.42	1528.4	0.06	8.63	1282.7	0.05
Thymol analogue I (isothymol?)	15.30*	2127.2	[32.31]	8.84	1296.9	0.13
Thymol	15.30*	2127.2	[32.31]	9.00	1307.7	32.33
Carvacrol	15.53	2149.5	2.83	9.08	1312.9	2.81
$\alpha$ -Terpinyl acetate	9.89	1643.8	0.04	9.56	1347.2	0.02
Thymyl acetate	11.69*	1793.1	[0.08]	9.64	1353.0	0.02
$\alpha$ -Copaene	7.33	1446.6	0.04	9.92	1372.2	0.06
$\beta$ -Bourbonene	7.67	1471.2	0.03	10.03	1380.0	0.05
Geranyl acetate	10.80	1717.6	0.02	10.13	1387.2	0.02
Unknown MEPU VII [m/z 148, 133 (66), 105 (46), 43 (33), 77 (15)...				10.16	1389.5	0.01
Isocaryophyllene	8.35*	1522.5	[0.04]	10.33	1401.3	0.01
$\alpha$ -Gurjunene	7.78	1479.8	0.10	10.37	1404.1	0.01
$\beta$ -Caryophyllene	8.62*	1543.3	[2.58]	10.50	1413.7	2.45
Aromadendrene	8.75*	1553.7	[2.44]	10.77	1433.5	0.08
Unknown CASA XV [m/z 79, 67 (75), 93 (47), 81 (47), 55 (46), 41 (43)...				10.92	1444.7	0.01
$\alpha$ -Humulene	9.47	1609.7	0.07	10.95	1447.0	0.07
allo-Aromadendrene	9.16	1585.2	0.01	11.00	1451.1	0.01
Thymohydroquinone isomer?				11.05	1454.4	0.01
( <i>E</i> )- $\beta$ -Farnesene	9.72	1630.0	0.12	11.09	1457.7	0.14
$\gamma$ -Muurolole	9.77*	1634.1	[0.15]	11.29	1472.5	0.10
Germacrene D	9.95*	1648.5	[1.48]	11.32	1475.1	0.41
allo-Aromadendr-9-ene	9.77*	1634.1	[0.15]	11.40*	1480.7	[0.04]

β-Selinene	10.09	1659.6	0.03	11.40*	1480.7	[0.04]
Viridiflorene	9.84	1639.0	0.01	11.52*	1489.9	[0.08]
β-Himachalene	10.06	1657.1	0.03	11.52*	1489.9	[0.08]
Bicyclogermacrene	10.27	1674.4	0.03	11.52*	1489.9	[0.08]
α-Muurolene	10.25	1672.3	0.02	11.61	1496.3	0.05
β-Bisabolene	10.34	1679.5	0.03	11.77*	1508.4	[0.18]
γ-Cadinene	10.58	1699.2	0.14	11.77*	1508.4	[0.18]
Cubebol	12.74	1884.9	0.01	11.77*	1508.4	[0.18]
δ-Cadinene	10.60	1701.3	0.19	11.91*	1519.3	[0.21]
<i>trans</i> -Calamenene	11.41	1769.4	0.01	11.91*	1519.3	[0.21]
<i>trans</i> -Cadina-1,4-diene	10.84	1721.5	0.02	12.01	1526.9	0.02
α-Cadinene	10.97	1732.3	0.02	12.08	1532.6	0.02
Geranyl butyrate	12.42	1857.3	0.01	12.47	1563.5	0.01
Caryophyllene oxide isomer	12.89	1898.6	0.02	12.60*	1573.7	[0.30]
Caryophyllene oxide	12.97	1905.7	0.27	12.60*	1573.7	[0.30]
Unknown THVU II [m/z 161, 187 (29), 105 (24), 91 (23), 93 (23)... 205 (19), 220? (2)]				12.64	1576.7	0.01
Humulene epoxide II	13.56	1960.6	0.01	12.93	1599.6	0.01
10-epi-γ-Eudesmol	14.32	2031.5	0.03	13.07	1610.5	0.03
1-epi-Cubenol	13.96	1997.5	0.02	13.20	1621.2	0.01
Caryophylladienol II	16.24	2221.4	0.03	13.30	1629.3	0.02
Isospathulenol	15.67*	2163.6	[0.04]	13.32	1631.5	0.01
τ-Cadinol	15.08	2105.5	0.07	13.37	1635.1	0.08
α-Cadinol	15.67*	2163.6	[0.04]	13.51	1646.5	0.01
(3 <i>Z</i> )-Caryophylla- 3,8(13)-dien-5β-ol	17.00	2300.6	0.02	13.74	1665.9	0.02
Shyobunol	16.54	2253.2	0.01	13.94	1682.2	0.01
Unknown UNKN XX [m/z 81, 136 (68), 135 (58), 150 (44), 93 (34), 121 (30)...]				15.69	1834.6	0.01
Unknown THVU XVI [m/z 81, 136 (62), 135 (56), 150 (39), 93 (33), 121 (24)...]				16.18	1878.8	0.03
Unknown THVU III [m/z 136, 81 (96), 135 (76), 93 (48), 150 (47), 121 (43), 137 (28)...]				16.37	1895.9	0.04
<i>meta</i> -Camphorene	15.57	2153.9	0.06	16.93	1948.5	0.06

Unknown THVU IV [m/z 201, 159 (37), 148 (27), 173 (22), 41 (20)... 284 (16)]				17.14	1969.1	0.02
Unknown THVU VI [m/z 135, 150 (61), 81 (45), 69 (37), 41 (24), 136 (21), 93 (19)...]				17.28	1982.0	0.04
Unknown THVU VII [m/z 135, 150 (67), 69 (57), 41 (24)...]				17.66	2018.5	0.01
Unknown ORVU VI [m/z 135, 150 (66), 43 (38), 109 (27), 93 (25), 137 (20)...]	18.63	2479.8	0.01	17.69	2022.1	0.01
Unknown UNKN XXIV [m/z 135, 43 (51), 150 (36), 109 (30), 93 (27), 95 (21)...]				17.83	2035.8	0.02
Unknown THVU VIII [m/z 173, 159 (29), 216 (27), 286 (15)]				18.06	2058.7	0.01
Unknown MOFI V [m/z 69, 41 (81), 91 (37), 166 (35), 105 (33), 43 (30)...]	20.17	2659.7	0.03	18.66	2119.0	0.01
Unknown MOFI VI [m/z 69, 41 (74), 166 (36), 91 (32), 105 (28), 43 (25)...]	20.22	2665.4	0.01	18.71	2124.0	0.02
Unknown THVU XI [m/z 163, 175 (91), 173 (83), 161 (82), 41 (66), 286 (66)]				19.05	2159.3	0.01
Total reported		97.81%			98.59%	

\*: 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