Date : August 3, 2023

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 22L09-PTH01
Customer identification : Arnica Flower CO2 - AU1100R
Type : CO2 extract
Source : *Arnica montana*
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 : Sylvain Mercier, M. Sc., Chimiste 2014-005
Analysis date : December 13, 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

This report is an update of the version first issued on December 19, 2022 to correct the customer identification.

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: Brown viscous liquid
Refractive index: 1.4916 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

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

To the best of our knowledge, there is no literature available with regards to the expected composition of *A. montana* supercritical extracts. The observed volatile compounds do not feature the thymol derivatives often described in *A. montana* essential oils,[1,2] but some publications describe a different composition with relatively little thymol and higher amounts of caryophyllene, caryophyllene oxide and germacrene D – as observed here.[3,4] This could therefore be the result of natural variability of the species.

REFERENCES

(1) Sugier, D.; Sugier, P.; Jakubowicz-Gil, J.; Winiarczyk, K.; Kowalski, R. Essential Oil from Arnica Montana L. Achenes: Chemical Characteristics and Anticancer Activity. *Molecules* **2019**, *24* (22), 1–13. https://doi.org/10.3390/molecules24224158.

(2) Sugier, P.; Jakubowicz-Gil, J.; Sugier, D.; Kowalski, R.; Gawlik-Dziki, U.; Kołodziej, B.; Dziki, D. Chemical Characteristics and Anticancer Activity of Essential Oil from Arnica Montana L. Rhizomes and Roots. *Molecules* **2020**, *25* (6), 1284. https://doi.org/10.3390/molecules25061284.

(3) Kowalski, R.; Sugier, D.; Sugier, P.; Kołodziej, B. Evaluation of the Chemical Composition of Essential Oils with Respect to the Maturity of Flower Heads of Arnica Montana L. and Arnica Chamissonis Less. Cultivated for Industry. *Ind. Crops Prod.* **2015**, *76*, 857–865. https://doi.org/10.1016/j.indcrop.2015.07.029.

(4) Judžentiene, A.; Budiene, J. Analysis of the Chemical Composition of Fower Essential Oils from Arnica Montana of Lithuanian Origin. *Chemija* **2009**, *20* (3), 190–194.

ANALYSIS SUMMARY

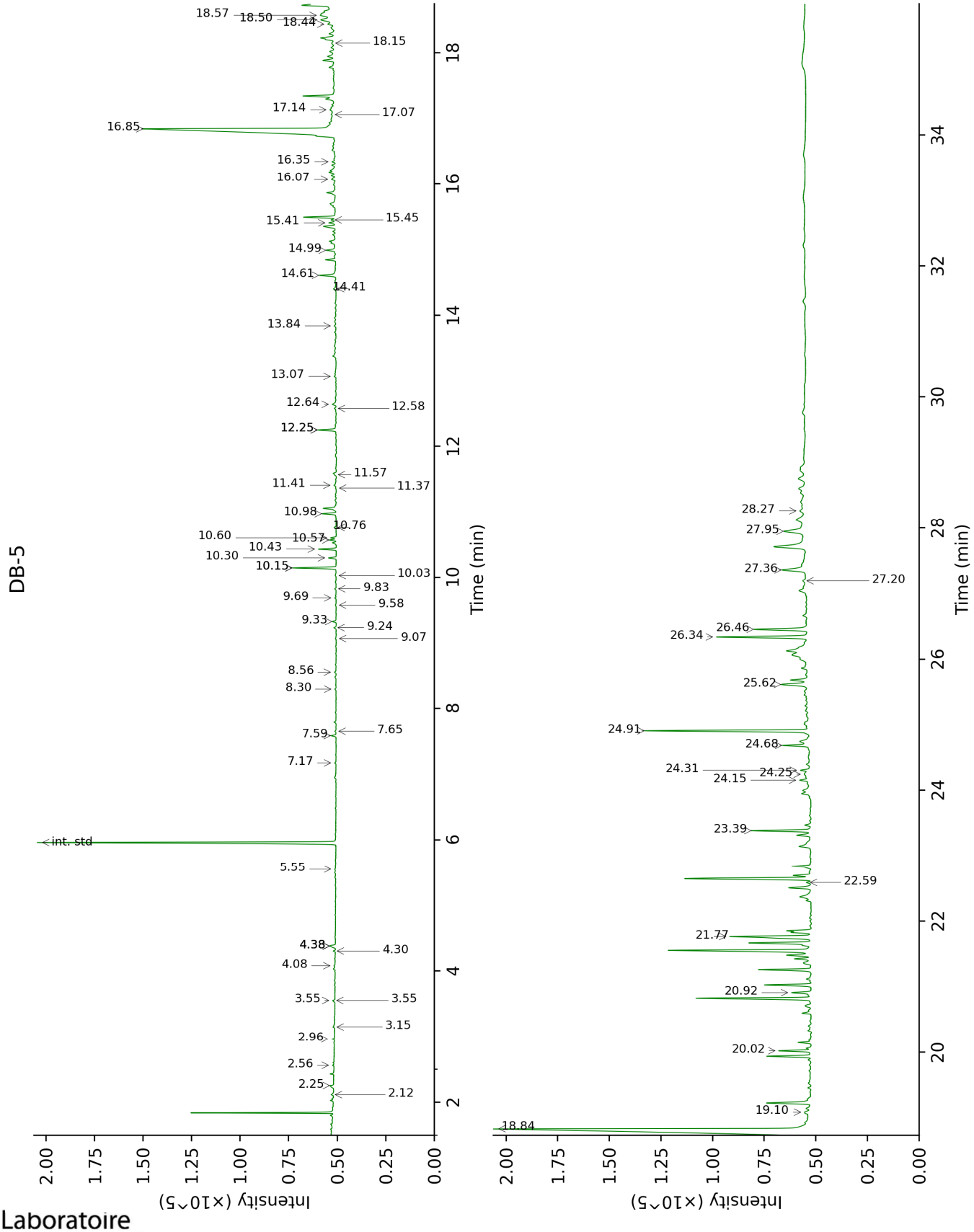
Identification	(mg/g)	% m/m	Classe
Isobutyric acid	2.28	0.23	Aliphatic acid
Isovaleric acid	0.46	0.05	Aliphatic acid
2-Methylbutyric acid	0.98	0.10	Aliphatic acid
2-Heptanol	0.12	0.01	Aliphatic alcohol
α-Pinene	0.19	0.02	Monoterpene
Camphene	0.28	0.03	Monoterpene
Sabinene	0.17	0.02	Monoterpene
β-Pinene	0.21	0.02	Monoterpene
Δ3-Carene	0.15	0.02	Monoterpene
para-Cymene	0.18	0.02	Monoterpene
Limonene	0.35	0.04	Monoterpene
β-Phellandrene	0.20	0.02	Monoterpene
1,8-Cineole	0.51	0.05	Monoterpenic ether
Linalool	0.18	0.02	Monoterpenic alcohol
Decanal	0.19	0.02	Aliphatic aldehyde
Thymol methyl ether	0.52	0.05	Monoterpenic ether
Carvone	0.19	0.02	Monoterpenic ketone
Bornyl acetate	0.18	0.02	Monoterpenic ester
Thymol	0.19	0.02	Monoterpenic alcohol
Silphin-1-ene	0.12	0.01	Sesquiterpene
α-Terpinyl acetate	0.33	0.03	Monoterpenic ester
Eugenol	0.50	0.05	Phenylpropanoid
α-Copaene	0.12	0.01	Sesquiterpene
α-Isocomene	0.15	0.02	Sesquiterpene
β-Elemene	0.16	0.02	Sesquiterpene
Tetradecane	0.12	0.01	Alkane
β-Caryophyllene	3.58	0.36	Sesquiterpene
cis-α-Bergamotene	0.23	0.02	Sesquiterpene
Thymohydroquinone dimethyl ether	0.80	0.08	Monoterpenic ether
trans-α-Bergamotene	1.48	0.15	Sesquiterpene
1,4-Dimethoxy-2-methyl-5-(prop-1-en-2-yl)benzene	0.69	0.07	Simple phenolic
α-Humulene	0.50	0.05	Sesquiterpene
(*E*)-β-Farnesene	0.22	0.02	Sesquiterpene
Germacrene D	1.25	0.13	Sesquiterpene
Pentadecane	0.11	0.01	Alkane
β-Bisabolene	0.41	0.04	Sesquiterpene
δ-Cadinene	0.16	0.02	Sesquiterpene
Caryophyllene oxide	1.69	0.17	Sesquiterpenic ether
Caryophyllene oxide isomer	0.14	0.01	Sesquiterpenic ether
Humulene epoxide II	0.25	0.03	Sesquiterpenic ether
Hexadecane	0.60	0.06	Alkane
Zingerone	0.23	0.02	Phenylbutanoid
Heptadecane	0.23	0.02	Alkane
Loliolide?	0.62	0.06	Terpenic lactone
Myristic acid	2.30	0.23	Aliphatic acid
Octadecane	1.07	0.11	Alkane
Neophytadiene	0.72	0.07	Diterpene

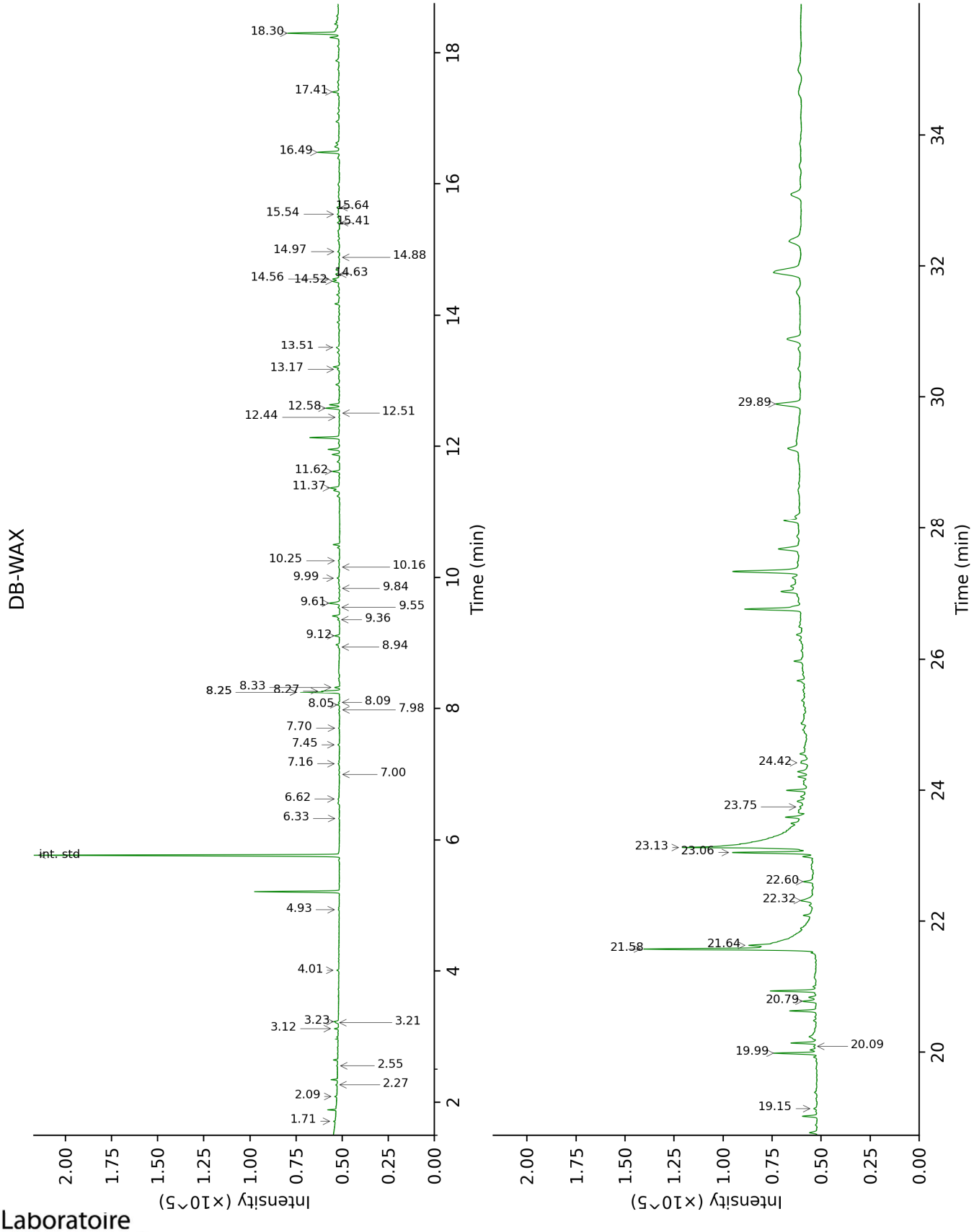
Phytone	0.44	0.04	Terpenic ketone
2-Heptadecanone	0.54	0.05	Aliphatic ketone
Methyl palmitate	0.34	0.03	Aliphatic ester
Palmitic acid	54.12	5.41	Aliphatic acid
9-(15,16-Dihydro-15-methyleneneryl)-α-terpinene?	0.45	0.05	Homoditerpene
Eicosane	0.69	0.07	Alkane
Heneicosane	0.34	0.03	Alkane
Unknown	0.97	0.10	Unknown
Linoleic acid	2.79	0.28	Aliphatic acid
Oleic acid	3.82	0.38	Aliphatic acid
Stearic acid	78.18	7.82	Aliphatic acid
Docosane	0.32	0.03	Alkane
Tricosane	2.91	0.29	Alkane
Tetracosane	2.03	0.20	Alkane
Pentacosane	10.03	1.00	Alkane
Hexacosane	0.47	0.05	Alkane
Heptacosane	5.61	0.56	Alkane
Octacosane	1.29	0.13	Alkane
(*E*)-Phytyl benzoate?	1.39	0.14	Phenolic ester
Squalene	1.01	0.10	Triterpene
Hexacosanol?	2.66	0.27	Aliphatic alcohol
Nonacosane	15.34	1.53	Alkane
Triacontane	3.94	0.39	Alkane
Untriacontane	9.44	0.94	Alkane
α-Tocopherol	6.46	0.65	Tocopherol
Dotriacontane	0.48	0.05	Alkane
Stigmasterol	4.23	0.42	Sterol
γ-Sitosterol?	3.72	0.37	Sterol
Tritriacontane	0.58	0.06	Alkane
Consolidated total	**240.93 mg/g**	**24.09%**	

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.


DB-5
18.57
18.50
18.44
18.15
17.14
17.07
16.85
16.35
16.07
15.41
15.45
14.99
14.61
14.41
13.84
13.07
12.64
12.58
12.25
11.57
11.41
11.37
10.98
10.76
10.60
10.57
10.43
10.30
10.15
10.03
9.83
9.69
9.58
9.33
9.24
9.07
8.56
8.30
7.59
7.65
7.17
int. std
5.55
4.38
4.30
4.08
3.55
3.55
3.15
2.96
2.56
2.25
2.12
Intensity (×10^5)
Time (min)
28.27
27.95
27.36
27.20
26.46
26.34
25.62
24.91
24.68
24.31
24.25
24.15
23.39
22.59
21.77
20.92
20.02
19.10
18.84


DB-WAX
Intensity (×10^5)
Time (min)
18.30
17.41
16.49
15.54
15.64
15.41
14.97
14.88
14.56
14.52
14.63
13.51
13.17
12.58
12.44
12.51
11.62
11.37
10.25
10.16
9.99
9.84
9.61
9.55
9.36
9.12
8.94
8.25
8.33
8.27
8.05
8.09
7.98
7.70
7.45
7.16
7.00
6.62
6.33
int. std
4.93
4.01
3.12
3.23
3.21
2.55
2.27
2.09
1.71
29.89
24.42
23.75
23.13
23.06
22.60
22.32
21.58
21.64
20.79
20.09
19.99
19.15

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g	R.T	R.I	mg/g
Isobutyric acid	1.32	794	2.28			
Isovaleric acid	2.12	868	0.46			
2-Methylbutyric acid	2.25	880	0.98			
2-Heptanol	2.56	906	0.12	4.93	1300	0.09
α-Pinene	2.96	934	0.19	1.41	1004	0.18
Camphene	3.15	946	0.28	1.71	1034	0.11
Sabinene	3.55*	974	0.28	2.26	1091	0.17
β-Pinene	3.55*	974	[0.28]	2.09	1073	0.21
Δ3-Carene	4.08	1009	0.15	2.55	1115	0.13
para-Cymene	4.30	1024	0.18	4.01	1231	0.22
Limonene	4.38*	1028	0.84	3.12	1161	0.35
β-Phellandrene	4.38*	1028	[0.84]	3.21	1169	0.20
1,8-Cineole	4.38*	1028	[0.96]	3.23	1170	0.51
Linalool	5.55	1103	0.18	7.98	1521	0.13
Decanal	7.17	1207	0.19	7.16	1459	0.26
Thymol methyl ether	7.59	1235	0.52	8.33	1548	0.49
Carvone	7.65	1240	0.19	9.84	1668	0.14
Bornyl acetate	8.30	1284	0.18	8.09	1530	0.18
Thymol	8.56	1301	0.19	14.97	2134	0.20
Silphin-1-ene	9.07	1337	0.12	6.62	1420	0.12
α-Terpinyl acetate	9.24	1348	0.33	9.55	1645	0.27
Eugenol	9.33	1355	0.50	14.63	2099	0.66
α-Copaene	9.58	1373	0.12	7.00	1447	0.07
α-Isocomene	9.69	1380	0.15	7.45	1481	0.20
β-Elemene	9.83	1390	0.16	8.25*†	1542	5.37
Tetradecane	10.03	1405	0.12	6.33	1398	0.07
β-Caryophyllene	10.15*	1413	3.81	8.25*†	1542	[5.37]
cis-α-Bergamotene	10.15*	1413	[3.81]	8.05	1527	0.23
Thymohydroquinone dimethyl ether	10.30	1425	0.80	11.62	1820	0.93
trans-α-Bergamotene	10.43	1435	1.48	8.27†	1544	[5.37]
1,4-Dimethoxy-2-methyl-5-(prop-1-en-2-yl)benzene	10.57	1445	0.69			
α-Humulene	10.60	1447	0.50	9.12	1610	0.53
(*E*)-β-Farnesene	10.76	1459	0.22	9.36	1630	0.22
Germacrene D	10.98	1476	1.25	9.61	1650	1.44
Pentadecane	11.37	1505	0.11	7.70	1500	0.12
β-Bisabolene	11.41	1508	0.41	9.99	1681	0.33
δ-Cadinene	11.57	1521	0.16	10.25	1703	0.19
Caryophyllene oxide	12.25*	1574	2.06	12.58	1905	1.69
Caryophyllene oxide isomer	12.25*	1574	[2.06]	12.51	1898	0.14
Humulene epoxide II	12.58	1600	0.25	13.17	1960	0.33
Hexadecane	12.64	1605	0.60	8.94	1596	0.18
Zingerone	13.07	1640	0.23	20.09	2700	0.66
Heptadecane	13.84	1705	0.23	10.16	1695	0.23

Loliolide?	14.41	1754	0.62			
Myristic acid	14.61	1772	2.30			
Octadecane	14.99	1805	1.07	11.37	1798	1.22
Neophytadiene	15.41	1843	0.72	12.44	1893	0.11
Phytone	15.45	1847	0.44	14.52	2088	0.83
2-Heptadecanone	16.07	1903	0.54	14.88	2125	0.16
Methyl palmitate	16.35	1929	0.34	15.41	2178	0.28
Palmitic acid	16.85	1977	54.12	21.64	2895	48.39
9-(15,16-Dihydro-15-methyleneneryl)-α-terpinene?	17.07	1998	0.45	15.64	2201	0.31
Eicosane	17.14	2005	0.69	13.51	1991	0.68
Heneicosane	18.15	2106	0.34	14.56	2092	0.80
Unknown [m/z 69, 81 (54), 93 (36), 41 (33), 121 (23), 95 (20)...]	18.44	2136	0.97			
Linoleic acid	18.50	2142	2.79			
Oleic acid	18.57	2150	3.82			
Stearic acid	18.84	2178	78.18	23.13	3097	81.08
Docosane	19.10	2204	0.32	15.54	2190	0.40
Tricosane	20.02	2304	2.91	16.49	2290	2.33
Tetracosane	20.92	2405	2.03	17.41	2389	0.79
Pentacosane	21.77	2504	10.03	18.30	2489	5.94
Hexacosane	22.59	2604	0.47	19.15	2587	0.41
Heptacosane	23.39	2704	5.61	19.99	2688	4.45
Octacosane	24.15	2804	1.29	20.79	2787	1.62
(*E*)-Phytyl benzoate?	24.24	2816	1.39			
Squalene	24.31	2824	1.01	22.60	3024	1.15
Hexacosanol?	24.68	2875	2.66			
Nonacosane	24.91	2905	15.34	21.58	2888	22.42
Triacontane	25.62	3004	3.94	22.32	2985	2.64
Untriacontane	26.34	3104	9.44	23.06	3086	9.21
α-Tocopherol	26.46	3118	6.46	29.89	3913	6.45
Dotriacontane	27.20	3204	0.48	23.75	3183	2.11
Stigmasterol	27.36	3219	4.23			
γ-Sitosterol?	27.95	3274	3.72			
Tritriacontane	28.27	3304	0.58	24.42	3280	1.32

*: 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
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