

Date : May 08, 2023

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 23D28-PTH02

**Customer identification :** Fir Needle - Russia - F20111R

**Type :** Essential oil

**Source :** *Abies sibirica*

**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 :** May 02, 2023

Checked and approved by :

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

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*PHYSICOCHEMICAL DATA*

**Physical aspect:** Clear liquid

**Refractive index:**  $1.4702 \pm 0.0003$  (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
Toluene	0.01	Simple phenolic
Santene	2.56	Normonoterpene
Unknown	0.02	Normonoterpene
Bornylene	0.01	Monoterpene
Tricyclene	2.27	Monoterpene
$\alpha$ -Thujene	0.09	Monoterpene
$\alpha$ -Pinene	12.58	Monoterpene
Camphene	22.67	Monoterpene
$\alpha$ -Fenchene	0.03	Monoterpene
Thuja-2,4(10)-diene	0.02	Monoterpene
3,7,7-Trimethylcyclohepta-1,3,5-triene	0.04	Monoterpene
$\beta$ -Pinene	1.94	Monoterpene
Sabinene	0.01	Monoterpene
Myrcene	0.65	Monoterpene
2-Carene	0.01	Monoterpene
$\alpha$ -Phellandrene	0.18	Monoterpene
Pseudolimonene	0.01	Monoterpene
$\Delta$ 3-Carene	12.72	Monoterpene
(3Z)-Hexenyl acetate	0.01	Aliphatic ester
$\alpha$ -Terpinene	0.11	Monoterpene
Carvomenthene	0.03	Aliphatic alcohol
para-Cymene	0.12	Monoterpene
$\beta$ -Phellandrene	3.15	Monoterpene
Limonene	4.63	Monoterpene
(Z)- $\beta$ -Ocimene	0.02	Monoterpene
$\gamma$ -Terpinene	0.16	Monoterpene
Octanol	0.01	Aliphatic alcohol
meta-Cymenene	0.01	Monoterpene
$\gamma$ -Campholenal	0.05	Aliphatic alcohol
Terpinolene	1.17	Monoterpene
para-Cymenene	0.04	Monoterpene
$\alpha$ -Pinene oxide	0.01	Monoterpenic ether
Unknown	0.01	Unknown
Unknown	0.03	Unknown
Linalool	0.05	Monoterpenic alcohol
endo-Fenchol	0.03	Monoterpenic alcohol
cis-para-Menth-2-en-1-ol	0.03	Monoterpenic alcohol
$\alpha$ -Campholenal	0.03	Monoterpenic aldehyde
Cosmene	0.01	Monoterpene
trans-Pinocarveol	0.03	Monoterpenic alcohol
Camphor	0.21	Monoterpenic ketone
Camphene hydrate	0.11	Monoterpenic alcohol
Isoborneol	0.04	Monoterpenic alcohol
Pinocarvone	0.01	Monoterpenic ketone
Borneol	1.94	Monoterpenic alcohol

Isopinocampone	0.05	Monoterpenic ketone
Terpinen-4-ol	0.12	Monoterpenic alcohol
meta-Cymen-8-ol	0.02	Monoterpenic alcohol
Cryptone	tr	Normonoterpenic ketone
para-Cymen-8-ol	0.04	Monoterpenic alcohol
$\alpha$ -Terpineol	0.16	Monoterpenic alcohol
Myrtenal	0.05	Monoterpenic aldehyde
Myrtenol	0.03	Monoterpenic alcohol
Unknown	0.04	Oxygenated monoterpene
Verbenone	0.03	Monoterpenic ketone
endo-Fenchyl acetate	0.03	Monoterpenic ester
Citronellol	0.02	Monoterpenic alcohol
Thymol methyl ether	0.07	Monoterpenic ether
Carvone	0.04	Monoterpenic ketone
Piperitone	0.02	Monoterpenic ketone
Geraniol	0.03	Monoterpenic alcohol
Phellandral	0.04	Monoterpenic aldehyde
Isobornyl acetate	0.23	Monoterpenic ester
Bornyl acetate	26.32	Monoterpenic ester
2-Undecanone	0.06	Aliphatic ketone
Isohexyl isocaproate	0.04	Aliphatic ester
Unknown	0.02	Unknown
Unknown	0.02	Unknown
$\alpha$ -Longipinene	0.03	Sesquiterpene
$\alpha$ -Terpinyl acetate	0.01	Monoterpenic ester
Citronellyl acetate	0.02	Monoterpenic ester
Neryl acetate	0.06	Monoterpenic ester
$\alpha$ -Ylangene	0.02	Sesquiterpene
$\alpha$ -Copaene	0.02	Sesquiterpene
Geranyl acetate	0.22	Monoterpenic ester
$\beta$ -Longipinene	0.03	Sesquiterpene
Longifolene	0.09	Sesquiterpene
Sibirene	0.03	Sesquiterpene
Methyleugenol	0.02	Phenylpropanoid
Dodecanal	0.16	Aliphatic aldehyde
$\beta$ -Caryophyllene	1.21	Sesquiterpene
Caryophylla-4(12),8(13)-diene	0.01	Sesquiterpene
<i>trans</i> - $\alpha$ -Bergamotene	0.01	Sesquiterpene
$\alpha$ -Himachalene	0.05	Sesquiterpene
$\alpha$ -Humulene	0.68	Sesquiterpene
( <i>E</i> )- $\beta$ -Farnesene	0.02	Sesquiterpene
$\gamma$ -Himachalene	0.03	Sesquiterpene
Unknown	0.08	Sesquiterpene
Unknown	0.05	Unknown
$\beta$ -Himachalene	0.04	Sesquiterpene
$\alpha$ -Muurolene	0.03	Sesquiterpene
( <i>Z</i> )- $\alpha$ -Bisabolene	0.03	Sesquiterpene
$\beta$ -Bisabolene	0.18	Sesquiterpene
( <i>Z</i> )- $\gamma$ -Bisabolene	0.06	Sesquiterpene
$\delta$ -Cadinene	0.03	Sesquiterpene
( <i>E</i> )- $\gamma$ -Bisabolene	0.09	Sesquiterpene
( <i>E</i> )- $\alpha$ -Bisabolene	0.02	Sesquiterpene

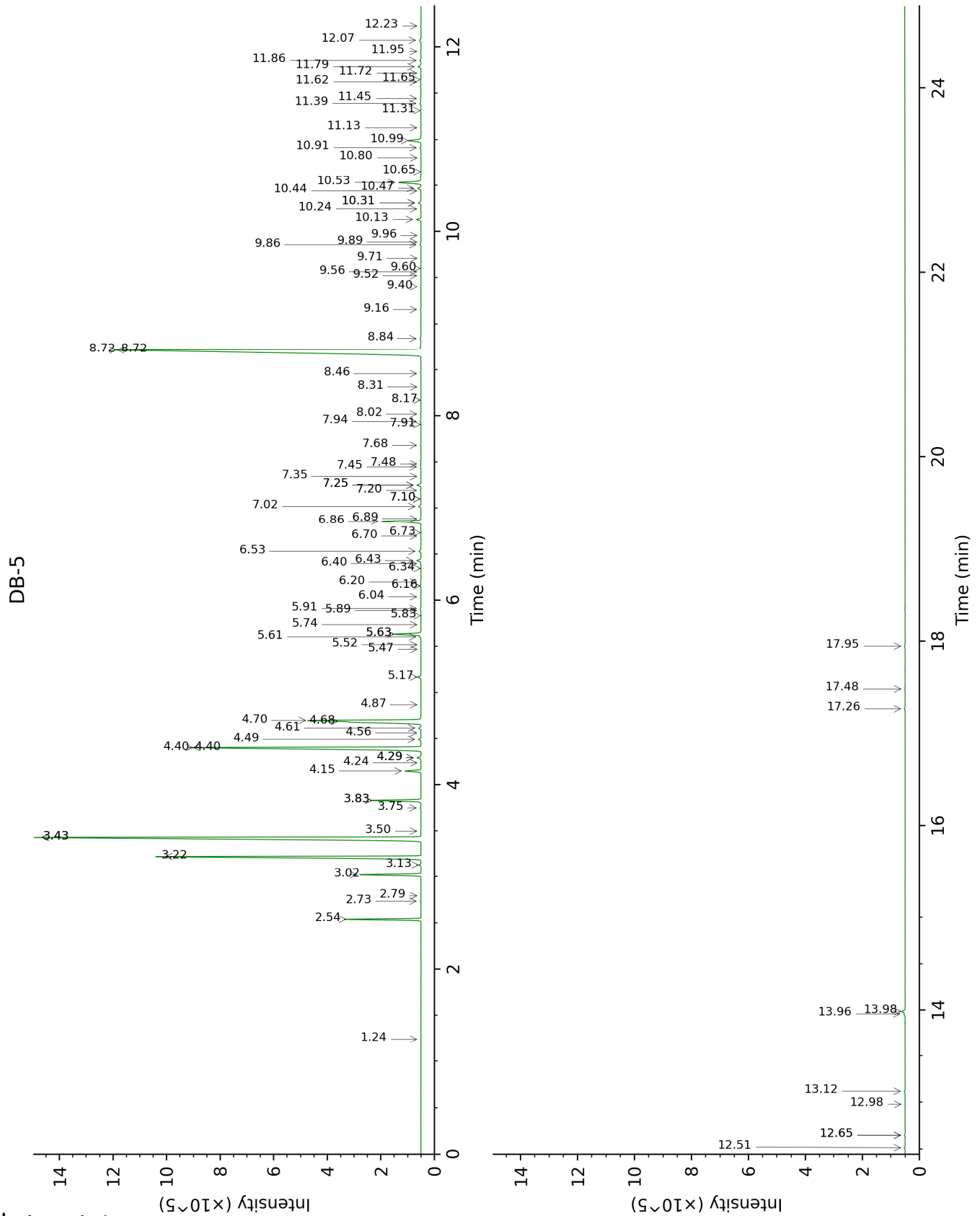
(E)-Nerolidol	0.03	Sesquiterpenic alcohol
Caryophyllene oxide	0.04	Sesquiterpenic ether
Caryophyllene oxide isomer	0.01	Sesquiterpenic ether
Humulene epoxide II	0.02	Sesquiterpenic ether
Selin-6-en-4 $\alpha$ -ol isomer	0.05	Sesquiterpenic alcohol
$\alpha$ -Bisabolol	0.07	Sesquiterpenic alcohol
epi- $\alpha$ -Bisabolol	0.18	Sesquiterpenic alcohol
Manoyl oxide	0.05	Diterpenic ether
13-epi-Manoyl oxide	0.03	Diterpenic ether
Manool	0.04	Diterpenic alcohol
<b>Consolidated total</b>	<b>99.18%</b>	

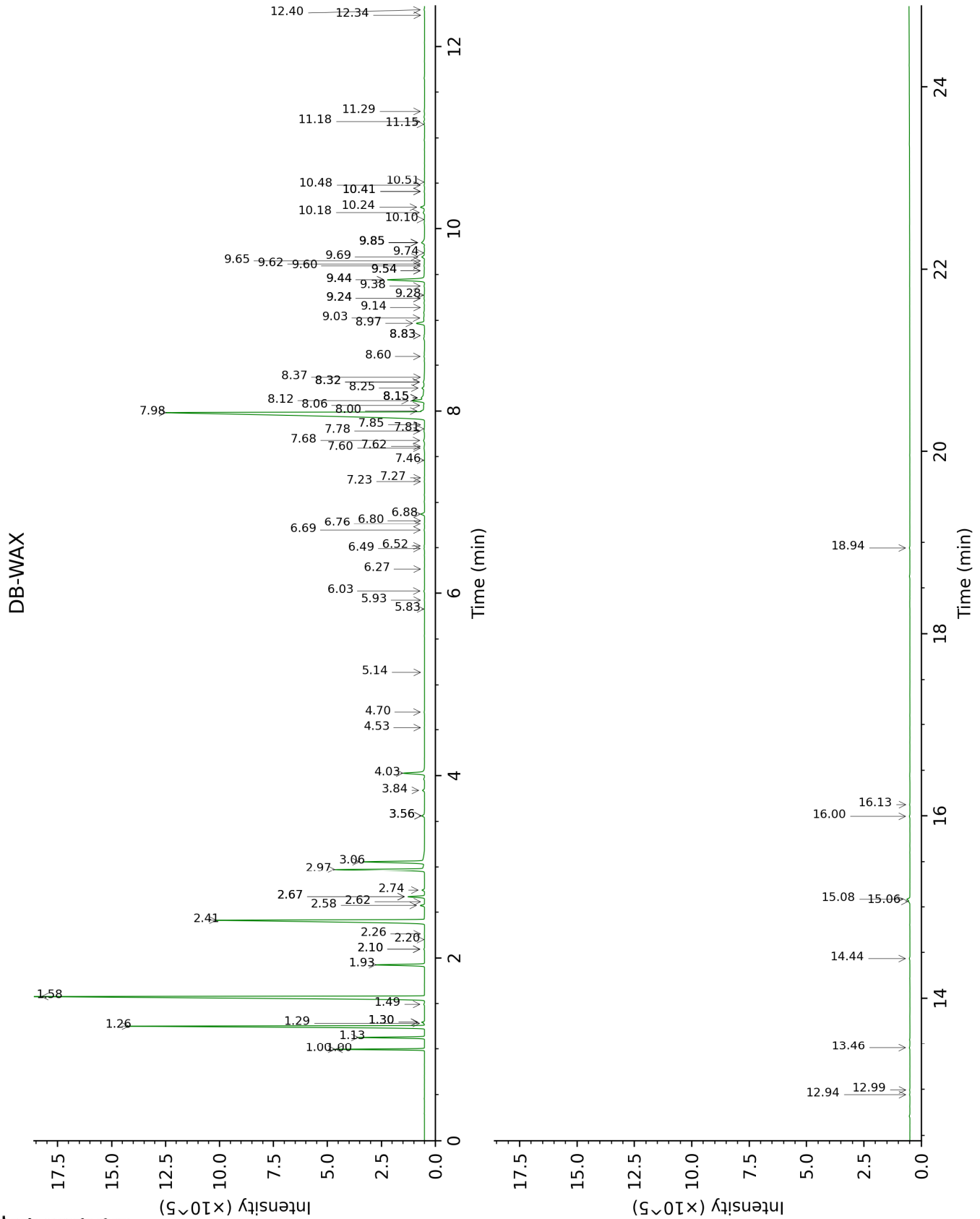
Note: no correction factor was applied

**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.







FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
Toluene	1.24	759	0.01	1.30*	1002	0.09
Santene	2.54	883	2.56	1.00*	949	2.59
Unknown [m/z 79, 93 (66), 94 (52), 91 (39), 77 (37), 122 (31)]	2.74	899	0.02	1.29	1000	0.02
Bornylene	2.79	904	0.01	1.00*	949	[2.59]
Tricyclene	3.02	919	2.27	1.13	973	2.25
$\alpha$ -Thujene	3.13	926	0.09	1.30*	1002	[0.09]
$\alpha$ -Pinene	3.22	932	12.58	1.26	994	12.66
Camphene	3.43*	946	22.60	1.58	1030	22.67
$\alpha$ -Fenchene	3.43*	946	[22.60]	1.49	1021	0.03
Thuja-2,4(10)-diene 3,7,7-	3.50	950	0.02	2.10*	1084	0.03
Trimethylcyclohepta-1,3,5-triene	3.75	967	0.04	2.67*	1134	0.69
$\beta$ -Pinene	3.83*	972	1.96	1.93	1066	1.94
Sabinene	3.83*	972	[1.96]	2.10*	1084	[0.03]
Myrcene	4.15	993	0.65	2.67*	1134	[0.69]
2-Carene	4.24	999	0.01	2.20	1095	0.01
$\alpha$ -Phellandrene	4.29*	1002	0.19	2.58	1127	0.18
Pseudolimonene	4.29*	1002	[0.19]	2.62	1130	0.01
$\Delta^3$ -Carene	4.40*	1010	12.64	2.41	1114	12.72
(3Z)-Hexenyl acetate	4.40*	1010	[12.64]	4.53	1283	0.01
$\alpha$ -Terpinene	4.49	1015	0.11	2.74	1140	0.11
Carvomenthene	4.56	1019	0.03	2.26	1101	0.01
para-Cymene	4.61	1023	0.12	3.84	1229	0.12
$\beta$ -Phellandrene	4.68†	1027	7.68	3.06	1166	3.15
Limonene	4.70†	1028	[7.68]	2.97	1159	4.63
(Z)- $\beta$ -Ocimene	4.86	1038	0.02	3.56*	1208	0.17
$\gamma$ -Terpinene	5.17	1058	0.16	3.56*	1208	[0.17]
Octanol	5.47	1076	0.01	7.85	1523	0.01
meta-Cymenene	5.52	1079	0.01	5.93	1378	0.02
$\gamma$ -Campholenal	5.61	1085	0.05	4.70	1296	0.03
Terpinolene	5.64*	1086	1.23	4.03	1244	1.17
para-Cymenene	5.64*	1086	[1.23]	6.03	1385	0.04
$\alpha$ -Pinene oxide	5.74	1093	0.01	5.14	1320	0.01
Unknown [m/z 109, 43 (65), 95 (54), 119 (50), 91 (47)... 149 (8)...]	5.84	1099	0.01	5.83	1371	0.02
Unknown [m/z 79, 94 (87), 77 (25), 91 (21), 93 (16), 95 (12), 138 (8)]	5.89	1102	0.03			
Linalool	5.91	1104	0.05	7.78	1518	0.04
endo-Fenchol	6.04	1112	0.03	8.06	1540	0.08
cis-para-Menth-2-en-1-ol	6.16	1119	0.03	7.81	1519	0.02

α-Campholenal	6.20	1122	0.03	6.69	1435	0.03
Cosmene	6.34	1131	0.01	6.27	1403	0.01
trans-Pinocarveol	6.40	1135	0.03	8.83*	1600	0.03
Camphor	6.43	1137	0.21	6.88	1449	0.20
Camphene hydrate	6.53	1143	0.11	8.15*†	1546	[1.20]
Isoborneol	6.70	1154	0.04	9.03	1616	0.12
Pinocarvone	6.73	1156	0.01	7.62	1504	0.02
Borneol	6.86	1164	1.94	9.44*	1650	2.15
Isopinocampone	6.89	1166	0.05	7.27	1478	0.01
Terpinen-4-ol	7.02	1174	0.12	8.25	1554	0.21
meta-Cymen-8-ol	7.10*	1180	0.04	11.15	1794	0.02
Cryptone	7.10*	1180	[0.04]	8.83*	1600	[0.03]
para-Cymen-8-ol	7.20	1185	0.04	11.18	1797	0.05
α-Terpineol	7.25*	1189	0.21	9.44*	1650	[2.15]
Myrtenal	7.25*	1189	[0.21]	8.37	1564	0.05
Myrtenol	7.35	1195	0.03	10.51	1739	0.02
Unknown [m/z 109, 91 (100), 81 (88), 94 (75), 119 (74), 96 (73), 41 (63)... 150 (2)]	7.45	1202	0.04	10.48	1736	0.03
Verbenone	7.48	1204	0.03	9.28	1636	0.03
endo-Fenchyl acetate	7.68	1217	0.03	6.52	1422	0.02
Citronellol	7.91	1232	0.02	10.41*	1730	0.03
Thymol methyl ether	7.94	1234	0.07	8.15*†	1546	[1.20]
Carvone	8.02	1239	0.04	9.65	1667	0.02
Piperitone	8.17	1249	0.02	9.54*	1658	0.05
Geraniol	8.31	1259	0.03	11.29	1806	0.04
Phellandral	8.46	1269	0.04	9.60	1662	0.04
Isobornyl acetate	8.72*	1286	26.76	8.00	1535	0.23
Bornyl acetate	8.72*	1286	[26.76]	7.98	1533	26.32
2-Undecanone	8.84	1294	0.06	8.32*	1560	0.13
Isohexyl isocaproate	9.16	1316	0.04	7.23	1475	0.02
Unknown [m/z 135, 91 (76), 43 (59), 77 (39), 93 (33)...]	9.40	1333	0.02			
Unknown [m/z 121, 93 (84), 43 (81), 79 (48), 117 (40), 56 (37)...]	9.52	1342	0.02			
α-Longipinene	9.56	1344	0.03	6.49	1420	0.03
α-Terpinyl acetate	9.60	1347	0.01	9.38	1644	0.04
Citronellyl acetate	9.71	1355	0.02	9.14	1625	0.03
Neryl acetate	9.86	1365	0.06	9.85*	1683	0.26
α-Ylangene	9.89	1367	0.02	6.76	1440	0.02
α-Copaene	9.96	1372	0.02	6.80	1443	0.01
Geranyl acetate	10.13	1384	0.22	10.24	1716	0.23
β-Longipinene	10.24	1392	0.03	7.46	1493	0.01
Longifolene	10.31*	1397	0.14	7.68	1510	0.09
Sibirene	10.31*	1397	[0.14]	7.60	1503	0.03
Methyleugenol	10.44	1406	0.02	13.00	1962	0.02
Dodecanal	10.47	1408	0.16	9.69	1671	0.18

β-Caryophyllene	10.53	1413	1.21	8.12†	1544	1.20
Caryophylla-4(12),8(13)-diene	10.65	1422	0.01	8.32*	1560	[0.13]
<i>trans</i> -α-Bergamotene	10.80	1433	0.01	8.15*†	1546	[1.20]
α-Himachalene	10.91	1441	0.05	8.60	1582	0.04
α-Humulene	10.99	1447	0.68	8.97	1611	0.51
( <i>E</i> )-β-Farnesene	11.13	1457	0.02	9.24*	1633	0.04
γ-Himachalene	11.31	1471	0.03	9.24*	1633	[0.04]
Unknown [m/z 91, 93 (92), 105 (71), 77 (69), 79 (68), 133 (63)... 204 (32)]	11.39	1477	0.08			
Unknown [m/z 43, 58 (75), 57 (58), 71 (55), 41 (41), 59 (31)...]	11.44	1481	0.05			
β-Himachalene	11.62	1494	0.04	9.54*	1658	[0.05]
α-Muurolene	11.65	1496	0.03	9.74	1674	0.03
( <i>Z</i> )-α-Bisabolene	11.72	1501	0.03	9.85*	1683	[0.26]
β-Bisabolene	11.79	1506	0.18	9.85*	1683	[0.26]
( <i>Z</i> )-γ-Bisabolene	11.86	1512	0.06	9.62	1664	0.02
δ-Cadinene	11.95	1519	0.03	10.10	1704	0.03
( <i>E</i> )-γ-Bisabolene	12.07	1529	0.09	10.18	1711	0.10
( <i>E</i> )-α-Bisabolene	12.23	1541	0.02	10.41*	1730	[0.03]
( <i>E</i> )-Nerolidol	12.51	1563	0.03	13.46	2004	0.04
Caryophyllene oxide	12.65*	1574	0.04	12.40	1906	0.04
Caryophyllene oxide isomer	12.65*	1574	[0.04]	12.34	1900	0.01
Humulene epoxide II	12.98	1600	0.02	12.94	1957	0.02
Selin-6-en-4α-ol isomer	13.12	1611	0.05	14.44	2100	0.04
α-Bisabolol	13.96	1680	0.07	15.06	2163	0.07
epi-α-Bisabolol	13.98	1683	0.18	15.08	2166	0.19
Manoyl oxide	17.26	1976	0.05	16.13	2274	0.02
13-epi-Manoyl oxide	17.48	1997	0.03	16.00	2260	0.03
Manool	17.95	2043	0.04	18.94	2590	0.03
<b>Total identified</b>		<b>98.88%</b>			<b>98.73%</b>	
<b>Total reported</b>		<b>99.16%</b>			<b>98.80%</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

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index