Date : February 08, 2022

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 21I13-PTH01
Customer identification : German Chamomile CO2 Extract - CA4108218R
Type : CO2 extract
Source : *Matricaria chamomilla*
Customer : Plant Therapy

Analysis

Method: Dilution of a known amount with an appropriate solvent, and addition of a methyl octanoate internal standard for quantitation. Application of a correction factor[1]. Analysis with PC-MAT-004 - Terpenes and volatiles profiling by response factor (in French); identifications validated by GC-MS.
Analyst : Sarah-Eve Tremblay, M. Sc. A., Chimiste
Analysis date : September 17, 2021

Checked and approved by :

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

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

This report is an update of the version first issued on September 17, 2021 to correct a mistake in the lot number.

Reference

(1) Cachet, T.; Brevard, H.; Chaintreau, A.; Demyttenaere, J.; French, L.; Gassenmeier, K.; Joulain, D.; Koenig, T.; Leijs, H.; Liddle, P.; et al. IOFI Recommended Practice for the Use of Predicted Relative-Response Factors for the Rapid Quantification of Volatile Flavouring *Compounds by GC-FID. Flavour Fragr. J. 2016, 31 (3), 191–194.*

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PHYSICOCHEMICAL DATA

Physical aspect: Dark green liquid
Refractive index: 1.5130 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

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

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ANALYSIS SUMMARY

Identification	(mg/g)	% m/m	Classe
Isovaleric acid	0.30	0.03	Aliphatic acid
α-Pinene	0.06	0.01	Monoterpene
Camphene	0.10	0.01	Monoterpene
Benzaldehyde	0.05	0.01	Simple phenolic
β-Pinene	0.04	tr	Monoterpene
Sabinene	0.47	0.05	Monoterpene
6-Methyl-5-hepten-2-one	0.28	0.03	Aliphatic ketone
Myrcene	0.08	0.01	Monoterpene
Yomogi alcohol	0.13	0.01	Monoterpenic alcohol
para-Cymene	0.30	0.03	Monoterpene
Limonene	0.28	0.03	Monoterpene
1,8-Cineole	0.63	0.06	Monoterpenic ether
β-Phellandrene	0.10	0.01	Monoterpene
(*Z*)-β-Ocimene	0.04	tr	Monoterpene
Seudenone?	0.05	0.01	Aliphatic ketone
(*E*)-β-Ocimene	0.28	0.03	Monoterpene
γ-Terpinene	0.26	0.03	Monoterpene
Artemisia ketone	0.80	0.08	Monoterpenic ketone
cis-Sabinene hydrate	0.07	0.01	Monoterpenic alcohol
Artemisia alcohol	0.47	0.05	Monoterpenic alcohol
trans-Sabinene hydrate	0.14	0.01	Monoterpenic alcohol
Linalool	0.12	0.01	Monoterpenic alcohol
Camphor	0.09	0.01	Monoterpenic ketone
Borneol	0.35	0.04	Monoterpenic alcohol
Artemisyl acetate	0.05	0.01	Monoterpenic ester
Terpinen-4-ol	0.12	0.01	Monoterpenic alcohol
α-Terpineol	0.37	0.04	Monoterpenic alcohol
Creosol	0.20	0.02	Simple phenolic
Carvone	0.15	0.02	Monoterpenic ketone
(*E*)-4,8-Dimethylnona-3,8-dien-2-one	0.08	0.01	Terpenic ketone
Thymol	0.14	0.01	Monoterpenic alcohol
Methyl decanoate	0.05	0.01	Aliphatic ester
7βH-Silphiperfol-5-ene	0.03	tr	Sesquiterpene
α-Cubebene	0.06	0.01	Sesquiterpene
Eugenol	0.09	0.01	Phenylpropanoid
α-Copaene	0.22	0.02	Sesquiterpene
Modhephene	0.14	0.01	Sesquiterpene
α-Isocomene	0.82	0.08	Sesquiterpene
β-Elemene	0.19	0.02	Sesquiterpene
β-Isocomene	0.13	0.01	Sesquiterpene
β-Caryophyllene	0.51	0.05	Sesquiterpene
β-Copaene	0.04	tr	Sesquiterpene
Aromadendrene	0.23	0.02	Sesquiterpene
α-Humulene	0.14	0.01	Sesquiterpene
allo-Aromadendrene	0.19	0.02	Sesquiterpene
(*E*)-β-Farnesene	53.50	5.35	Sesquiterpene
Dehydrosesquicineole	0.19	0.02	Sesquiterpenic ether
γ-Muurolene	0.16	0.02	Sesquiterpene

Germacrene D	3.45	0.35	Sesquiterpene
Unknown	0.29	0.03	Sesquiterpene
β-Selinene	0.93	0.09	Sesquiterpene
ar-Curcumene	0.34	0.03	Sesquiterpene
epi-Cubebol	0.19	0.02	Sesquiterpenic alcohol
Bicyclogermacrene	1.24	0.12	Sesquiterpene
α-Selinene	0.19	0.02	Sesquiterpene
Viridiflorene	0.17	0.02	Sesquiterpene
β-Himachalene	0.13	0.01	Sesquiterpene
(3*Z*,6*E*)-α-Farnesene	0.35	0.04	Sesquiterpene
Cubebol	0.51	0.05	Sesquiterpenic alcohol
(3*E*,6*E*)-α-Farnesene	2.49	0.25	Sesquiterpene
γ-Cadinene	0.12	0.01	Sesquiterpene
δ-Cadinene	0.05	0.01	Sesquiterpene
β-Sesquiphellandrene	0.13	0.01	Sesquiterpene
(*E*)-α-Bisabolene	0.12	0.01	Sesquiterpene
Dihydrocaryophyllen-5-one?	0.23	0.02	Sesquiterpenic ketone
Salviadienol?	0.17	0.02	Sesquiterpenic alcohol
(*E*)-Nerolidol	0.64	0.06	Sesquiterpenic alcohol
Spathulenol	4.93	0.49	Sesquiterpenic alcohol
Dendrolasin	0.60	0.06	Sesquiterpenic ether
Salvial-4(14)-en-1-one	0.28	0.03	Aliphatic alcohol
Torilenol	0.26	0.03	Oxygenated sesquiterpene
cis-Zingiberenol	0.33	0.03	Sesquiterpenic alcohol
(2,7*Z*)-Bisaboladien-4-ol	0.11	0.01	Sesquiterpenic alcohol
τ-Cadinol	0.40	0.04	Sesquiterpenic alcohol
Unknown	0.48	0.05	Unknown
α-Bisabolol oxide B, epimer 1	0.57	0.06	Sesquiterpenic alcohol
α-Bisabolol oxide B, epimer 2	0.28	0.03	Sesquiterpenic alcohol
Ageratochromene	0.67	0.07	Chromane
Bisabolone oxide A	1.06	0.11	Sesquiterpenic ketone
α-Bisabolol	125.88	12.59	Sesquiterpenic alcohol
Herniarin	11.48	1.15	Coumarin
Chamazulene	4.54	0.45	Azulene
α-Bisabolol oxide A	8.96	0.90	Sesquiterpenic alcohol
Myristic acid	2.64	0.26	Aliphatic acid
Unknown	0.53	0.05	Unknown
Unknown	0.27	0.03	Unknown
Phytone	0.37	0.04	Terpenic ketone
(*Z*)-Spiroether	162.34	16.23	Polyyne
(*E*)-Spiroether	23.14	2.31	Polyyne
(*Z*)-Tibetin spiroether	1.23	0.12	Polyyne
Unknown	0.28	0.03	Unknown
Methyl palmitate	0.36	0.04	Aliphatic ester
(*E*)-Tibetin spiroether	3.74	0.37	Polyyne
Palmitic acid	35.97	3.60	Aliphatic acid
Methyl linoleate	1.38	0.14	Aliphatic ester
Methyl petroselinate?	0.65	0.07	Aliphatic ester
Heneicosane	0.16	0.02	Alkane
Phytol	1.60	0.16	Diterpenic alcohol
Linoleic acid	109.96	11.00	Aliphatic acid
Oleic acid	47.24	4.72	Aliphatic acid

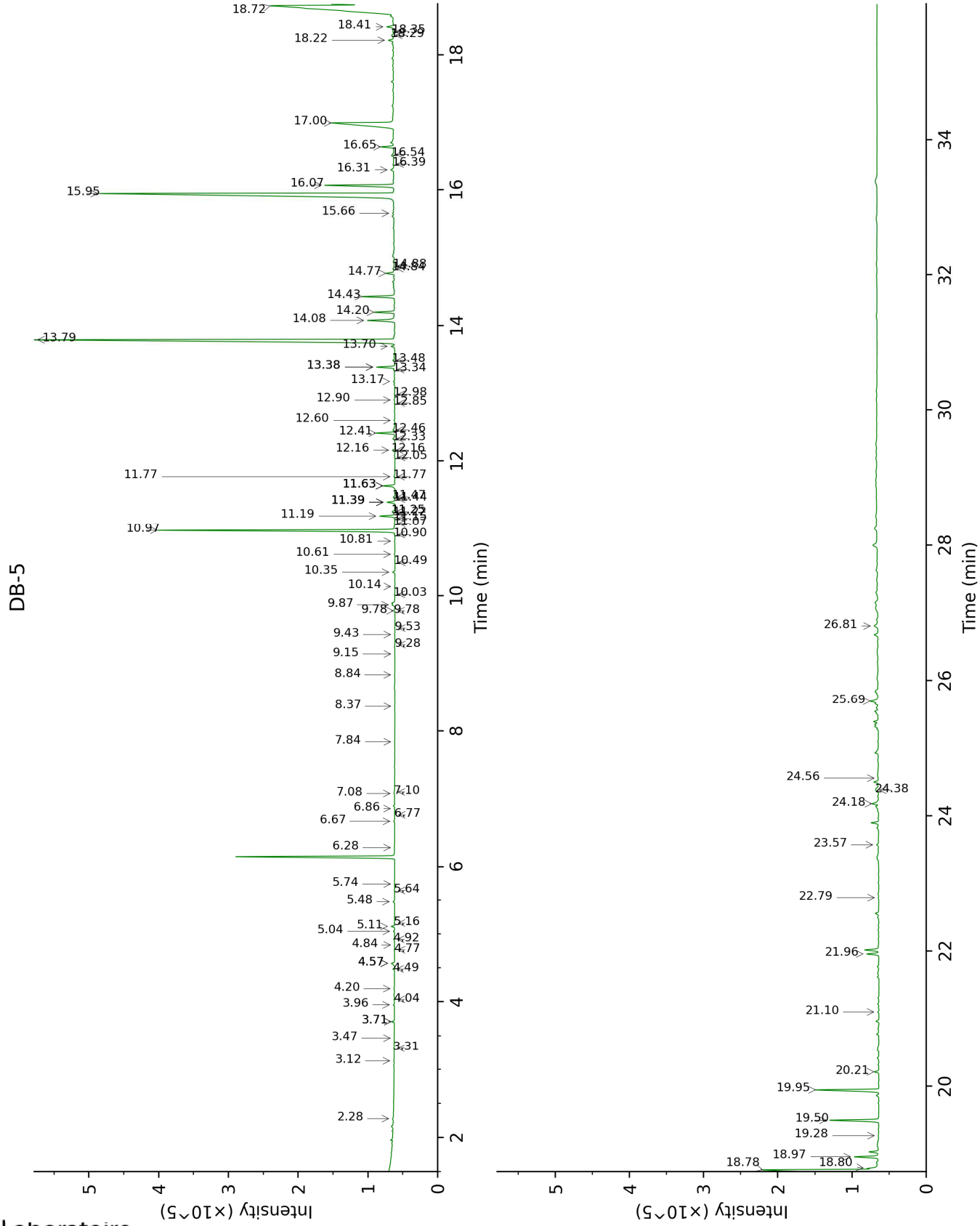
α-Linolenic acid	3.02	0.30	Aliphatic acid
Stearic acid	6.83	0.68	Aliphatic acid
Docosane	0.30	0.03	Alkane
Unknown	15.48	1.55	Unknown
Unknown	21.00	2.10	Unknown
Tricosane	1.02	0.10	Alkane
Tetracosane	0.30	0.03	Alkane
Pentacosane	2.83	0.28	Alkane
Hexacosane	0.11	0.01	Alkane
Heptacosane	0.62	0.06	Alkane
6,8-Pentacosanedione?	2.35	0.24	β-Diketone
Octacosane	0.76	0.08	Alkane
Squalene	0.11	0.01	Triterpene
6,8-Heptacosanedione?	2.79	0.28	β-Diketone
α-Tocopherol	1.75	0.18	Tocopherol
Consolidated total	**687.02 mg/g**	**68.70%**	

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

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: 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.



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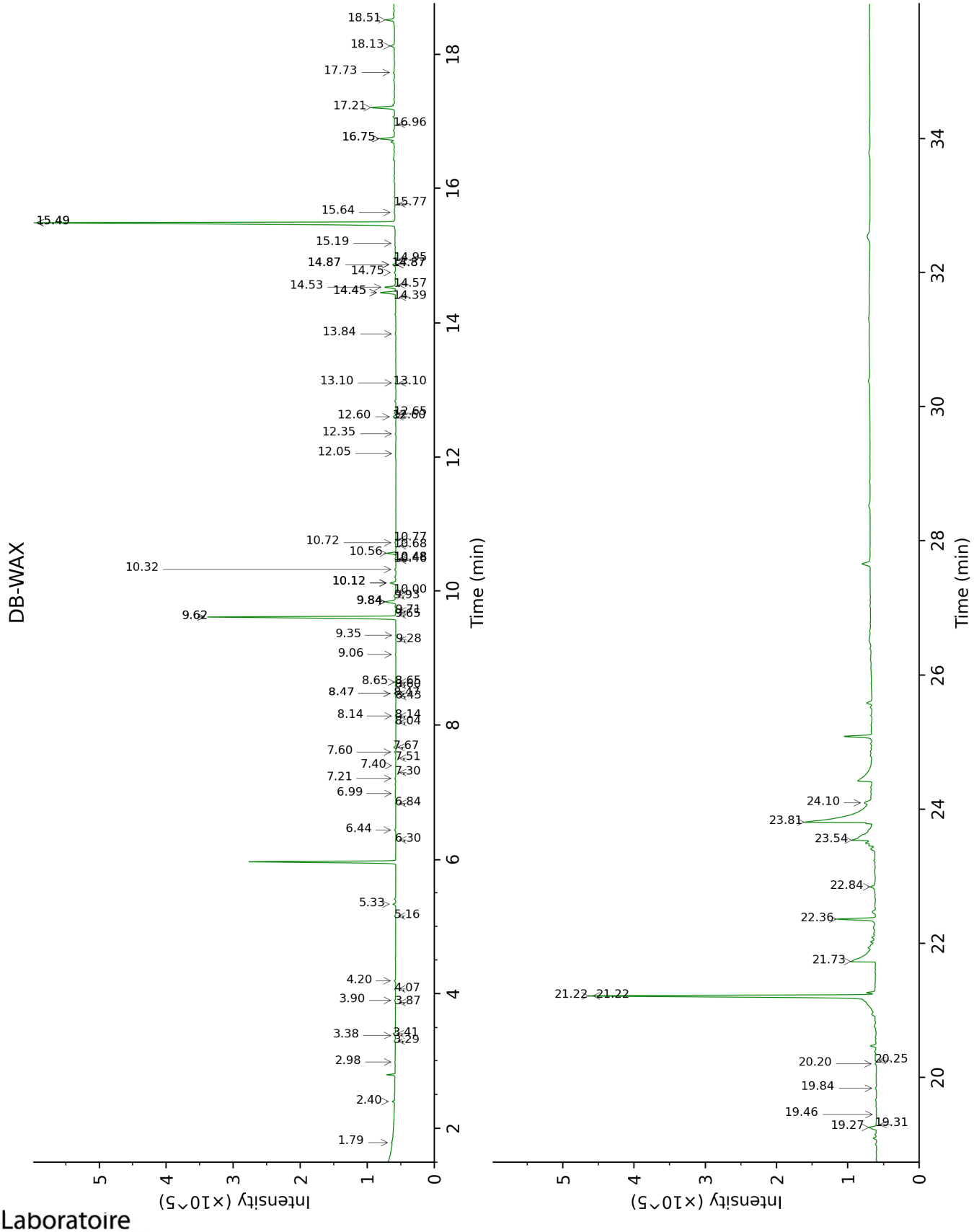
DB-WAX
Intensity (×10^5)
Time (min)
18.51
18.13
17.73
17.21
16.96
16.75
15.77
15.64
15.49
15.19
14.95
14.87
14.75
14.57
14.53
14.45
14.39
13.84
13.10
13.10
12.65
12.60
12.60
12.35
12.05
10.77
10.72
10.68
10.56
10.48
10.32
10.12
10.00
9.93
9.84
9.71
9.62
9.65
9.35
9.28
9.06
8.65
8.65
8.60
8.47
8.43
8.14
8.14
8.04
7.67
7.60
7.51
7.40
7.30
7.21
6.99
6.84
6.44
6.30
5.33
5.16
4.20
4.07
3.90
3.87
3.41
3.38
3.29
2.98
2.40
1.79
24.10
23.81
23.54
22.84
22.36
21.73
21.22
21.22
20.25
20.20
19.84
19.46
19.31
19.27

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g	R.T	R.I	mg/g
Isovaleric acid	2.28	869	0.30	9.65	1635	0.21
α-Pinene	3.12	933	0.06			
Camphene	3.31	945	0.10	1.79	1030	0.11
Benzaldehyde	3.47	955	0.05	7.40	1461	0.09
β-Pinene	3.71*	972	0.50			
Sabinene	3.71*	972	[0.50]	2.40	1090	0.47
6-Methyl-5-hepten-2-one	3.96	988	0.28	5.16	1298	0.28
Myrcene	4.04	994	0.08	2.98	1137	0.06
Yomogi alcohol	4.20	1004	0.13	6.30	1380	0.06
para-Cymene	4.49	1023	0.30	4.20	1231	0.32
Limonene	4.57*	1028	0.98	3.29	1161	0.28
1,8-Cineole	4.57*	1028	[1.11]	3.41	1170	0.63
β-Phellandrene	4.57*	1028	[0.98]	3.38	1168	0.10
(*Z*)-β-Ocimene	4.77	1040	0.04	3.87	1207	0.09
Seudenone?	4.84	1045	0.05	8.42	1539	0.17
(*E*)-β-Ocimene	4.92	1050	0.28	4.07	1222	0.19
γ-Terpinene	5.04	1058	0.26	3.90	1209	0.21
Artemisia ketone	5.11	1062	0.80	5.33	1310	0.77
cis-Sabinene hydrate	5.16	1066	0.07	6.99	1430	0.24
Artemisia alcohol	5.48	1086	0.47	7.60	1476	0.36
trans-Sabinene hydrate	5.64	1096	0.14	8.04	1509	0.13
Linalool	5.74	1102	0.12	8.14*	1516	0.19
Camphor	6.28	1138	0.09	7.30	1453	0.05
Borneol	6.67	1163	0.35	9.84*	1651	4.74
Artemisyl acetate	6.77	1169	0.05	6.44	1390	0.38
Terpinen-4-ol	6.86	1175	0.12	8.65*	1556	0.23
α-Terpineol	7.08	1189	0.37	9.84*	1651	[4.74]
Creosol	7.10	1191	0.20	12.60*	1886	1.22
Carvone	7.84	1241	0.15	10.12*	1673	2.24
(*E*)-4,8-Dimethylnona-3,8-dien-2-one	8.37	1276	0.08	9.28	1605	0.06
Thymol	8.84	1304	0.14	15.19	2132	0.13
Methyl decanoate	9.15	1326	0.05	8.65*	1556	[0.25]
7βH-Silphiperfol-5-ene	9.28	1336	0.03			
α-Cubebene	9.43	1346	0.06	6.84	1419	0.06
Eugenol	9.53	1353	0.09	14.87*	2100	1.20
α-Copaene	9.78*	1371	0.36	7.21	1447	0.22
Modhephene	9.78*	1371	[0.36]	7.51	1469	0.14
α-Isocomene	9.87	1378	0.82	7.67	1481	0.55
β-Elemene	10.02	1388	0.19	8.47*	1542	0.66
β-Isocomene	10.14	1397	0.13	8.14*	1516	[0.17]
β-Caryophyllene	10.35	1412	0.51	8.47*	1542	[0.66]
β-Copaene	10.50	1423	0.04	8.47*	1542	[0.66]
Aromadendrene	10.61	1432	0.23	8.60	1552	0.20
α-Humulene	10.81	1446	0.14	9.35	1611	0.08

allo-Aromadendrene	10.90	1454	0.19	9.06	1588	0.18
(*E*)-β-Farnesene	10.97	1459	53.50	9.62*	1633	52.37
Dehydrosesquicineole	11.07	1466	0.19	10.12*	1673	[2.05]
γ-Muurolene	11.15	1472	0.16	9.62*	1633	[52.37]
Germacrene D	11.19	1475	3.45	9.84*	1651	[4.10]
Unknown [m/z 119, 132 (91), 105 (60), 91 (34), 41 (33), 131 (32)...202 (18)]	11.22	1478	0.29	10.48*	1703	0.35
β-Selinene	11.25*	1480	0.94	9.93	1658	0.93
ar-Curcumene	11.25*	1480	[0.88]	10.72	1723	0.34
epi-Cubebol	11.39*	1490	1.94	12.05	1838	0.19
Bicyclogermacrene	11.39*	1490	[1.78]	10.12*	1673	[1.86]
α-Selinene	11.39*	1490	[1.78]	1tr	1664	0.19
Viridiflorene	11.39*	1490	[1.78]	9.71	1640	0.17
β-Himachalene	11.44	1494	0.13	9.84*	1651	[4.10]
(3*Z*,6*E*)-α-Farnesene	11.47	1496	0.35	10.32	1690	0.36
Cubebol	11.63*	1509	3.15	12.65	1891	0.51
(3*E*,6*E*)-α-Farnesene	11.63*	1509	[2.89]	10.56	1710	2.49
γ-Cadinene	11.63*	1509	[2.89]	10.46	1701	0.12
δ-Cadinene	11.77*	1519	0.37	10.48*	1703	[0.27]
β-Sesquiphellandrene	11.77*	1519	[0.37]	10.68	1719	0.13
(*E*)-α-Bisabolene	12.05	1542	0.12	10.77	1728	0.13
Dihydrocaryophyllen-5-one?	12.16*	1550	0.69	12.35	1864	0.23
Salviadienol?	12.16*	1550	[0.69]	14.39	2053	0.17
(*E*)-Nerolidol	12.33	1563	0.64	13.84	2001	0.18
Spathulenol	12.41	1570	4.93	14.45*	2060	5.45
Dendrolasin	12.46	1574	0.60	12.60*	1886	[1.04]
Salvial-4(14)-en-1-one	12.60	1585	0.28	13.10*	1932	0.21
Torilenol	12.85	1605	0.26	15.49*	2162	124.66
cis-Zingiberenol	12.90	1609	0.33	14.53	2067	3.50
(2,7*Z*)-Bisaboladien-4-ol	12.98	1616	0.11	14.87*	2100	[1.04]
τ-Cadinol	13.17	1632	0.40	14.95	2108	0.06
Unknown [m/z 123, 43 (86), 81 (75), 95 (73), 82 (68), 161 (64), 105 (63)... 220 (6)]	13.34	1646	0.48	13.10*	1932	[0.25]
α-Bisabolol oxide B, epimer 1	13.38*	1649	4.79	14.45*	2060	[5.91]
α-Bisabolol oxide B, epimer 2	13.38*	1649	[4.79]	14.57	2071	0.28
Ageratochromene	13.48	1657	0.67	16.96	2316	0.20
Bisabolone oxide A	13.70	1675	1.06	14.87*	2100	[1.16]
α-Bisabolol	13.80	1683	125.88	15.49*	2162	[123.06]
Herniarin	14.08	1707	11.48	21.22*	2812	163.92
Chamazulene	14.20	1718	4.54	16.75*	2292	4.55
α-Bisabolol oxide A	14.43	1738	8.96	17.21	2342	8.86
Myristic acid	14.77	1768	2.64	20.25	2692	1.47

Unknown [m/z 82, 43 (99), 95 (50), 67 (38), 139 (41)...]	14.84	1774	0.53	19.31	2578	0.34
Unknown [m/z 128, 158 (74), 199 (63), 115 (61), 129 (57), 200 (50)...]	14.88	1777	0.27			
Phytone	15.66	1846	0.37	14.75	2088	0.42
(*Z*)-Spiroether	15.95	1873	162.34	21.22*	2812	[147.77]
(*E*)-Spiroether	16.07	1884	23.14	22.36	2960	15.80
(*Z*)-Tibetin spiroether	16.31	1906	1.23			
Unknown [m/z 109, 110 (63), 69 (49), 43 (43), 41 (37)...]	16.39	1914	0.28	19.84	2642	0.57
Methyl palmitate	16.54	1928	0.36	15.64	2178	0.33
(*E*)-Tibetin spiroether	16.65	1938	3.74			
Palmitic acid	17.00	1972	35.97	21.73	2877	29.56
Methyl linoleate	18.22	2091	1.38	18.13	2443	1.45
Methyl petroselinate?	18.29	2099	0.65			
Heneicosane	18.35	2105	0.16	14.87*	2100	[0.91]
Phytol	18.41	2111	1.60	19.27	2573	3.24
Linoleic acid	18.72	2144	109.96	23.81	3158	80.45
Oleic acid	18.78	2149	47.24	23.54	3121	25.66
α-Linolenic acid	18.80	2151	3.02	24.10	3199	4.04
Stearic acid	18.97	2169	6.83			
Docosane	19.28	2201	0.30	15.77	2191	0.05
Unknown [m/z 228, 199 (92), 171 (85), 43 (68), 143 (45)...]	19.50	2225	15.48			
Unknown [m/z 228, 213 (85), 185 (81), 43 (77), 172 (75)...]	19.95	2273	21.00			
Tricosane	20.21	2301	1.02	16.75*	2292	[4.48]
Tetracosane	21.10	2401	0.30	17.73	2399	0.40
Pentacosane	21.96	2500	2.83	18.51	2486	2.64
Hexacosane	22.78	2599	0.11	19.46	2596	0.12
Heptacosane	23.58	2697	0.62	20.20	2685	0.34
6,8-Pentacosanedione?	24.18	2775	2.35			
Octacosane	24.38	2801	0.76			
Squalene	24.56	2824	0.11	22.84	3024	2.04
6,8-Heptacosanedione?	25.69	2977	2.79			
α-Tocopherol	26.81	3119	1.75			

*: 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.

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.
R.T.: Retention time (minutes)
R.I.: Retention index