

**Date :** August 16, 2022

**CERTIFICATE OF ANALYSIS – GC PROFILING**

*SAMPLE IDENTIFICATION*

**Internal code :** 22H09-PTH04

**Customer identification :** Thyme Thymol (Red) - Greece - T40111R

**Type :** Essential oil

**Source :** *Thymus vulgaris* ct. Thymol

**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 :** August 12, 2022

Checked and approved by :

---

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

*Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia. This report is digitally signed, it is only considered valid if the digital signature is intact. The results only describe the samples that were submitted to the assays.*

*PHYSICOCHEMICAL DATA*

**Physical aspect:** Light orange yellow liquid

**Refractive index:**  $1.5032 \pm 0.0003$  (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
Isobutyral	0.01	Aliphatic aldehyde
Isovaleral	0.02	Aliphatic aldehyde
2-Methylbutyral	0.02	Aliphatic aldehyde
2-Ethylfuran	tr	Furan
Isoamyl alcohol	tr	Aliphatic alcohol
2-Methylbutanol	tr	Aliphatic alcohol
Methyl 2-methylbutyrate	0.04	Aliphatic ester
Octane	tr	Alkane
Unknown	0.01	Unknown
(3Z)-Hexenol	0.01	Aliphatic alcohol
Hexanol	0.01	Aliphatic alcohol
Hashishene	0.01	Monoterpene
Tricyclene	0.03	Monoterpene
$\alpha$ -Thujene	0.37	Monoterpene
$\alpha$ -Pinene	1.44	Monoterpene
$\alpha$ -Fenchene	0.01	Monoterpene
Camphene	0.35	Monoterpene
Benzaldehyde	0.01	Simple phenolic
$\beta$ -Pinene	0.12	Monoterpene
Sabinene	0.01	Monoterpene
4-Pentenyl propionate	0.02	Aliphatic ester
Octen-3-ol	0.20	Aliphatic alcohol
Octan-3-one	0.06	Aliphatic ketone
Myrcene	1.66	Monoterpene
Octan-3-ol	0.01	Aliphatic alcohol
Pseudolimonene	0.03	Monoterpene
$\alpha$ -Phellandrene	0.11	Monoterpene
<i>cis</i> -Dehydroxylinalool oxide	0.03	Monoterpenic ether
$\Delta^3$ -Carene	0.10	Monoterpene
$\alpha$ -Terpinene	1.17	Monoterpene
meta-Cymene	0.05	Monoterpene
para-Cymene	19.44	Monoterpene
$\beta$ -Phellandrene	1.21	Monoterpene
1,8-Cineole	0.01	Monoterpenic ether
Limonene	0.39	Monoterpene
ortho-Cymene	0.03	Monoterpene
(Z)- $\beta$ -Ocimene	0.05	Monoterpene
(E)- $\beta$ -Ocimene	0.07	Monoterpene
$\gamma$ -Terpinene	6.94	Monoterpene
2-Methylbutyl butyrate	0.01	Aliphatic ester
<i>cis</i> -Sabinene hydrate	0.13	Monoterpenic alcohol
3-Methyl-3-butenyl butyrate?	0.02	Aliphatic ester
<i>cis</i> -Linalool oxide (fur.)	0.02	Monoterpenic alcohol
Octanol	0.01	Aliphatic alcohol
meta-Cymenene	0.01	Monoterpene

Fenchone	0.01	Monoterpenic ketone
Terpinolene	0.09	Monoterpene
para-Cymenene	0.04	Monoterpene
<i>trans</i> -Linalool oxide (fur.)	0.01	Monoterpenic alcohol
<i>trans</i> -Sabinene hydrate	0.07	Monoterpenic alcohol
Linalool	3.00	Monoterpenic alcohol
Nonanal	0.01	Aliphatic aldehyde
Hotrienol	0.03	Monoterpenic alcohol
endo-Fenchol	0.02	Monoterpenic alcohol
Unknown	0.03	Unknown
<i>trans</i> -Pinocarveol	0.02	Monoterpenic alcohol
Camphor	0.05	Monoterpenic ketone
Camphene hydrate	0.04	Monoterpenic alcohol
<i>trans</i> -Chrysanthemal	0.01	Monoterpenic aldehyde
Unknown	0.03	Oxygenated monoterpene
Isoborneol	0.03	Monoterpenic alcohol
Unknown	0.01	Unknown
Borneol	0.63	Monoterpenic alcohol
Lavandulol	0.04	Monoterpenic alcohol
Terpinen-4-ol	1.22	Monoterpenic alcohol
para-Cymen-8-ol	0.03	Monoterpenic alcohol
Unknown	0.02	Unknown
$\alpha$ -Terpineol	0.30	Monoterpenic alcohol
<i>cis</i> -Dihydrocarvone	0.03	Monoterpenic ketone
<i>trans</i> -Dihydrocarvone	0.03	Monoterpenic ketone
Verbenone	0.02	Monoterpenic ketone
Bornyl formate	0.01	Monoterpenic ester
Thymol methyl ether	0.42	Monoterpenic ether
Neral	0.12	Monoterpenic aldehyde
Carvacrol methyl ether	0.07	Monoterpenic ether
( <i>E</i> )-Isogeraniol?	0.02	Monoterpenic alcohol
Geraniol	0.17	Monoterpenic alcohol
Geranial	0.10	Monoterpenic aldehyde
Thymol analogue I (isothymol?)	0.15	Monoterpenic alcohol
Thymol	46.95	Monoterpenic alcohol
Carvacrol	4.46	Monoterpenic alcohol
Thymyl acetate	0.07	Monoterpenic ester
Eugenol	0.05	Phenylpropanoid
Isodauca-4,7(14)-diene?	0.01	Sesquiterpene
$\alpha$ -Copaene	0.21	Sesquiterpene
$\beta$ -Bourbonene	0.02	Sesquiterpene
Geranyl acetate	0.01	Monoterpenic ester
Unknown	0.02	Unknown
Isocaryophyllene	0.01	Sesquiterpene
$\alpha$ -Gurjunene	0.03	Sesquiterpene
$\beta$ -Caryophyllene	2.73	Sesquiterpene
Aromadendrene	0.30	Sesquiterpene
$\alpha$ -Humulene	1.00	Sesquiterpene
Unknown	0.09	Oxygenated monoterpene
allo-Aromadendrene	0.05	Sesquiterpene
Thymohydroquinone isomer?	0.02	Simple phenolic
$\gamma$ -Muurolole	0.06	Sesquiterpene

Germacrene D	0.04	Sesquiterpene
β-Selinene	0.02	Sesquiterpene
allo-Aromadendr-9-ene	0.03	Sesquiterpene
Bicyclogermacrene	0.04	Sesquiterpene
Viridiflorene	0.21	Sesquiterpene
α-Muurolene	0.03	Sesquiterpene
β-Bisabolene	0.02	Sesquiterpene
γ-Cadinene	0.07	Sesquiterpene
trans-Calamenene	0.02	Sesquiterpene
δ-Cadinene	0.17	Sesquiterpene
trans-Cadina-1,4-diene	0.02	Sesquiterpene
α-Cadinene	0.01	Sesquiterpene
Thymohydroquinone	0.01	Monoterpenic alcohol
Caryophyllenyl alcohol	0.01	Sesquiterpenic alcohol
Spathulenol	0.04	Sesquiterpenic alcohol
Caryophyllene oxide	0.20	Sesquiterpenic ether
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Unknown	0.03	Oxygenated sesquiterpene
Neryl 2-methylbutyrate?	0.01	Monoterpenic ester
Humulene epoxide II	0.07	Sesquiterpenic ether
10-epi-γ-Eudesmol	0.02	Sesquiterpenic alcohol
Caryophylladienol I?	0.02	Sesquiterpenic alcohol
Isospathulenol	0.01	Sesquiterpenic alcohol
τ-Cadinol	0.03	Sesquiterpenic alcohol
α-Cadinol	0.01	Sesquiterpenic alcohol
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	0.02	Sesquiterpenic alcohol
Unknown	0.01	Unknown
Unknown	0.03	Unknown
Unknown	0.06	Unknown
Unknown	0.01	Unknown
meta-Camphorene	0.03	Diterpene
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Unknown	0.03	Unknown
Unknown	0.01	Unknown
Unknown	0.01	Unknown
Unknown	0.02	Unknown
Unknown	0.02	Unknown
Unknown	0.02	Unknown
<b>Consolidated total</b>	<b>98.63%</b>	

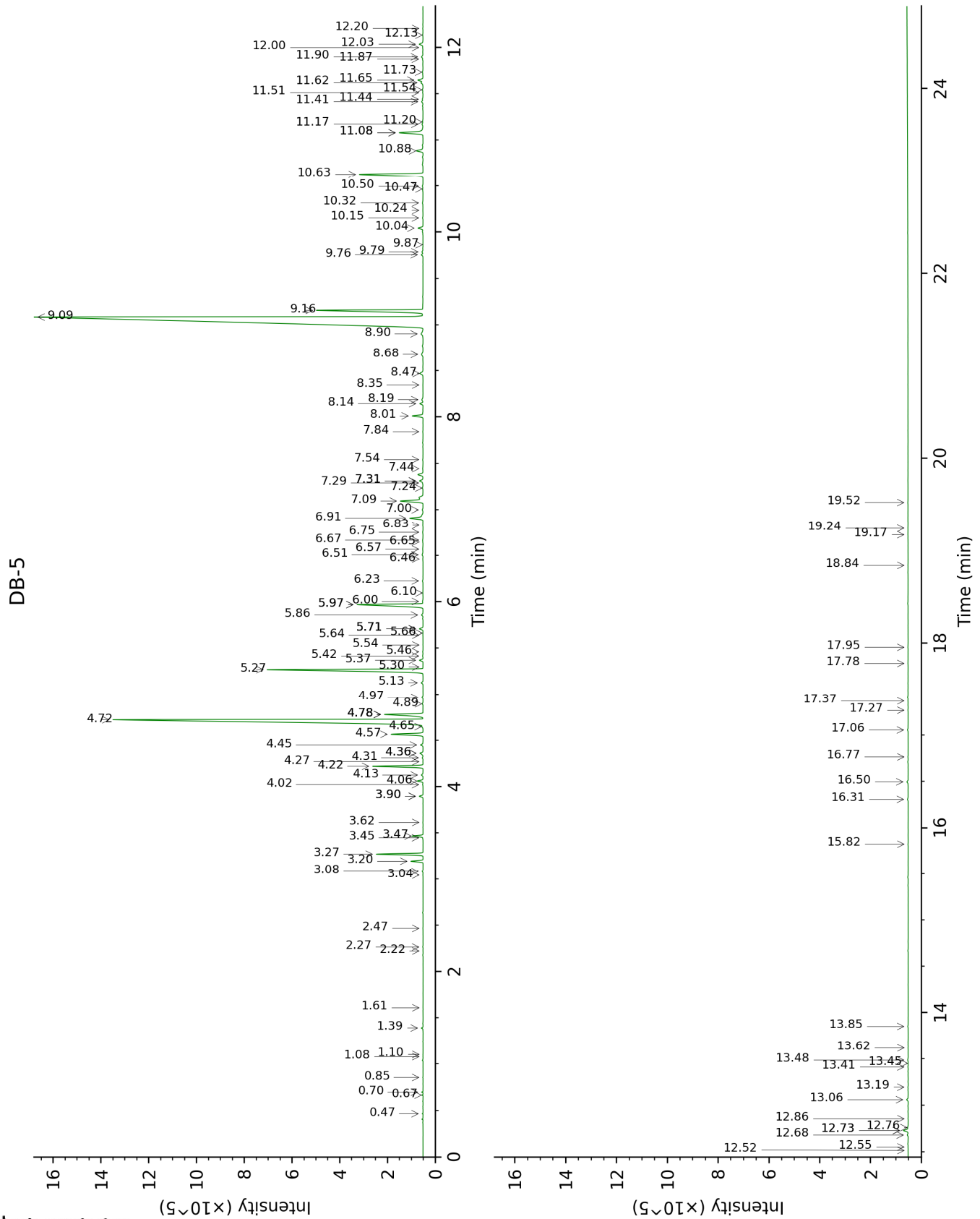
tr: The compound has been detected below 0.005% of total signal.

Note: no correction factor was applied

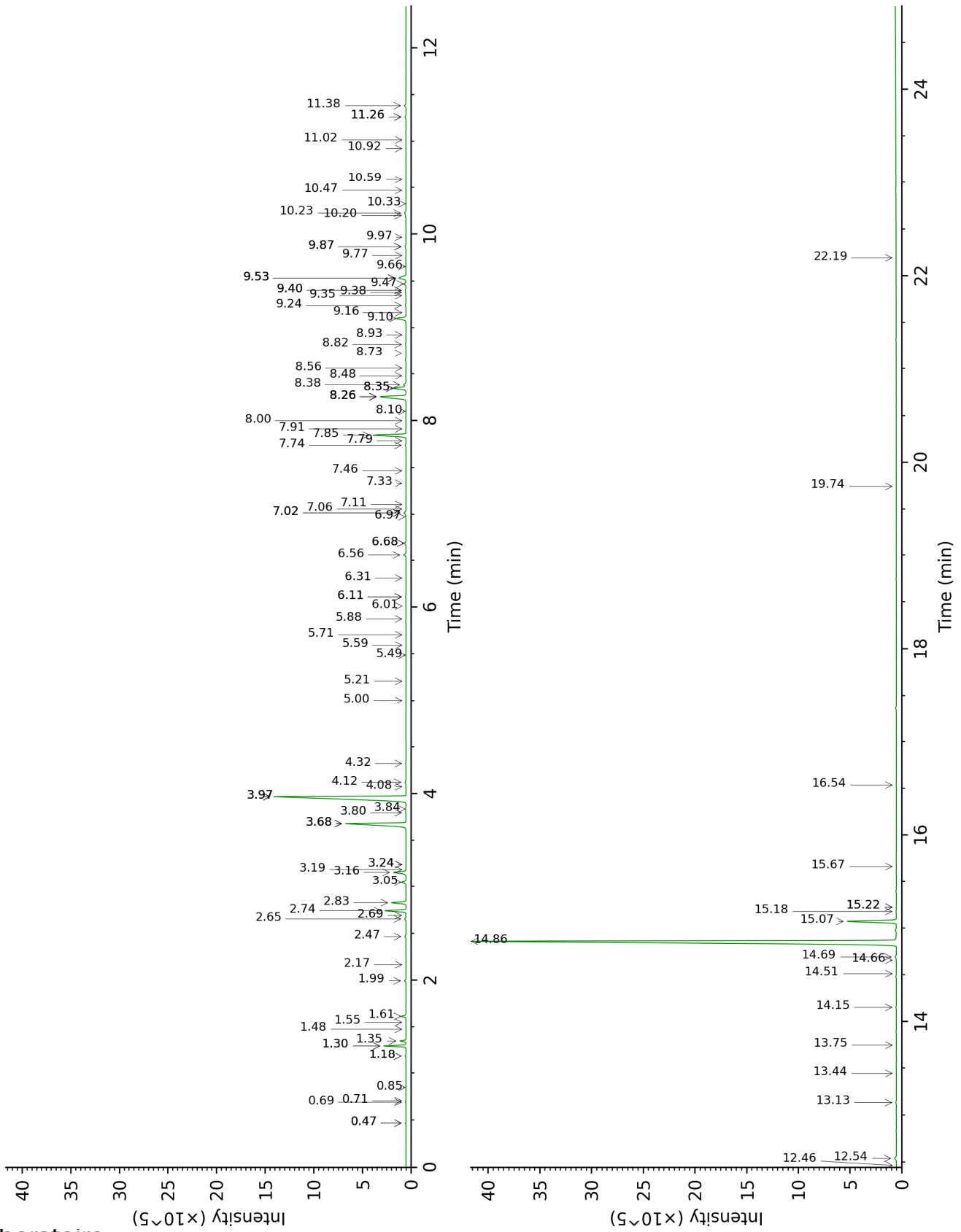
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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

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



DB-WAX





FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Isobutylal	0.47	541	0.01	0.47*	782	0.02
Isovaleral	0.66	642	0.02	0.71	885	0.02
2-Methylbutylal	0.70	653	0.02	0.69	879	0.02
2-Ethylfuran	0.85	703	tr	0.85	920	tr
Isoamyl alcohol	1.08	734	tr	3.24*	1174	0.01
2-Methylbutanol	1.10	737	tr	3.24*	1174	[0.01]
Methyl 2-methylbutyrate	1.39	776	0.04	1.18*	974	0.06
Octane	1.61	804	tr	0.47*	782	[0.02]
Unknown [m/z 109, 43 (28), 124 (28), 41 (14), 55 (11), 79 (9), 81 (8)...]	2.22	854	0.01	1.48	1016	0.01
(3Z)-Hexenol	2.26	857	0.01	5.60	1345	0.01
Hexanol	2.47	874	0.01	5.21	1317	0.01
Hashishene	3.04	917	0.01	1.30*	994	1.44
Tricyclene	3.08	920	0.03	1.18*	974	[0.06]
$\alpha$ -Thujene	3.20	927	0.37	1.35	1002	0.37
$\alpha$ -Pinene	3.27	932	1.44	1.30*	994	[1.44]
$\alpha$ -Fenchene	3.45†	944	0.37	1.55	1023	0.01
Camphene	3.47†	945	[0.37]	1.61	1030	0.35
Benzaldehyde	3.62	954	0.01	7.11	1458	0.03
$\beta$ -Pinene	3.90*	973	0.13	1.99	1067	0.12
Sabinene	3.90*	973	[0.13]	2.17	1084	0.01
4-Pentenyl propionate	4.02	981	0.02	3.97*	1230	19.48
Octen-3-ol	4.06	984	0.20	6.56	1416	0.20
Octan-3-one	4.13	988	0.06	3.80	1217	0.05
Myrcene	4.22	994	1.66	2.74	1134	1.66
Octan-3-ol	4.27	997	0.01	5.88	1366	0.02
Pseudolimonene	4.31	1000	0.03	2.69	1130	0.03
$\alpha$ -Phellandrene	4.36*	1003	0.14	2.65	1127	0.11
<i>cis</i> -Dehydroxylinalool oxide	4.36*	1003	[0.14]	3.68*	1209	7.02
$\Delta^3$ -Carene	4.45	1009	0.10	2.47	1112	0.09
$\alpha$ -Terpinene	4.57	1016	1.17	2.83	1141	1.17
meta-Cymene	4.65	1021	0.05	3.97*	1230	[19.48]
para-Cymene	4.72	1026	19.44	3.97*	1230	[19.48]
$\beta$ -Phellandrene	4.78*	1029	1.61	3.16	1167	1.21
1,8-Cineole	4.78*	1029	[1.61]	3.19	1170	0.01
Limonene	4.78*	1029	[1.61]	3.05	1158	0.39
ortho-Cymene	4.90	1036	0.03	4.32	1256	0.03
(Z)- $\beta$ -Ocimene	4.97	1041	0.05	3.68*	1209	[7.02]
(E)- $\beta$ -Ocimene	5.13	1051	0.07	3.84	1220	0.07
$\gamma$ -Terpinene	5.27	1060	6.94	3.68*	1209	[7.02]
2-Methylbutyl butyrate	5.30	1062	0.01	4.08	1238	0.02

<i>cis</i> -Sabinene hydrate	5.37	1066	0.13	6.68*	1426	0.14
3-Methyl-3-butenyl butyrate?	5.42	1069	0.02	5.00	1307	0.02
<i>cis</i> -Linalool oxide (fur.)	5.46	1072	0.02	6.31	1398	0.02
Octanol	5.54	1076	0.01	7.91	1519	0.01
meta-Cymenene	5.64	1083	0.01	6.11*	1383	0.05
Fenchone	5.66	1084	0.01	5.49	1337	0.01
Terpinolene	5.71*	1087	0.14	4.12	1241	0.09
para-Cymenene	5.71*	1087	[0.14]	6.11*	1383	[0.05]
<i>trans</i> -Linalool oxide (fur.)	5.71*	1087	[0.14]	6.68*	1426	[0.14]
<i>trans</i> -Sabinene hydrate	5.86	1096	0.07	7.74	1506	0.08
Linalool	5.97*	1104	3.00	7.85	1514	3.00
Nonanal	5.97*	1104	[3.00]	5.71	1353	0.01
Hotrienol	6.00	1106	0.03	8.56	1571	0.01
endo-Fenchol	6.10	1112	0.02	8.10	1534	0.01
Unknown [m/z 81, 79 (19), 41 (12), 92 (8), 77 (8)...]	6.23	1120	0.03	6.01	1376	0.01
<i>trans</i> -Pinocarveol	6.46	1135	0.02	8.92	1599	0.01
Camphor	6.51	1138	0.05	6.98	1448	0.05
Camphene hydrate	6.57	1142	0.04	8.26*	1547	3.21
<i>trans</i> -Chrysanthemal	6.65	1146	0.01	7.02*	1451	0.20
Unknown [m/z 123, 81 (60), 67 (49), 95 (36), 41 (29), 68 (25)...152 (2)]	6.67	1148	0.03	7.06	1454	0.01
Isoborneol	6.75	1153	0.03	9.16	1619	0.01
Unknown [m/z 123, 81 (46), 43 (45), 95 (34), 166 (30)]	6.83	1158	0.01	8.73	1584	0.02
Borneol	6.91	1163	0.63	9.53*	1649	0.97
Lavandulol	7.00	1169	0.04	9.38†	1636	0.14
Terpinen-4-ol	7.10	1175	1.22	8.35*	1554	1.31
para-Cymen-8-ol	7.24	1184	0.03	11.26*	1795	0.11
Unknown [m/z 43, 135 (73), 59 (46), 93 (39), 91 (35), 81 (32)...]	7.29	1188	0.02			
α-Terpineol	7.31*†	1189	0.39	9.53*	1649	[0.97]
<i>cis</i> -Dihydrocarvone	7.31*†	1189	[0.39]	8.26*	1547	[3.21]
<i>trans</i> -Dihydrocarvone	7.44	1197	0.03	8.48	1564	0.03
Verbenone	7.54	1204	0.02	9.34	1634	0.03
Bornyl formate	7.84	1224	0.01	7.79	1509	0.01
Thymol methyl ether	8.01	1235	0.42	8.26*	1547	[3.21]
Neral	8.14	1244	0.12	9.24	1625	0.09
Carvacrol methyl ether	8.19	1247	0.07	8.35*	1554	[1.31]
( <i>E</i> )-Isogeraniol?	8.35	1257	0.02	10.92	1766	0.01

Geraniol	8.47	1266	0.17	11.38	1806	0.16
Geranial	8.68	1279	0.10	9.87*	1677	0.13
Thymol analogue I (isothymol?)	8.90	1294	0.15	14.69	2115	0.13
Thymol	9.09	1307	46.95	14.86	2132	46.90
Carvacrol	9.16	1312	4.46	15.07	2154	4.48
Thymyl acetate	9.76	1354	0.07	11.26*	1795	[0.11]
Eugenol	9.79	1356	0.05	14.51	2098	0.02
Isodauca-4,7(14)-diene?	9.87	1362	0.01			
α-Copaene	10.04	1374	0.21	7.02*	1451	[0.20]
β-Bourbonene	10.15	1382	0.02	7.33	1475	0.02
Geranyl acetate	10.24	1388	0.01	10.33	1715	0.01
Unknown [m/z 148, 133 (66), 105 (46), 43 (33), 77 (15)...]	10.32	1393	0.02			
Isocaryophyllene	10.47	1404	0.01	8.00	1526	0.01
α-Gurjunene	10.50	1406	0.03	7.46	1485	0.02
β-Caryophyllene	10.63	1416	2.73	8.26*	1547	[3.21]
Aromadendrene	10.88	1435	0.30	8.38	1557	0.24
α-Humulene	11.08*	1450	1.09	9.10	1613	1.00
Unknown [m/z 151, 166 (40), 105 (26)...]	11.08*	1450	[1.09]			
allo-Aromadendrene	11.17	1456	0.05	8.82	1591	0.07
Thymohydroquinone isomer?	11.20	1458	0.02			
γ-Murolene	11.41	1474	0.06	9.40*†	1638	[0.14]
Germacrene D	11.44	1476	0.04	9.53*	1649	[0.97]
β-Selinene	11.51	1482	0.02	9.66	1659	0.04
allo-Aromadendr-9-ene	11.54	1484	0.03	9.40*†	1638	[0.14]
Bicyclogermacrene	11.62†	1490	0.32	9.77	1669	0.04
Viridiflorene	11.65†	1492	[0.32]	9.47	1644	0.21
α-Murolene	11.73	1498	0.03	9.87*	1677	[0.13]
β-Bisabolene	11.87	1509	0.02	9.97	1685	0.02
γ-Cadinene	11.90	1511	0.07	10.20	1704	0.06
trans-Calamenene	12.00	1518	0.02	11.02	1774	0.01
δ-Cadinene	12.03	1521	0.17	10.23	1706	0.16
trans-Cadina-1,4-diene	12.13	1529	0.02	10.47	1727	0.02
α-Cadinene	12.20	1535	0.01	10.59	1737	0.02
Thymohydroquinone	12.52	1559	0.01	22.19	2980	0.01
Caryophyllenyl alcohol	12.55	1562	0.01	13.44	1994	0.01
Spathulenol	12.68	1572	0.04	14.15	2063	0.04
Caryophyllene oxide	12.73*	1576	0.20	12.54	1910	0.20
Caryophyllene oxide isomer	12.73*	1576	[0.20]	12.46	1903	0.01
Unknown [m/z 161, 187 (29), 105 (24), 91 (23), 93 (23)... 205 (19), 220? (2)]	12.76	1578	0.03			

Neryl 2-methylbutyrate?	12.86	1586	0.01			
Humulene epoxide II	13.06	1602	0.07	13.13	1965	0.06
10-epi- $\gamma$ -Eudesmol	13.19	1613	0.02	13.75	2024	0.02
Caryophylladienol I?	13.41	1630	0.02			
Isospathulenol	13.45	1634	0.01	15.22*	2169	0.02
$\tau$ -Cadinol	13.48	1637	0.03	14.66	2112	0.02
$\alpha$ -Cadinol	13.62	1648	0.01	15.22*	2169	[0.02]
(3Z)-Caryophylla-3,8(13)-dien-5 $\beta$ -ol	13.85	1667	0.02	16.54	2306	0.02
Unknown [m/z 81, 136 (68), 135 (58), 150 (44), 93 (34), 121 (30)...]	15.82	1837	0.01			
Unknown [m/z 81, 136 (62), 135 (56), 150 (39), 93 (33), 121 (24)...]	16.31	1881	0.03			
Unknown [m/z 136, 81 (96), 135 (76), 93 (48), 150 (47), 121 (43), 137 (28)...]	16.50	1898	0.06			
Unknown [m/z 136, 81 (81), 150 (74), 135 (52), 93 (46), 121 (42)...]	16.77	1924	0.01	15.67	2214	0.01
meta-Camphorene	17.06	1951	0.03	15.18	2165	0.05
Unknown [m/z 201, 159 (37), 148 (27), 173 (22), 41 (20)... 284 (16)]	17.27	1971	0.01			
Unknown [m/z 135, 150 (61), 81 (45), 69 (37), 41 (24), 136 (21), 93 (19)...]	17.37	1981	0.01			
Unknown [m/z 135, 150 (67), 69 (57), 41 (24)...]	17.78	2021	0.03			
Unknown [m/z 135, 43 (51), 150 (36), 109 (30), 93 (27), 95 (21)...]	17.96	2038	0.01			
Unknown [m/z 69, 41 (74), 166 (36), 91 (32), 105 (28), 43 (25)...]	18.84	2127	0.01	19.74	2670	0.01
Unknown [m/z 163, 175 (91), 173 (83), 161 (82), 41 (66), 286 (66)]	19.17	2161	0.02			
Unknown [m/z 267, 282 (24), 268 (21), 117 (16), 126 (11)...]	19.24	2168	0.02			

Unknown [m/z 175, 163 (78), 161 (33), 41 (32)... 286 (18)]	19.52	2197	0.02	
<b>Total identified</b>		<b>98.36%</b>		<b>97.87%</b>
<b>Total reported</b>		<b>98.75%</b>		<b>97.94%</b>

\*: 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