

Date : December 18, 2018

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 18L10-PTH01-1-CC

**Customer identification :** Helichrysum Italicum - Herzegovina - H2010786R

**Type :** Essential oil

**Source :** *Helichrysum italicum*

**Customer :** Plant Therapy

ANALYSIS

**Method:** PC-PA-014-17J19 - Analysis of the composition of an essential oil, or other volatile liquid, by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Sylvain Mercier, M. Sc., Chimiste

**Analysis date :** December 11, 2018

Checked and approved by :



Alexis St-Gelais, M. Sc., chimiste 2013-174

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#### PYHSICOCHEMICAL DATA

**Physical aspect:** Faintly yellow liquid

**Refractive index:**  $1.4753 \pm 0.0003$  (20 °C)

#### CONCLUSION

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

## ANALYSIS SUMMARY

Identification	DB-5 (%)	DB-WAX (%)	Classe
2-Methylbutyral	tr	tr	Aliphatic aldehyde
3-Pentanone	0.01	0.01	Aliphatic ketone
2-Ethylfuran	0.01	tr	Furan
2-Methyl-3-pantanone	0.02	0.02	Aliphatic ketone
Unknown	tr		Unknown
Unknown	0.01	0.01	Unknown
Hexanal	tr	0.01	Aliphatic aldehyde
Octane	0.01	0.01	Alkane
2-Methyl-2-heptene	0.04	0.04	Alkene
4-Methyl-3-hexanone	0.05	0.05	Aliphatic ketone
Hexanol	tr	0.02*	Aliphatic alcohol
Isoamyl acetate	tr	0.01	Aliphatic ester
Nonane	0.03*	0.01	Alkane
Bornylene	[0.03]*	0.01	Monoterpene
$\alpha$ -Thujene	0.01	0.01	Monoterpene
$\alpha$ -Pinene	10.54	10.39	Monoterpene
Camphepane	0.23	0.09	Monoterpene
Thuja-2,4(10)-diene	0.02	0.02*	Monoterpene
Sabinene	0.23*	[0.02]*	Monoterpene
$\beta$ -Pinene	[0.23]*	0.23	Monoterpene
6-Methyl-5-hepten-2-one	0.02	0.01	Aliphatic ketone
Myrcene	0.05*	0.04	Monoterpene
trans-Dehydroxylinalool oxide	[0.05]*	0.02	Monoterpenic ether
2-Carene	0.01	0.02	Monoterpene
6-Methyl-5-hepten-2-ol	0.02	0.04*	Aliphatic alcohol
Unknown	0.02*	0.01	Monoterpene
$\alpha$ -Phellandrene	[0.02]*	0.02	Monoterpene
Isobutyl 2-methylbutyrate	0.03	0.04	Aliphatic ester
(3Z)-Hexenyl acetate	0.01	0.01	Aliphatic ester
$\alpha$ -Terpinene	0.10	0.10	Monoterpene
para-Methylanisole	0.01	0.01	Simple phenolic
para-Cymene	0.15	0.15	Monoterpene
Limonene	1.79*	1.52	Monoterpene
1,8-Cineole	[1.79]*	0.25	Monoterpenic ether
(Z)- $\beta$ -Ocimene	0.01	0.01	Monoterpene
(E)- $\beta$ -Ocimene	0.02	0.02	Monoterpene
Isobutyl angelate	0.19	0.19	Aliphatic ester
$\gamma$ -Terpinene	0.27	0.26	Monoterpene
Octanol	0.01	0.10*	Aliphatic alcohol
Terpinolene	0.12*	0.11	Monoterpene
para-Cymenene	[0.12]*	0.01	Monoterpene
2-Nonanone	0.04*	0.03	Aliphatic ketone
Isobutyl tiglate	[0.04]*	[0.02]*	Aliphatic ester
2,4-Dimethylheptane-3,5-dione	0.04	0.04	$\beta$ -Diketone
Linalool	0.55	0.55	Monoterpenic alcohol
Nonanal	0.06	0.06	Aliphatic aldehyde
2-Methylbutyl 2-methylbutyrate	0.08	0.08	Aliphatic ester
endo-Fenchol	0.07	0.11	Monoterpenic alcohol

α-Campholenal	0.02	0.41*	Monoterpenic aldehyde
trans-Pinocarveol	0.07	0.06	Monoterpenic alcohol
trans-Verbenol	0.04	0.16	Monoterpenic alcohol
para-Vinylanisole	0.02	0.15*	Simple phenolic
Isoamyl angelate	0.03	0.67*	Aliphatic ester
Nerol oxide	0.02	0.03	Aliphatic ether
Pinocarvone	0.68*	0.32*	Monoterpenic ketone
2-Methylbutyl angelate	[0.68]*	[0.67]*	Aliphatic ester
Borneol	0.07	10.36*	Monoterpenic alcohol
Unknown	0.02	0.02	Aliphatic ester
Nonanol	0.23*	0.02	Aliphatic alcohol
Terpinen-4-ol	[0.23]*	0.29	Monoterpenic alcohol
4,6-Dimethyloctane-3,5-dione epimer I	0.15	0.12	β-Diketone
4,6-Dimethyloctane-3,5-dione epimer II	0.16	0.15*	β-Diketone
α-Terpineol	0.24	[10.36]*	Monoterpenic alcohol
Myrtenol	0.04	0.03	Monoterpenic alcohol
2-Methylbutyl tiglate	0.03	[0.04]*	Aliphatic ester
Unknown	0.03	0.62	Unknown
Dodecane	0.01	0.02	Alkane
Decanal	0.06	0.05	Aliphatic aldehyde
Nerol	0.40	0.43	Monoterpenic alcohol
Unknown	0.11		β-Diketone
Hexyl isovalerate	0.01	0.01	Aliphatic ester
Isoamyl hexanoate	0.01	0.09*	Aliphatic ester
3-Methylpentyl angelate	0.04	0.03	Aliphatic ester
Unknown	0.06	[0.09]*	Aliphatic ester
Unknown	0.03	0.06	Aliphatic ester
(3Z)-Hexenyl angelate	0.03	0.93	Aliphatic ester
Hexyl angelate	0.29	[0.32]*	Aliphatic ester
2-Undecanone	0.04	[0.15]*	Aliphatic ketone
Tridecane	0.04	0.03	Alkane
Myrtenyl acetate	0.01	0.80*	Monoterpenic ester
Hexyl tiglate	0.03	0.02	Aliphatic ester
α-Terpinyl acetate	0.17	0.19	Monoterpenic ester
Cyclosativene II	0.27	[0.41]*	Sesquiterpene
Neryl acetate	26.13*	26.44*	Monoterpenic ester
α-Ylangene	[26.13]*	[0.41]*	Sesquiterpene
α-Copaene	2.20*	1.43*	Sesquiterpene
Italicene isomer	[2.20]*	0.81	Sesquiterpene
7-Cubebene	0.03	[1.43]*	Sesquiterpene
Geranyl acetate	0.28	0.25	Monoterpenic ester
α-Funebrene	0.21*	0.14	Sesquiterpene
Hexyl hexanoate	[0.21]*	0.04	Aliphatic ester
Sativene	[0.21]*	0.03	Sesquiterpene
Isoitalicene	0.15	0.14	Sesquiterpene
Italicene	3.01	3.02	Sesquiterpene
Isocaryophyllene	0.09*	[0.10]*	Sesquiterpene
α-Gurjunene	[0.09]*	0.03	Sesquiterpene
cis-α-Bergamotene	5.08*	0.03	Sesquiterpene
β-Ylangene	[5.08]*	0.03	Sesquiterpene

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β-Caryophyllene	[5.08]*	5.16*	Sesquiterpene
β-Copaene	0.05	[5.16]*	Sesquiterpene
trans-α-Bergamotene	0.90	[5.16]*	Sesquiterpene
6,9-Guaiadiene	2.29*	0.02	Sesquiterpene
Italidione I	[2.29]*		β-Diketone
Cadina-4,11-diene	0.20*	0.08	Sesquiterpene
Unknown	[0.20]*	0.06	Sesquiterpene
α-Humulene	0.39*	0.33	Sesquiterpene
Neryl propionate	[0.39]*	0.01	Monoterpenic ester
allo-Aromadendrene	1.38*	0.12	Sesquiterpene
Muurola-4,11-diene	[1.38]*	0.11	Sesquiterpene
α-Acoradiene	[1.38]*	1.52*	Sesquiterpene
(E)-β-Farnesene	[1.38]*	[0.80]*	Sesquiterpene
β-Acoradiene	[1.38]*	[1.52]*	Sesquiterpene
4,5-diepi-Aristolochene	0.37	[1.52]*	Sesquiterpene
Unknown	0.13	[0.15]*	Sesquiterpene
Selina-4,11-diene	1.68*	[1.52]*	Sesquiterpene
trans-Cadina-1(6),4-diene	[1.68]*	0.28	Sesquiterpene
γ-Curcumene	20.20*	[10.36]*	Sesquiterpene
α-Amorphene	[20.20]*	[0.80]*	Sesquiterpene
ar-Curcumene	[20.20]*	2.66*	Sesquiterpene
β-Selinene	[20.20]*	5.54*	Sesquiterpene
Italidione II isomer I	[20.20]*	7.14*	β-Diketone
Italidione II isomer II	2.02	[7.14]*	β-Diketone
Valencene	3.69*	[5.54]*	Sesquiterpene
α-Selinene	[3.69]*	3.58*	Sesquiterpene
Italidione II analog	0.39*	1.39*	β-Diketone
Eudesma-2,4(15),11-triene	[0.39]*	0.02	Sesquiterpene
δ-Amorphene	0.34	[3.58]*	Sesquiterpene
10-epi-Italicene ether	0.18*	0.02	Sesquiterpenic ether
β-Bisabolene	[0.18]*	[26.44]*	Sesquiterpene
γ-Cadinene	[0.18]*	1.16*	Sesquiterpene
β-Curcumene	1.49*	[26.44]*	Sesquiterpene
7-epi-α-Selinene	[1.49]*	[1.16]*	Sesquiterpene
Sesquicineole	0.93*	0.41	Sesquiterpenic ether
δ-Cadinene	[0.93]*	[1.16]*	Sesquiterpene
trans-Calamenene	[0.93]*	0.07	Sesquiterpene
Zonarene	[0.93]*	[1.16]*	Sesquiterpene
cis-Calamenene?	0.03	0.03	Sesquiterpene
trans-Cadina-1,4-diene	0.21	[2.66]*	Sesquiterpene
Italicene ether	0.09	0.06	Sesquiterpenic ether
α-Cadinene	0.13*	0.06	Sesquiterpene
(E)-γ-Bisabolene	[0.13]*	[1.16]*	Sesquiterpene
Phenylethyl angelate?	[0.13]*	0.03	Phenolic ester
Selina-3,7(11)-diene	0.08*	0.05	Sesquiterpene
α-Calacorene	[0.08]*	0.26*	Sesquiterpene
(E)-α-Bisabolene	0.12	0.12	Sesquiterpene
Isocaryophyllene epoxide B	0.04	[0.26]*	Sesquiterpenic ether
(E)-Nerolidol	0.17*	0.15	Sesquiterpenic alcohol
Caryophyllenyl alcohol	[0.17]*	0.03	Sesquiterpenic alcohol
Italidione III isomer I	0.52	[1.39]*	β-Diketone
Italidione III isomer II	0.36	[1.39]*	β-Diketone

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Italidione III isomer III	0.23		β-Diketone
Guaiol	0.14	0.17	Sesquiterpenic alcohol
Eudesm-5-en-11-ol	0.27	0.28	Sesquiterpenic alcohol
Copaborneol	0.28	0.27	Sesquiterpenic alcohol
Unknown	0.12	0.12	Oxygenated sesquiterpene
Unknown	0.16	0.07	Oxygenated sesquiterpene
Unknown	0.16	0.16	Unknown
Neryl angelate?	0.09*		Monoterpenic ester
1-epi-Cubenol	[0.09]*	0.03	Sesquiterpenic alcohol
Caryophylladienol I	0.09	0.02	Sesquiterpenic alcohol
γ-Eudesmol	0.17	0.14	Sesquiterpenic alcohol
τ-Cadinol	0.10*	0.04	Sesquiterpenic alcohol
τ-Muurolol	[0.10]*	0.03	Sesquiterpenic alcohol
α-Muurolol	0.10*	0.03	Sesquiterpenic alcohol
β-Eudesmol	[0.10]*	0.02	Sesquiterpenic alcohol
α-Eudesmol	0.27*	0.14	Sesquiterpenic alcohol
Selin-11-en-4α-ol	[0.27]*	0.18	Sesquiterpenic alcohol
Bulnesol	0.04	0.07	Sesquiterpenic alcohol
β-Bisabolol	0.13	0.10	Sesquiterpenic alcohol
α-Bisabolol	0.05	0.04	Sesquiterpenic alcohol
Neryl 4-methylvalerate?	0.06	0.04	Monoterpenic ester
Unknown	0.03	0.03	Unknown
Geranyl 4-methylvalerate?	0.04	0.11	Monoterpenic ester
Unknown	0.12		Oxygenated sesquiterpene
Unknown	0.04		Oxygenated sesquiterpene
Unknown	0.30		Oxygenated sesquiterpene
Unknown	0.13*		Oxygenated sesquiterpene
Unknown	[0.13]*	0.02	Oxygenated sesquiterpene
Unknown	0.05	0.04	Oxygenated sesquiterpene
Unknown	0.17	0.08	Oxygenated sesquiterpene
Unknown	0.18		Unknown
Octyl angelate		[1.16]*	Aliphatic ester
<b>Total identified</b>	<b>95.71%</b>	<b>94.60%</b>	

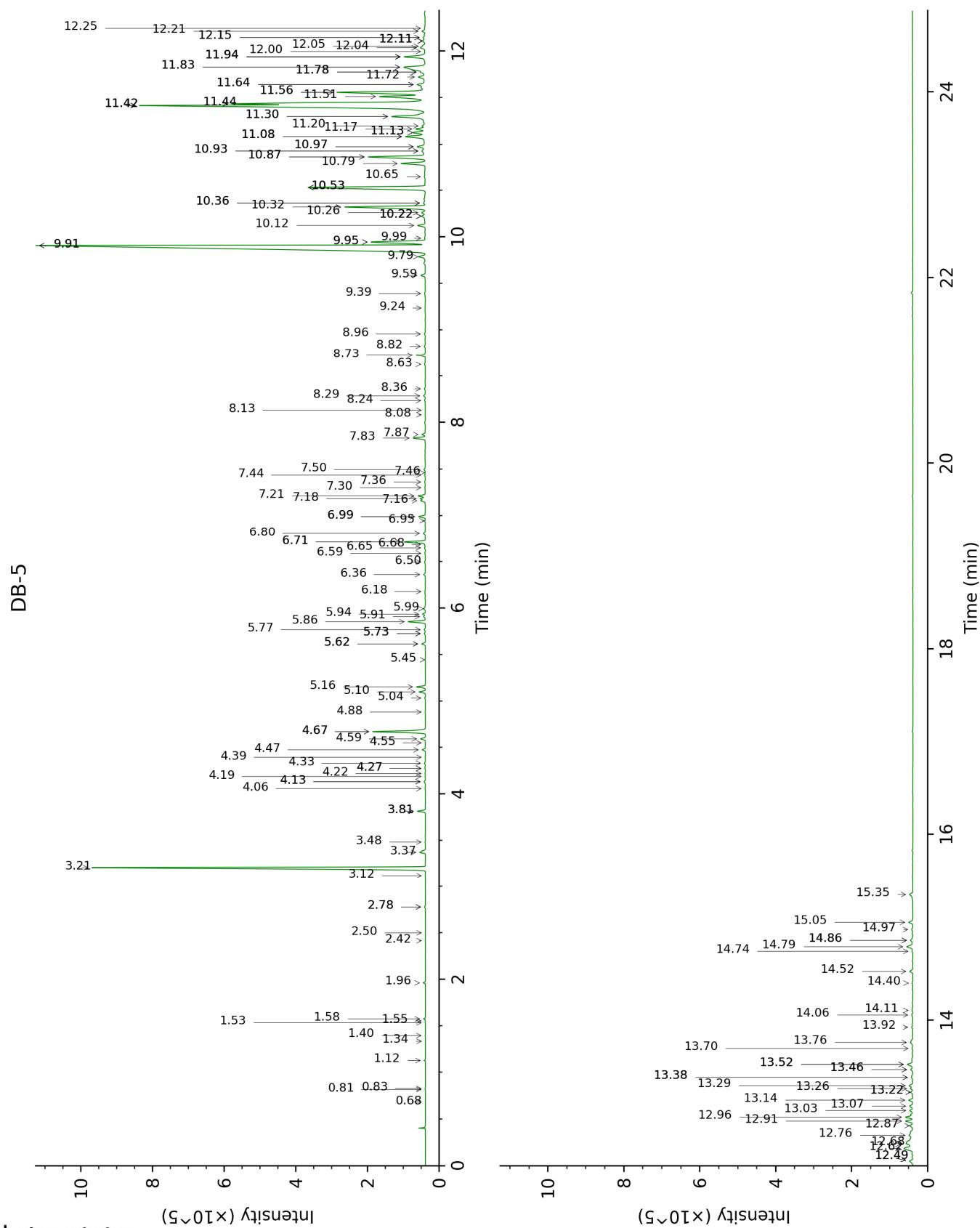
\*: Two or more compounds are coeluting on this column

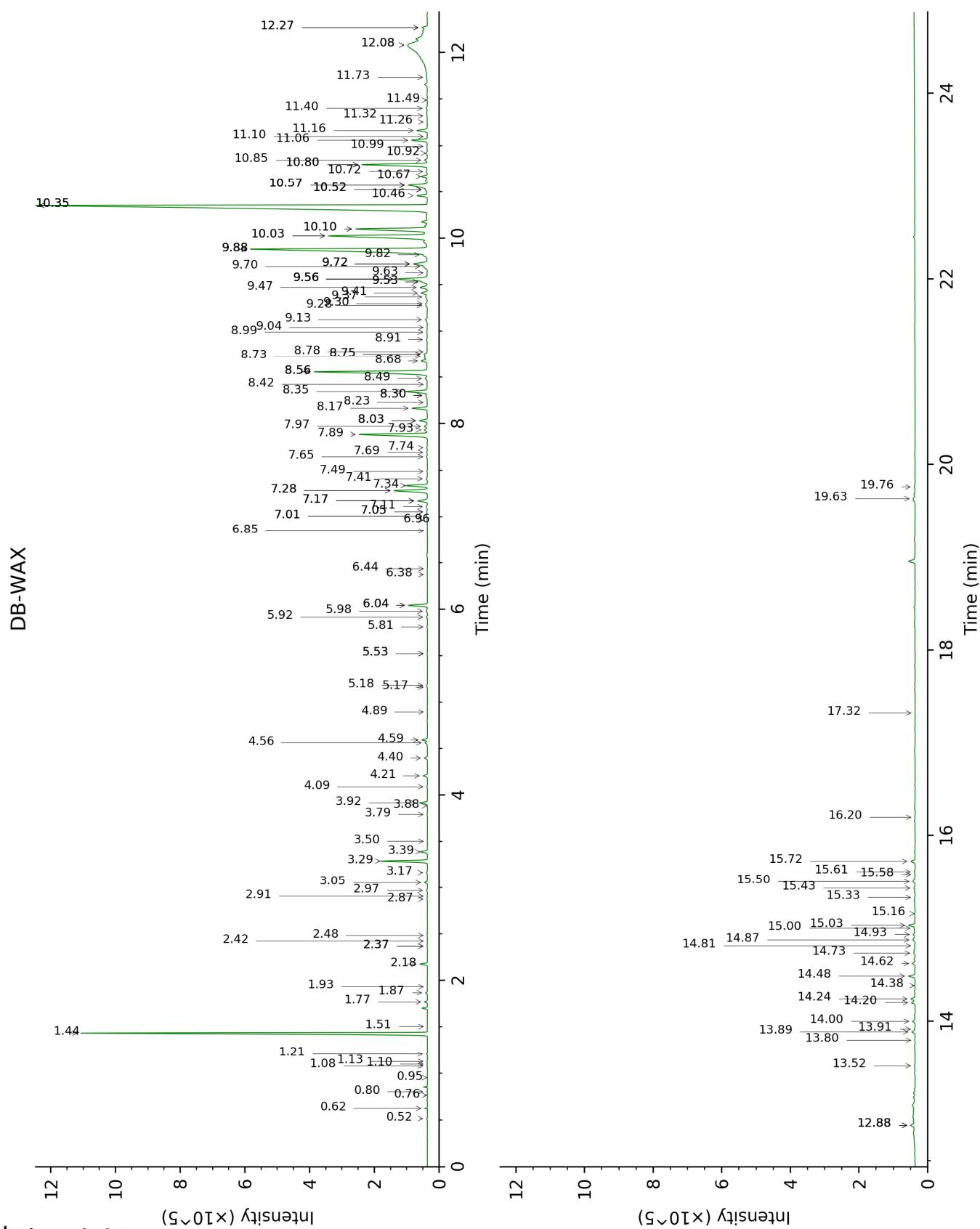
[xx]: Duplicate percentage due to coelutions, not taken account in the identified total

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

Note: no correction factor was applied

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FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	%	R.T	R.I	%
2-Methylbutyral	0.68	650	tr	0.76	881	tr
3-Pentanone	0.81	689	0.01	1.08	941	0.01
2-Ethylfuran	0.83	693	0.01	0.95	922	tr
2-Methyl-3-pentanone	1.12	742	0.02	1.21	960	0.02
Unknown [m/z 73, 41 (54), 87 (50), 56 (47), 54 (29), 55 (25), 100 (23)... 115? (6)]	1.34	770	tr			
Unknown [m/z 73, 87 (52), 41 (45), 56 (42), 100 (29)...]	1.40	778	0.01	1.10	944	0.01
Hexanal	1.54	797	tr	1.93	1042	0.01
Octane	1.56	800	0.01	0.52	786	0.01
2-Methyl-2-heptene	1.58	803	0.04	0.62	838	0.04
4-Methyl-3-hexanone	1.96	835	0.05	1.87	1036	0.05
Hexanol	2.42	872	tr	5.52*	1321	0.02
Isoamyl acetate	2.50	879	tr	2.42	1089	0.01
Nonane	2.78*	902	0.03	0.80	893	0.01
Bornylene	2.78*	902	[0.03]	1.13	948	0.01
$\alpha$ -Thujene	3.12	924	0.01	1.51	1002	0.01
$\alpha$ -Pinene	3.21	930	10.54	1.44	994	10.39
Camphepane	3.37	941	0.23	1.77	1027	0.09
Thuja-2,4(10)-diene	3.48	948	0.02	2.37*	1084	0.02
Sabinene	3.81*	970	0.23	2.37*	1084	[0.02]
$\beta$ -Pinene	3.81*	970	[0.23]	2.18	1066	0.23
6-Methyl-5-hepten-2-one	4.06	986	0.02	5.16	1302	0.01
Myrcene	4.13*	991	0.05	2.97	1133	0.04
<i>trans</i> -Dehydroxylinalool oxide	4.13*	991	[0.05]	3.50	1175	0.02
2-Carene	4.19	995	0.01	2.48	1095	0.02
6-Methyl-5-hepten-2-ol	4.22	997	0.02	7.05*	1432	0.04
Unknown [m/z = 123, 43 (16), 152 (14), 124 (9), 137 (6)]	4.27*	1000	0.02	2.91	1128	0.01
$\alpha$ -Phellandrene	4.27*	1000	[0.02]	2.87	1125	0.02
Isobutyl 2-methylbutyrate	4.33	1004	0.03	3.17	1148	0.04
(3Z)-Hexenyl acetate	4.39	1008	0.01	4.89	1280	0.01

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$\alpha$ -Terpinene	4.47	1013	0.10	3.05	1139	0.10
para-Methylanisole	4.55	1018	0.01	6.38	1382	0.01
para-Cymene	4.59	1020	0.15	4.21	1229	0.15
Limonene	4.67*	1025	1.79	3.29	1158	1.52
1,8-Cineole	4.67*	1025	[1.79]	3.39	1166	0.25
(Z)- $\beta$ -Ocimene	4.88	1038	0.01	3.88	1204	0.01
(E)- $\beta$ -Ocimene	5.04	1048	0.02	4.09	1220	0.02
Isobutyl angelate	5.10	1052	0.19	4.59	1258	0.19
$\gamma$ -Terpinene	5.16	1056	0.27	3.92	1207	0.26
Octanol	5.45	1074	0.01	8.30*	1526	0.10
Terpinolene	5.62*	1085	0.12	4.40	1243	0.11
para-Cymenene	5.62*	1085	[0.12]	6.44	1386	0.01
2-Nonanone	5.73*	1092	0.04	5.92	1349	0.03
Isobutyl tiglate	5.73*	1092	[0.04]	5.52*	1321	[0.02]
2,4-Dimethylheptane-3,5-dione	5.77	1095	0.04	7.65	1476	0.04
Linalool	5.86	1100	0.55	8.17	1515	0.55
Nonanal	5.91	1104	0.06	5.98	1354	0.06
2-Methylbutyl 2-methylbutyrate	5.94	1105	0.08	4.56	1255	0.08
endo-Fenchol	5.99	1109	0.07	8.49	1540	0.11
$\alpha$ -Campholenal	6.18	1121	0.02	7.17*	1441	0.41
trans-Pinocarveol	6.36	1133	0.07	9.30	1602	0.06
trans-Verbenol	6.50	1141	0.04	9.70	1635	0.16
para-Vinylanisole	6.59	1148	0.02	9.53*	1621	0.15
Isoamyl angelate	6.65	1151	0.03	6.04*	1358	0.67
Nerol oxide	6.68	1154	0.02	6.96	1425	0.03
Pinocarvone	6.71*	1155	0.68	8.03*	1505	0.32
2-Methylbutyl angelate	6.71*	1155	[0.68]	6.04*	1358	[0.67]
Borneol	6.80	1161	0.07	9.88*	1650	10.36
Unknown [m/z 83, 100 (34), 55 (33), 43 (21), 84 (21)...]	6.94	1171	0.02	5.81	1342	0.02
Nonanol	6.99*	1174	0.23	9.63	1629	0.02
Terpinen-4-ol	6.99*	1174	[0.23]	8.68	1554	0.29
4,6-Dimethyloctane-3,5-dione epimer I	7.16	1185	0.15	8.73	1558	0.12
4,6-Dimethyloctane-3,5-dione epimer II	7.18	1186	0.16	8.75*	1560	0.15
$\alpha$ -Terpineol	7.21	1188	0.24	9.88*	1650	[10.36]
Myrtenol	7.30	1194	0.04	10.99	1741	0.03
2-Methylbutyl tiglate	7.36	1198	0.03	7.05*	1432	[0.04]
Unknown [m/z 95, 93 (32), 121 (24), 79 (22), 91 (21),	7.44	1203	0.03	11.06	1747	0.62

105 (16)... 154 (2)]						
Dodecane	7.46	1204	0.01	3.79	1198	0.02
Decanal	7.50	1206	0.06	7.41	1458	0.05
Nerol	7.83	1230	0.40	11.16	1756	0.43
Unknown [m/z 113, 57 (55), 85 (16), 170 (16)]	7.87	1232	0.11			
Hexyl isovalerate	8.08	1247	0.01	6.85	1416	0.01
Isoamyl hexanoate	8.13	1250	0.01	7.01*	1428	0.09
3-Methylpentyl angelate	8.24	1257	0.04	7.49	1464	0.03
Unknown [m/z 83, 55 (29), 57 (24), 100 (21), 104 (13) ...]	8.29	1261	0.06	7.01*	1428	[0.09]
Unknown [m/z 83, 55 (30), 57 (23), 100 (20), 98 (14) ...]	8.36	1266	0.03	7.11	1436	0.06
(3Z)-Hexenyl angelate	8.63	1284	0.03	8.35	1529	0.93
Hexyl angelate	8.73	1291	0.29	8.03*	1505	[0.32]
2-Undecanone	8.82	1298	0.04	8.75*	1560	[0.15]
Tridecane	8.96	1307	0.04	5.18	1297	0.03
Myrtenyl acetate	9.24	1320	0.01	9.72*	1637	0.80
Hexyl tiglate	9.39	1332	0.03	9.04	1582	0.02
$\alpha$ -Terpinyl acetate	9.59	1346	0.17	9.82	1645	0.19
Cyclosativene II	9.79	1360	0.27	7.17*	1441	[0.41]
Neryl acetate	9.91*	1368	26.13	10.35*	1688	26.44
$\alpha$ -Ylangene	9.91*	1368	[26.13]	7.17*	1441	[0.41]
$\alpha$ -Copaene	9.94*	1371	2.20	7.28*	1449	1.43
Italicene isomer	9.94*	1371	[2.20]	7.34	1453	0.81
7-Cubebene	9.99	1374	0.03	7.28*	1449	[1.43]
Geranyl acetate	10.12	1384	0.28	10.67	1714	0.25
$\alpha$ -Funebrene	10.22*	1391	0.21	7.97	1500	0.14
Hexyl hexanoate	10.22*	1391	[0.21]	8.99	1578	0.04
Sativene	10.22*	1391	[0.21]	7.69	1479	0.03
Isoitalicene	10.26	1394	0.15	7.94	1497	0.14
Italicene	10.32	1398	3.01	7.89	1493	3.02
Isocaryophyllene	10.36*	1401	0.09	8.30*	1526	[0.10]
$\alpha$ -Gurjunene	10.36*	1401	[0.09]	7.74	1483	0.03
<i>cis</i> - $\alpha$ -Bergamotene	10.53*	1413	5.08	8.42	1535	0.03
$\beta$ -Ylangene	10.53*	1413	[5.08]	8.23	1520	0.03
$\beta$ -Caryophyllene	10.53*	1413	[5.08]	8.56*	1545	5.16
$\beta$ -Copaene	10.65	1423	0.05	8.56*	1545	[5.16]
<i>trans</i> - $\alpha$ -Bergamotene	10.80	1433	0.90	8.56*	1545	[5.16]
6,9-Guaiadiene	10.87*	1439	2.29	8.78	1562	0.02
Italidione I	10.87*	1439	[2.29]			
Cadina-4,11-diene	10.93*	1443	0.20	9.28	1601	0.08
Unknown [m/z 91,	10.93*	1443	[0.20]	8.91	1572	0.06

161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)]					
α-Humulene	10.98*	1447	0.39	9.47	1616 0.33
Neryl propionate	10.98*	1447	[0.39]	11.10	1750 0.01
allo-Aromadendrene	11.08*†	1455	1.38	9.13	1589 0.12
Muurola-4,11-diene	11.08*†	1455	[1.38]	9.37	1608 0.11
α-Acoradiene	11.08*†	1455	[1.38]	9.56*	1624 1.52
(E)-β-Farnesene	11.13*†	1458	[1.38]	9.72*	1637 [0.80]
β-Acoradiene	11.13*†	1458	[1.38]	9.56*	1624 [1.52]
4,5-diepi-Aristolochene	11.17	1461	0.37	9.56*	1624 [1.52]
Unknown [m/z 119, 91 (85), 93 (77), 105 (76), 79 (61), 134 (60), 94 (49), 204 (46)]	11.20	1464	0.13	9.53*	1621 [0.15]
Selina-4,11-diene	11.30*	1471	1.68	9.56*	1624 [1.52]
trans-Cadina-1(6),4-diene	11.30*	1471	[1.68]	9.41	1612 0.28
γ-Curcumene	11.42*†	1480	20.20	9.88*	1650 [10.36]
α-Amorphene	11.42*†	1480	[20.20]	9.72*	1637 [0.80]
ar-Curcumene	11.42*†	1480	[20.20]	10.80*	1725 2.66
β-Selinene	11.44*†	1482	[20.20]	10.03*	1661 5.54
Italidione II isomer I	11.44*†	1482	[20.20]	12.08*	1835 7.14
Italidione II isomer II	11.51	1487	2.02	12.08*	1835 [7.14]
Valencene	11.56*	1491	3.69	10.03*	1661 [5.54]
α-Selinene	11.56*	1491	[3.69]	10.10*	1667 3.58
Italidione II analog	11.64*	1497	0.39	12.88*	1906 1.39
Eudesma-2,4(15),11-triene	11.64*	1497	[0.39]	11.26	1764 0.02
δ-Amorphene	11.72	1503	0.34	10.10*	1667 [3.58]
10-epi-Italicene ether	11.78*	1507	0.18	11.49	1783 0.02
β-Bisabolene	11.78*	1507	[0.18]	10.35*	1688 [26.44]
γ-Cadinene	11.78*	1507	[0.18]	10.52*†	1702 1.16
β-Curcumene	11.83*	1511	1.49	10.35*	1688 [26.44]
7-epi-α-Selinene	11.83*	1511	[1.49]	10.57*†	1706 [1.16]
Sesquicineole	11.94*	1520	0.93	10.46	1696 0.41
δ-Cadinene	11.94*	1520	[0.93]	10.57*†	1706 [1.16]
trans-Calamenene	11.94*	1520	[0.93]	11.40	1776 0.07
Zonarene	11.94*	1520	[0.93]	10.52*†	1702 [1.16]
cis-Calamenene?	12.00	1525	0.03	11.32	1769 0.03
trans-Cadina-1,4-diene	12.04	1528	0.21	10.80*	1725 [2.66]
Italicene ether	12.05	1529	0.09	11.74	1804 0.06
α-Cadinene	12.11*	1534	0.13	10.92	1735 0.06

(E)-γ-Bisabolene	12.11*	1534	[0.13]	10.57*†	1706	[1.16]
Phenylethyl angelate?	12.11*	1534	[0.13]	14.38	2046	0.03
Selina-3,7(11)-diene	12.15*	1537	0.08	10.72	1718	0.05
α-Calacorene	12.15*	1537	[0.08]	12.27*	1851	0.26
(E)-α-Bisabolene	12.22	1542	0.12	10.85	1729	0.12
Isocaryophyllene epoxide B	12.25	1544	0.04	12.27*	1851	[0.26]
(E)-Nerolidol	12.49*	1564	0.17	13.89	1999	0.15
Caryophyllenyl alcohol	12.49*	1564	[0.17]	13.80	1990	0.03
Italidione III isomer I	12.62	1574	0.52	12.88*	1906	[1.39]
Italidione III isomer II	12.68	1578	0.36	12.88*	1906	[1.39]
Italidione III isomer III	12.76	1585	0.23			
Guaiol	12.87	1594	0.14	14.24	2033	0.17
Eudesm-5-en-11-ol	12.91	1597	0.27	14.48	2056	0.28
Copaborneol	12.96	1601	0.28	15.03	2109	0.27
Unknown [m/z 43, 81 (97), 135 (71), 95 (62), 204 (61), 71 (59), 207 (56)... 222 (3)]	13.03	1606	0.12	14.62	2069	0.12
Unknown [m/z 179, 161 (66), 119 (44), 95 (38), 105 (35)... 204 (24), 222 (1)]	13.07	1610	0.16	14.73	2080	0.07
Unknown [m/z 182, 109 (58), 69 (50), 41 (42), 43 (40), 139 (31)... 235 (17), 250 (1)...]	13.14	1616	0.16	14.20	2029	0.16
Neryl angelate?	13.22*	1623	0.09			
1-epi-Cubenol	13.22*	1623	[0.09]	13.92	2002	0.03
Caryophylladienol I	13.26	1626	0.09	16.20	2227	0.02
γ-Eudesmol	13.29	1628	0.17	14.87	2094	0.14
τ-Cadinol	13.38*	1636	0.10	15.00	2106	0.04
τ-Muurolol	13.38*	1636	[0.10]	15.16	2122	0.03
α-Muurolol	13.46*	1643	0.10	15.33	2139	0.03
β-Eudesmol	13.46*	1643	[0.10]	15.58	2164	0.02
α-Eudesmol	13.52*	1647	0.27	15.50	2156	0.14
Selin-11-en-4α-ol	13.52*	1647	[0.27]	15.72	2178	0.18
Bulnesol	13.70	1662	0.04	15.43	2149	0.07
β-Bisabolol	13.76	1667	0.13	14.93	2099	0.10
α-Bisabolol	13.92	1681	0.05	15.61	2167	0.04
Neryl 4-	14.06	1692	0.06	13.52	1964	0.04

methylvalerate?						
Unknown [m/z 196, 69 (62), 109 (58), 41 (54), 139 (41)... 249 (21)....]	14.10	1696	0.03	14.81	2087	0.03
Geranyl 4-methylvalerate?	14.40	1721	0.04	14.00	2010	0.11
Unknown [m/z 43, 69 (32), 198 (29), 41 (27), 93 (26)... 202 (20)....]	14.52	1732	0.12			
Unknown [m/z 109, 127 (46), 138 (45), 81 (27), 123 (25)... 220? (2)]	14.74	1751	0.04			
Unknown [m/z 136, 121 (74), 135 (55), 218 (36), 148 (33), 40 (42)... 236? (1)]	14.79	1755	0.30			
Unknown [m/z 109, 138 (71), 82 (42), 123 (41), 127 (38)....]	14.86*	1761	0.13			
Unknown [m/z 96, 41 (29), 178 (28), 43 (27)... 236 (2)]	14.86*	1761	[0.13]	17.32	2345	0.02
Unknown [m/z 109, 138 (75), 123 (45), 127 (42), 81 (30)....]	14.97	1771	0.05	19.76	2622	0.04
Unknown [m/z 98, 82 (77), 83 (42), 137 (37), 41 (28)... 238 (1)]	15.05	1778	0.17	19.63	2607	0.08
Unknown [m/z 43, 82 (69), 41 (66), 93 (62), 96 (55), 55 (49), 67 (45), 154 (44)....]	15.35	1804	0.18			
Octyl angelate				10.52*†	1702	[1.16]
<b>Total identified</b>	<b>95.71%</b>			<b>94.60%</b>		
<b>Total reported</b>	<b>97.44%</b>			<b>95.90%</b>		

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken account in the identified 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