

Date : 2024-08-12

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 24G29-NSO01

Customer Identification : CO2 Extract : Fir subcritical - Siberian - Lot: 09-24

Type : CO2 Extract

Source : *Abies sibirica*

Customer : Natural Sourcing LLC

Checked and approved by:

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

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GAS CHROMATOGRAPHIC ANALYSIS

Method : PC-MAT-004 - Terpenes and volatiles profiling by response factor

Results : See analysis summary (next page)

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

Date : 2024-08-08

PHYSICOCHEMICAL DATA

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

ANALYSIS SUMMARY

Identification	mg/g	% m/m	Class
Toluene	0.03	0.0	Simple phenolic
(2E)-Hexenal	0.16	0.02	Aliphatic aldehyde
(3Z)-Hexenol	0.87	0.09	Aliphatic alcohol
Hexanol	0.12	0.01	Aliphatic alcohol
Santene	0.92	0.09	Normonoterpene
Tricyclene	9.80	0.98	Monoterpene
2,5-Hexanedione	0.04	0.0	Aliphatic ketone
α -Thujene	0.62	0.06	Monoterpene
α -Pinene	57.05	5.71	Monoterpene
α -Fenchene	0.13	0.01	Monoterpene
Camphene	98.56	9.86	Monoterpene
Thuja-2,4(10)-diene	0.03	0.0	Monoterpene
Cymene isomer?	1.04	0.1	Monoterpene
β -Pinene	22.78	2.28	Monoterpene
Sabinene	0.08	0.01	Monoterpene
6-Methyl-5-hepten-2-one	0.07	0.01	Aliphatic ketone
Myrcene	2.30	0.23	Monoterpene
2-Carene	0.04	0.0	Monoterpene
Menthatriene isomer I	0.02	0.0	Monoterpene
Pseudolimonene	0.02	0.0	Monoterpene
α -Phellandrene	0.18	0.02	Monoterpene
Δ^3 -Carene	73.05	7.3	Monoterpene
(3Z)-Hexenyl acetate	0.65	0.07	Aliphatic ester
α -Terpinene	0.10	0.01	Monoterpene
Hexyl acetate	0.20	0.02	Aliphatic ester
<i>meta</i> -Cymene	0.17	0.02	Monoterpene
<i>para</i> -Cymene	1.08	0.11	Monoterpene
β -Phellandrene	24.14	2.41	Monoterpene
Limonene	25.03	2.5	Monoterpene
γ -Terpinene	0.14	0.01	Monoterpene
<i>cis</i> -Sabinene hydrate	0.11	0.01	Monoterpenic alcohol
<i>meta</i> -Cymenene	0.02	0.0	Monoterpene
Camphenilone	0.04	0.0	Normonoterpenic ketone
Isoterpinolene	0.17	0.02	Monoterpene
<i>para</i> -Cymenene	0.20	0.02	Monoterpene
Terpinolene	2.04	0.2	Monoterpene
2-Nonanone	0.12	0.01	Aliphatic ketone
Undecane	0.13	0.01	Alkane
Verbenol analog?	0.06	0.01	Monoterpenic alcohol
Maltol	3.48	0.35	Aliphatic alcohol
endo-Fenchol	0.37	0.04	Monoterpenic alcohol

(E)-4,8-Dimethyl-1,3,7-nonatriene	0.03	0.0	Monoterpene
<i>cis-para</i> -Menth-2-en-1-ol	0.42	0.04	Monoterpenic alcohol
α -Campholenal	0.11	0.01	Monoterpenic aldehyde
Nopinone	0.46	0.05	Normonoterpenic ketone
<i>cis</i> -Limonene oxide	0.20	0.02	Monoterpenic ether
<i>trans</i> -Pinocarveol	0.45	0.04	Monoterpenic alcohol
Camphor	1.76	0.18	Monoterpenic ketone
Camphene hydrate	0.67	0.07	Monoterpenic alcohol
Epoxyterpinolene	0.29	0.03	Monoterpenic ether
Isoborneol	0.11	0.01	Monoterpenic alcohol
Pinocamphone	0.10	0.01	Monoterpenic ketone
Phellandrenol analog I	0.44	0.04	Monoterpenic alcohol
Borneol	31.65	3.17	Monoterpenic alcohol
Unknown	0.39	0.04	Oxygenated monoterpene
Terpinen-4-ol	0.21	0.02	Monoterpenic alcohol
<i>trans</i> -2-Caren-4-ol	0.53	0.05	Monoterpenic alcohol
Cryptone	0.86	0.09	Normonoterpenic ketone
<i>meta</i> -Cymen-8-ol	0.47	0.05	Monoterpenic alcohol
<i>para</i> -Cymen-8-ol	1.25	0.12	Monoterpenic alcohol
α -Terpineol	0.58	0.06	Monoterpenic alcohol
Myrtenol	0.10	0.01	Monoterpenic alcohol
<i>para</i> -Mentha-1,5-dien-7-ol	0.04	0.0	Monoterpenic alcohol
Methylchavicol	0.03	0.0	Phenylpropanoid
Verbenone	0.56	0.06	Monoterpenic ketone
endo-Fenchyl acetate	0.20	0.02	Monoterpenic ester
Unknown	0.05	0.01	Oxygenated monoterpene
Bornyl formate	2.91	0.29	Monoterpenic ester
Thymol methyl ether	0.72	0.07	Monoterpenic ether
Nojigiku acetate	[0.11]	0.01	Monoterpenic ester
Carvone	[0.10]	0.01	Monoterpenic ketone
2-Nonyl acetate	0.16	0.02	Aliphatic ester
Car-3-en-2-one	0.19	0.02	Monoterpenic ketone
Piperitone	0.10	0.01	Monoterpenic ketone
Linalyl acetate	0.42	0.04	Monoterpenic ester
<i>trans</i> -Verbenyl acetate	0.13	0.01	Monoterpenic ester
<i>cis</i> -Verbenyl acetate	0.06	0.01	Monoterpenic ester
Bornyl acetate	137.53	13.75	Monoterpenic ester
2-Undecanone	0.16	0.02	Aliphatic ketone
<i>trans</i> -Pinocarvyl acetate	0.47	0.05	Monoterpenic ester
Unknown	0.70	0.07	Unknown
4-Hydroxycryptone	0.26	0.03	Normonoterpenic alcohol
Terpinyl acetate analog	0.08	0.01	Monoterpenic ester
Limonene <i>trans</i> -glycol	0.12	0.01	Monoterpenic alcohol
α -Longipinene	0.39	0.04	Sesquiterpene
α -Terpinyl acetate	0.14	0.01	Monoterpenic ester

Citronellyl acetate	0.28	0.03	Monoterpenic ester
Neryl acetate	0.42	0.04	Monoterpenic ester
α -Ylangene	0.27	0.03	Sesquiterpene
α -Copaene	0.25	0.03	Sesquiterpene
Geranyl acetate	1.56	0.16	Monoterpenic ester
Sativene	0.11	0.01	Sesquiterpene
Sibirene	0.16	0.02	Sesquiterpene
Longifolene	1.62	0.16	Sesquiterpene
Ethyl decanoate	0.04	0.0	Aliphatic ester
Isocaryophyllene	0.01	0.0	Sesquiterpene
Acora-3,7(14)-diene	0.40	0.04	Sesquiterpene
Dodecanal	0.29	0.03	Aliphatic aldehyde
β -Cedrene	0.05	0.01	Sesquiterpene
β -Caryophyllene	10.36	1.04	Sesquiterpene
Unknown	0.10	0.01	Unknown
<i>trans</i> - α -Bergamotene	0.38	0.04	Sesquiterpene
6,9-Guaiadiene	0.05	0.01	Sesquiterpene
α -Himachalene	0.61	0.06	Sesquiterpene
α -Humulene	5.35	0.53	Sesquiterpene
γ -Himachalene	0.47	0.05	Sesquiterpene
γ -Humulene?	0.93	0.09	Sesquiterpene
β -Selinene	0.15	0.01	Sesquiterpene
Unknown	0.24	0.02	Sesquiterpene
2-Tridecanone	0.14	0.01	Aliphatic ketone
β -Alaskene	0.64	0.06	Sesquiterpene
α -Muurolene	0.13	0.01	Sesquiterpene
β -Himachalene	0.36	0.04	Sesquiterpene
Limona ketone	0.05	0.01	Normonoterpenic ketone
β -Bisabolene	3.18	0.32	Sesquiterpene
(<i>Z</i>)- γ -Bisabolene	0.60	0.06	Sesquiterpene
δ -Cadinene	0.22	0.02	Sesquiterpene
α -Cadinene	0.15	0.01	Sesquiterpene
(<i>E</i>)- γ -Bisabolene	0.86	0.09	Sesquiterpene
α -Calacorene	0.05	0.01	Sesquiterpene
(<i>E</i>)- α -Bisabolene	0.22	0.02	Sesquiterpene
Isocaryophyllene epoxide B	0.04	0.0	Sesquiterpenic ether
Raspberry ketone	0.22	0.02	Simple phenolic
(<i>E</i>)-Nerolidol	0.72	0.07	Sesquiterpenic alcohol
β -Calacorene	0.14	0.01	Sesquiterpene
Caryophyllene oxide isomer	0.04	0.0	Sesquiterpenic ether
Caryophyllene oxide	5.36	0.54	Sesquiterpenic ether
Longiborneol	0.33	0.03	Sesquiterpenic alcohol
Humulol	0.28	0.03	Sesquiterpenic alcohol
Humulene epoxide II	2.50	0.25	Sesquiterpenic ether
β -Himachalene oxide	0.22	0.02	Sesquiterpenic ether

Selin-6-en-4 α -ol isomer	0.96	0.1	Sesquiterpenic alcohol
Lauryl acetate	0.34	0.03	Aliphatic ester
1-epi-Cubenol	0.22	0.02	Sesquiterpenic alcohol
Humulene 9,10-epoxide	0.15	0.01	Sesquiterpenic ether
Unknown	0.04	0.0	Oxygenated sesquiterpene
Humulenol II	0.23	0.02	Sesquiterpenic alcohol
Gossonorol	0.22	0.02	Sesquiterpenic alcohol
Unknown	0.42	0.04	Oxygenated sesquiterpene
α -Bisabolol oxide B, epimer 2	0.19	0.02	Sesquiterpenic alcohol
α -Bisabolol oxide B, epimer 1	0.11	0.01	Sesquiterpenic alcohol
(3Z)-Caryophylla-3,8(13)-dien-5 β -ol	1.73	0.17	Sesquiterpenic alcohol
(6Z)-Pentadecen-2-one	0.13	0.01	Aliphatic ketone
α -Bisabolol	2.92	0.29	Sesquiterpenic alcohol
epi- α -Bisabolol	6.87	0.69	Sesquiterpenic alcohol
2-Pentadecanone	0.20	0.02	Aliphatic ketone
Atracic acid	0.29	0.03	Phenolic ester
Oplopanone	0.14	0.01	Sesquiterpenic alcohol
(E)-Coniferaldehyde	0.14	0.01	Phenylpropanoid
Unknown	0.14	0.01	Phenylpropanoid
Caryolane-1,9 β -diol	0.19	0.02	Sesquiterpenic alcohol
Farnesyl acetate isomer I	0.11	0.01	Sesquiterpenic ester
(2E,6E)-Farnesyl acetate	0.32	0.03	Sesquiterpenic ester
Unknown	0.33	0.03	Unknown
Pimaradiene	0.28	0.03	Diterpene
Palmitic acid	1.72	0.17	Aliphatic acid
Manoyl oxide	3.16	0.32	Diterpenic ether
Unknown	0.19	0.02	Diterpene
13-epi-Manoyl oxide	1.40	0.14	Diterpenic ether
Unknown	0.56	0.06	Diterpene
4-Hydroxy-4-methylcyclohex-2-enone	0.18	0.02	Aliphatic alcohol
ar-Abietatriene	0.18	0.02	Diterpene
Manool	12.27	1.23	Diterpenic alcohol
Sclareolide?	0.20	0.02	Terpenic lactone
7,13-Abietadiene	0.62	0.06	Diterpene
Unknown	0.69	0.07	Unknown
Unknown	2.72	0.27	Oxygenated diterpene
Unknown	1.32	0.13	Oxygenated diterpene
(Z)-Abienol	29.14	2.91	Diterpenic alcohol
Abienol isomer	1.22	0.12	Diterpenic lactone
Sclareol	0.44	0.04	Diterpenic alcohol
Palustral	0.46	0.05	Diterpenic aldehyde
Dehydroabietal	1.02	0.1	Diterpenic aldehyde
Abietal	1.44	0.14	Diterpenic aldehyde
8,13-Abietadien-18-ol?	0.51	0.05	Diterpenic alcohol
Tricosane	1.35	0.14	Alkane

Methyl dehydroabietate	0.36	0.04	Diterpenic ester
Dehydroabietol?	0.67	0.07	Diterpenic alcohol
Pentacosane	0.60	0.06	Alkane
Methyl abietate	0.57	0.06	Diterpenic ester
γ -Sitosterol?	0.25	0.03	Sterol
γ -Sitostenone?	0.99	0.1	Triterpenic ketone
Consolidated total	634.21	63.42	

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

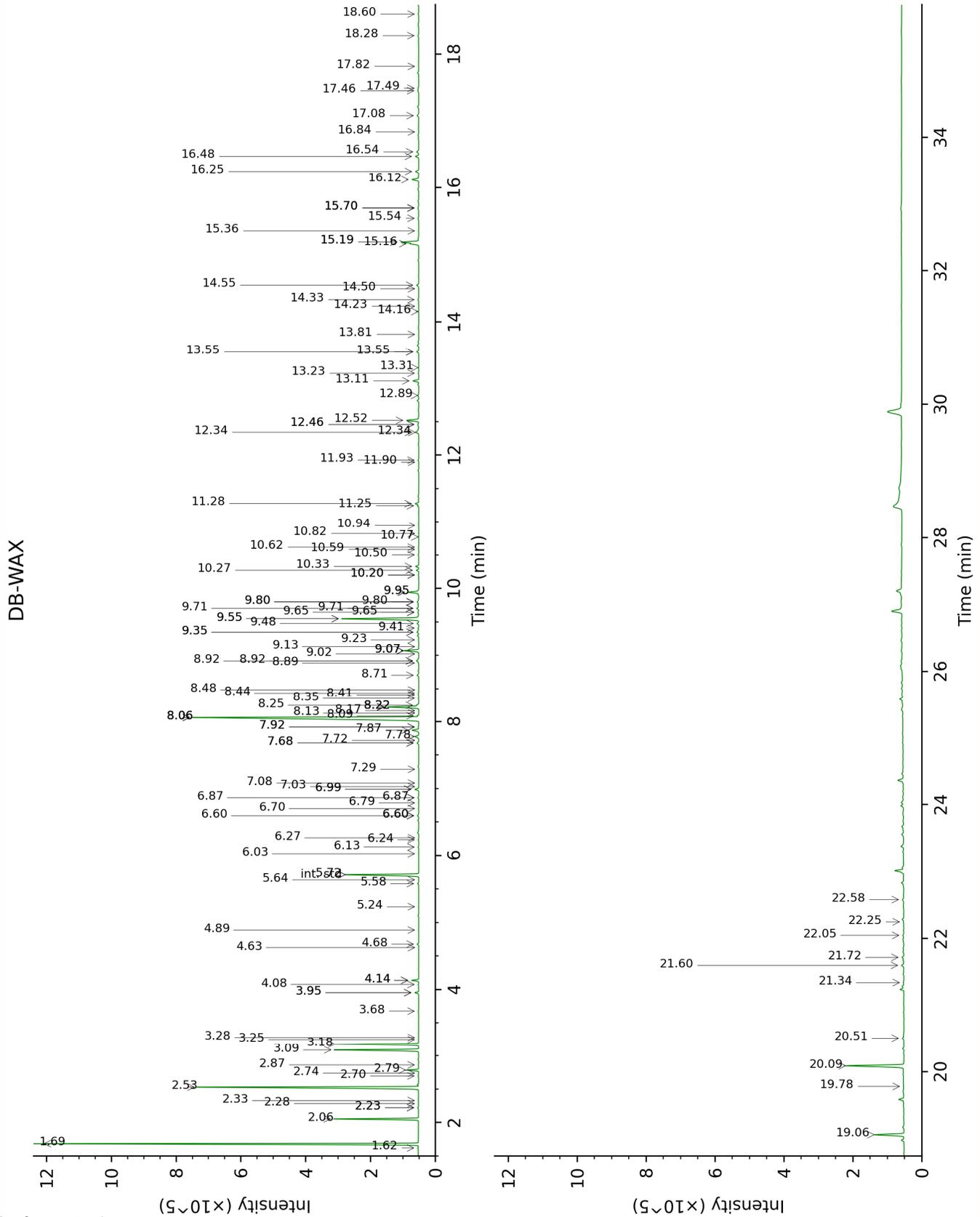
Note: Individual compounds contents were corrected following the method of Cachet et al., 2016 (Flavour and Fragrance Journal guidelines).

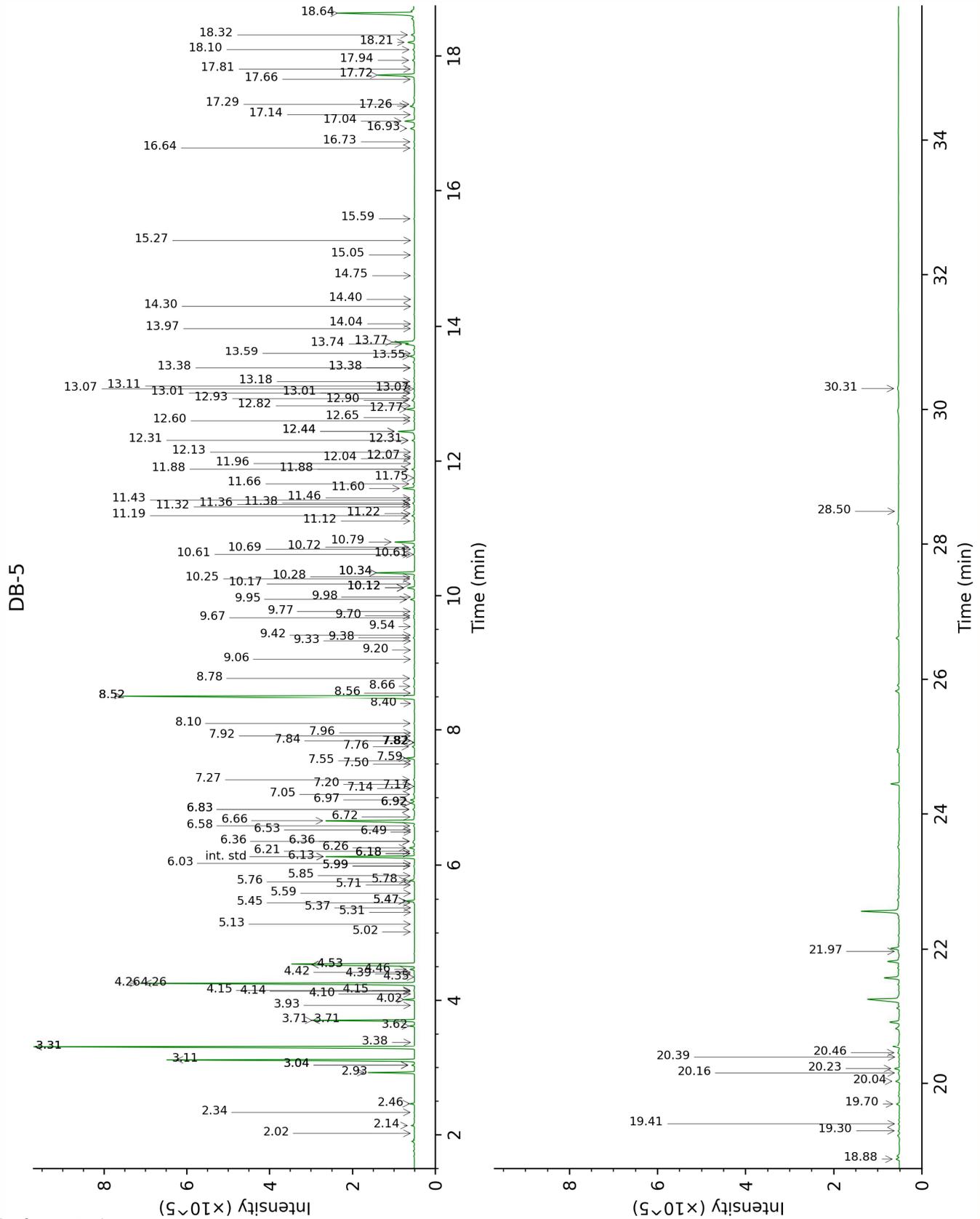
Unknown compounds are expressed in equivalents of internal standard without correction.

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: 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.





FULL ANALYSIS DATA

Toluene	Column DB-WAX			Column DB-5		
				1.25	770.1	tr
(2E)-Hexenal	3.25	1172.4	0.01	2.02	849.2	0.02
(3Z)-Hexenol	5.58	1344.6	0.06	2.14	859.0	0.10
Hexanol	5.24	1319.4	0.01	2.34	875.5	0.01
Santene	0.98	936.1	0.19	2.46	886.3	0.13
Tricyclene	1.28	987.5	1.37	2.93	921.0	1.37
2,5-Hexanedione	7.03	1452.0	tr	3.04*	928.4	[0.09]
α-Thujene	1.44	1009.6	0.09	3.04*	928.4	[0.09]
α-Pinene	1.40	1004.9	7.99	3.11	933.7	7.95
α-Fenchene	1.62	1027.8	0.02	3.31*	946.7	[13.68]
Camphene	1.69	1034.3	13.71	3.31*	946.7	[13.68]
Thuja-2,4(10)-diene	2.22*	1088.9	[0.04]	3.38	951.7	tr
Cymene isomer?				3.62	968.0	0.16
β-Pinene	2.06	1071.9	3.17	3.71*	973.6	[3.19]
Sabinene	2.22*	1088.9	[0.04]	3.71*	973.6	[3.19]
6-Methyl-5-hepten-2-one	4.89	1291.9	0.02	3.93	988.5	0.01
Myrcene	2.79	1136.1	0.48	4.02	994.3	0.32
2-Carene	2.28	1094.9	0.01	4.10	999.8	tr
Menthatriene isomer I	3.28	1174.8	tr	4.14*†	1002.5	[0.01]
Pseudolimonene	2.74	1132.5	tr	4.15*†	1003.5	[0.03]
α-Phellandrene	2.70	1129.2	0.03	4.15*†	1003.5	[0.03]
Δ3-Carene	2.53	1116.1	10.16	4.26*	1010.1	[10.19]
(3Z)-Hexenyl acetate	4.68	1276.9	0.06	4.26*	1010.1	[10.19]
α-Terpinene	2.86	1142.2	0.01	4.35	1016.0	0.01
Hexyl acetate	4.14*	1238.4	[0.30]	4.39	1018.8	0.02
meta-Cymene	3.95*	1225.2	[0.17]	4.42	1020.5	0.03
para-Cymene	3.95*	1225.2	[0.17]	4.46	1023.3	0.17
β-Phellandrene	3.18	1166.9	3.36	4.53*†	1027.7	[3.08]
Limonene	3.09	1160.0	3.48	4.53*†	1027.7	[3.08]
γ-Terpinene	3.68	1205.4	0.02	5.02	1058.5	0.02
cis-Sabinene hydrate	6.70	1427.3	0.02	5.13	1065.7	0.01
meta-Cymenene	6.03	1377.2	0.02	5.31	1076.9	tr
Camphenilone	6.27	1394.5	tr	5.37	1081.1	tr
Isoterpinolene	4.08	1234.0	0.03	5.45	1085.8	0.02
para-Cymenene	6.13	1384.5	0.03	5.47*	1087.5	[0.31]
Terpinolene	4.14*	1238.4	[0.30]	5.47*	1087.5	[0.31]
2-Nonanone	5.64	1348.8	0.01	5.59	1094.8	0.02
Undecane	2.33	1099.7	tr	5.71	1102.5	0.02

Verbenol analog?	8.13	1536.2	tr	5.76	1105.6	0.01
Maltol	12.34*	1889.9	[0.28]	5.78	1106.9	0.21
endo-Fenchol	8.22*	1543.2	[1.51]	5.85	1111.4	0.04
(E)-4,8-Dimethyl-1,3,7-nonatriene	4.63	1273.3	tr	5.99*	1120.7	[0.06]
cis-para-Menth-2-en-1-ol	7.92*	1519.8	[0.04]	5.99*	1120.7	[0.06]
α-Campholenal	6.79	1433.7	0.02	6.03	1123.2	0.01
Nopinone	8.09	1532.8	0.05	6.18*	1132.7	[0.03]
cis-Limonene oxide	6.24	1392.5	0.02	6.18*	1132.7	[0.03]
trans-Pinocarveol	8.92*	1598.0	[0.17]	6.21	1134.9	0.05
Camphor	6.99*	1449.0	[0.19]	6.26	1138.2	0.21
Camphene hydrate	8.25	1545.3	0.08	6.36*†	1144.4	[0.04]
Epoxyterpinolene	6.60*	1419.3	[0.08]	6.36*†	1144.4	[0.04]
Isoborneol	9.13	1615.2	0.01	6.49	1153.3	0.01
Pinocamphone	7.08	1456.0	0.01	6.53	1155.5	0.01
Phellandrenol analog I	9.80*	1670.0	[0.13]	6.58	1159.3	0.05
Borneol	9.55*	1649.4	[3.92]	6.66	1164.2	3.88
Unknown AFGI I [m/z 109, 79 (18), 81 (15), 91 (12), 77 (10)... 152 (3)]				6.72	1167.9	0.04
Terpinen-4-ol	8.35	1553.6	0.03	6.83*	1175.1	[0.09]
trans-2-Caren-4-ol	7.68*	1501.0	[0.09]	6.83*	1175.1	[0.09]
Cryptone	8.92*	1598.0	[0.17]	6.92*	1181.1	[0.16]
meta-Cymen-8-ol	11.25	1792.3	0.06	6.92*	1181.1	[0.16]
para-Cymen-8-ol	11.28	1795.0	0.18	6.97	1184.2	0.17
α-Terpineol	9.55*	1649.4	[3.92]	7.05	1189.5	0.07
Myrtenol	10.62	1738.6	0.03	7.14	1195.1	0.01
para-Mentha-1,5-dien-7-ol	10.77	1751.6	0.01	7.17	1197.2	tr
Methylchavicol	9.07*	1610.3	[0.75]	7.20	1199.2	0.01
Verbenone	9.41	1637.9	0.04	7.27	1203.6	0.07
endo-Fenchyl acetate	6.60*	1419.3	[0.08]	7.50	1219.1	0.02
Unknown DACA VI [m/z 119, 43 (52), 59 (45), 91 (36), 79 (24), 134 (23)...]	10.82	1756.0	0.02	7.55	1222.4	0.01
Bornyl formate	7.87	1516.0	0.37	7.59	1225.2	0.31

Thymol methyl ether	8.22*	1543.2	[1.51]	7.76	1236.6	0.10
Nojigiku acetate				7.82*	1240.9	[0.01]
Carvone				7.82*	1240.9	[0.01]
2-Nonyl acetate	6.87*	1439.5	[0.04]	7.84	1242.6	0.02
Car-3-en-2-one	10.20*	1702.9	[0.02]	7.92	1247.5	0.02
Piperitone	9.70*	1662.1	[0.13]	7.96	1250.6	0.01
Linalyl acetate	7.92*	1519.8	[0.04]	8.10	1260.2	0.05
<i>trans</i> -Verbenyl acetate	9.07*	1610.3	[0.75]	8.40	1280.2	0.01
<i>cis</i> -Verbenyl acetate	8.48	1563.8	0.01	8.52*	1288.3	[15.32]
Bornyl acetate	8.06*	1531.0	[15.29]	8.52*	1288.3	[15.32]
2-Undecanone	8.41	1558.0	0.02	8.56	1291.4	0.02
<i>trans</i> -Pinocarvyl acetate	8.89	1595.4	0.02	8.66	1298.1	0.05
Unknown CASA XVII [m/z 93, 111 (86), 43 (70), 110 (55), 59 (53), 69 (52), 41 (47)...]	13.23	1971.8	0.03	8.78	1306.2	0.08
4-Hydroxycryptone	15.36	2180.0	0.02	9.06	1322.8	0.03
Terpinyl acetate analog	9.35*	1632.9	[0.13]	9.20	1332.5	0.01
Limonene <i>trans</i> -glycol	15.70*	2214.8	[0.08]	9.33	1342.2	0.01
α -Longipinene	6.60*	1419.3	[0.08]	9.38	1345.4	0.06
α -Terpinyl acetate	9.48	1643.6	0.09	9.42	1348.2	0.02
Citronellyl acetate	9.23	1623.5	0.02	9.54	1357.3	0.03
Neryl acetate	9.94*	1681.8	[0.56]	9.67	1366.5	0.05
α -Ylangene	6.87*	1439.5	[0.04]	9.70	1368.6	0.04
α -Copaene	6.99*	1449.0	[0.19]	9.77	1373.1	0.04
Geranyl acetate	10.33	1713.9	0.15	9.94	1385.8	0.17
Sativene	7.29	1471.4	tr	9.98	1388.3	0.02
Sibirene	7.68*	1501.0	[0.09]	10.12*	1397.9	[0.29]
Longifolene	7.78	1508.5	0.23	10.12*	1397.9	[0.29]
Ethyl decanoate	9.02	1606.3	tr	10.12*	1397.9	[0.29]
Isocaryophyllene	8.06*	1531.0	[15.29]	10.17	1402.1	tr
Acora-3,7(14)-diene	8.06*	1531.0	[15.29]	10.25	1407.6	0.06
Dodecanal	9.80*	1670.0	[0.13]	10.28	1409.7	0.04
β -Cedrene	8.17	1538.9	0.01	10.34*	1414.2	[1.48]

β-Caryophyllene	8.22*	1543.2	[1.51]	10.34*	1414.2	[1.48]
Unknown ZIOF XIV [m/z 41, 97 (78), 69 (77), 43 (71), 125 (67), 55 (56)... 168 (39)]	16.84	2335.9	0.01	10.61*	1434.6	[0.06]
<i>trans</i> -α- Bergamotene	8.22*	1543.2	[1.51]	10.61*	1434.6	[0.06]
6,9-Guaiadiene	8.44	1560.0	0.02	10.69	1440.4	0.01
α-Himachalene	8.70	1581.1	0.10	10.72	1442.6	0.09
α-Humulene	9.07*	1610.3	[0.75]	10.79	1448.4	0.76
γ-Himachalene	9.35*	1632.9	[0.13]	11.12	1472.4	0.07
γ-Humulene?	9.70*	1662.1	[0.13]	11.19	1478.3	0.13
β-Selinene	9.65*	1657.3	[0.07]	11.22	1480.7	0.02
Unknown ZAAR VI [m/z 81, 82 (62), 41 (37), 69 (36), 43 (36), 110 (33), 71 (32)...204 (1)]	18.60	2532.5	0.03	11.32	1488.1	0.03
2-Tridecanone	10.94	1766.4	0.01	11.36	1490.7	0.02
β-Alaskene				11.38	1492.3	0.09
α-Murolene	9.80*	1670.0	[0.13]	11.43	1495.7	0.02
β-Himachalene	9.65*	1657.3	[0.07]	11.46	1498.0	0.05
Limona ketone	7.72	1504.0	0.01			
β-Bisabolene	9.94*	1681.8	[0.56]	11.60	1508.7	0.45
(<i>Z</i>)-γ-Bisabolene				11.66	1514.0	0.08
δ-Cadinene	10.20*	1702.9	[0.02]	11.75	1521.0	0.03
α-Cadinene	10.58	1735.6	0.02	11.88*	1531.1	[0.11]
(<i>E</i>)-γ-Bisabolene	10.27	1709.0	0.12	11.88*	1531.1	[0.11]
α-Calacorene	11.90	1850.0	tr	11.96	1537.7	0.01
(<i>E</i>)-α-Bisabolene	10.50	1728.6	0.03	12.04	1543.6	0.03
Isocaryophyllene epoxide B	11.93	1852.8	0.04	12.07	1545.8	0.01
Raspberry ketone				12.14	1551.2	0.02
(<i>E</i>)-Nerolidol	13.55*	2001.7	[0.12]	12.31*	1564.9	[0.11]
β-Calacorene	12.46*	1900.4	[0.09]	12.31*	1564.9	[0.11]
Caryophyllene oxide isomer	12.46*	1900.4	[0.09]	12.44*	1575.4	[0.69]
Caryophyllene oxide	12.52	1906.1	0.69	12.44*	1575.4	[0.69]
Longiborneol	14.33	2077.8	0.04	12.60	1587.6	0.04
Humulol	14.50	2093.5	0.02	12.65	1591.6	0.04
Humulene epoxide II	13.11	1961.1	0.31	12.77	1601.2	0.32

β-Himachalene oxide	12.90	1940.8	0.07	12.82	1605.3	0.03
Selin-6-en-4α-ol isomer	14.55	2098.6	0.13	12.90	1611.9	0.13
Lauryl acetate				12.92	1614.0	0.04
1-epi-Cubenol	13.55*	2001.7	[0.12]	13.01*	1620.9	[0.05]
Humulene 9,10-epoxide	13.31	1979.5	0.02	13.01*	1620.9	[0.05]
Unknown JUVI XII [m/z 132, 175 (22), 119 (18), 91 (18), 157 (18)... 219 (10)]				13.07*	1626.0	[0.03]
Humulenol II	15.70*	2214.8	[0.08]	13.07*	1626.0	[0.03]
Gossonorol				13.11	1629.4	0.03
Unknown JUVI XIII [m/z 132, 91 (24), 119 (22), 105 (21), 133 (17), 117 (16)... 219 (3)]				13.18	1635.0	0.05
α-Bisabolol oxide B, epimer 2	14.24	2068.3	0.02	13.38*	1651.8	[0.05]
α-Bisabolol oxide B, epimer 1	14.16	2060.7	0.01	13.38*	1651.8	[0.05]
(3Z)-Caryophylla-3,8(13)-dien-5β-ol	16.54	2303.5	0.14	13.55	1666.1	0.22
(6Z)-Pentadecen-2-one	12.34*	1889.9	[0.28]	13.59	1669.5	0.02
α-Bisabolol	15.16	2160.7	0.39	13.74	1681.8	0.38
epi-α-Bisabolol	15.19*	2163.2	[0.92]	13.77	1684.3	0.89
2-Pentadecanone				13.97	1700.9	0.03
Atracic acid				14.04	1706.5	0.02
Oplopanone	17.82	2443.7	0.02	14.30	1728.9	0.02
(E)-Coniferaldehyde				14.40	1738.0	0.01
Unknown WTAR IX [m/z 137, 164 (59), 224 (42), 149 (33)]				14.75	1768.4	0.01
Caryolane-1,9β-diol	19.78	2672.2	0.04	15.05	1794.8	0.02
Farnesyl acetate isomer I	15.54	2198.9	0.05	15.27	1813.8	0.01
(2E,6E)-Farnesyl	15.70*	2214.8	[0.08]	15.59	1843.0	0.04

acetate						
Unknown FRAG MXX [m/z 137, 43 (96), 95 (81), 81 (79), 107 (54)...]	17.49	2407.0	0.04	16.64	1940.5	0.04
Pimaradiene	15.19*	2163.2	[0.92]	16.73	1949.3	0.04
Palmitic acid				16.93	1968.2	0.21
Manoyl oxide	16.25	2272.6	0.19	17.04	1978.4	0.43
Unknown PIGL IV [m/z 197, 239 (66), 254 (35)]				17.14	1987.5	0.02
13-epi-Manoyl oxide	16.12	2259.1	0.40	17.26	1999.4	0.19
Unknown PIGL III [m/z 159, 241 (87), 69 (60), 185 (34), 81 (31), 256 (26)...]				17.29	2002.1	0.06
4-Hydroxy-4- methylcyclohex- 2-enone	13.82	2027.5	0.02			
ar-Abietatriene	17.46	2402.8	0.07	17.66	2038.5	0.03
Manool	19.06	2585.9	1.53	17.72	2044.8	1.67
Sclareolide?	21.34	2867.4	0.05	17.81	2053.5	0.02
7,13-Abietadiene	17.08	2362.3	0.10	17.94	2066.6	0.09
Unknown MISC CXXXV [m/z 204, 109 (57), 80 (50), 93 (32), 81 (28), 161 (26)..]				18.10	2082.2	0.07
Unknown ABBA XIII [m/z 191, 95 (32), 69 (26), 123 (26), 109 (24)...290 (9)]				18.21	2093.0	0.29
Unknown ABBA XII [m/z 177, 95 (36), 43 (35), 69 (34), 71 (32), 121 (26)...290 (13)]				18.32	2104.0	0.14
(Z)-Abienol	20.09	2709.8	3.22	18.64	2137.1	3.91
Abienol isomer				18.88	2162.4	0.16
Sclareol	22.58	3031.0	0.10	19.30	2205.7	0.06
Palustral	20.51	2762.0	0.10	19.40	2216.8	0.06
Dehydroabietal	21.72	2916.2	0.11	19.70	2248.4	0.13

Abietal	21.60	2900.5	0.15	20.04	2284.7	0.19
8,13-Abietadien-18-ol?				20.16	2298.1	0.06
Tricosane	16.48	2296.4	0.19	20.22	2305.1	0.20
Methyl dehydroabietate	22.25	2986.2	0.04	20.39	2324.0	0.04
Dehydroabietol?				20.46	2331.2	0.09
Pentacosane	18.28	2495.2	0.05	21.97	2503.5	0.09
Methyl abietate	22.05	2959.6	0.07			
γ-Sitosterol?				28.50	3279.0	0.03
γ-Sitostenone?				30.31	3402.3	0.14
Total reported		83.15%			85.65%	

*: 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