Date : May 09, 2022

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 22D19-PTH02
Customer identification : Caraway CO2 Extract - Germany - CC5103R
Type : CO2 extract
Source : *Carum carvi*
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 : Seydou Ka, Ph. D.
Analysis date : April 20, 2022

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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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 April 21, 2022 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: Yellow liquid
Refractive index: 1.4835 ± 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
α-Pinene	0.39	0.04	Monoterpene
β-Pinene	0.06	0.01	Monoterpene
Sabinene	0.59	0.06	Monoterpene
Octan-3-one	0.04	tr	Aliphatic ketone
Myrcene	3.26	0.33	Monoterpene
Octanal	0.10	0.01	Aliphatic aldehyde
para-Cymene	0.88	0.09	Monoterpene
1,8-Cineole	0.06	0.01	Monoterpenic ether
β-Phellandrene	0.25	0.03	Monoterpene
Limonene	401.41	40.14	Monoterpene
(*Z*)-β-Ocimene	0.08	0.01	Monoterpene
(*E*)-β-Ocimene	0.18	0.02	Monoterpene
γ-Terpinene	0.88	0.09	Monoterpene
Fenchone	0.03	tr	Monoterpenic ketone
Linalool	0.28	0.03	Monoterpenic alcohol
Unknown	0.06	0.01	Unknown
trans-para-Mentha-2,8-dien-1-ol	1.68	0.17	Monoterpenic alcohol
cis-para-Mentha-2,8-dien-1-ol	1.10	0.11	Monoterpenic alcohol
trans-Limonene oxide	1.16	0.12	Monoterpenic ether
Unknown	0.45	0.05	Oxygenated monoterpene
trans-Isocarveol	0.56	0.06	Monoterpenic alcohol
α-Terpineol	0.74	0.07	Monoterpenic alcohol
Unknown	1.03	0.10	Unknown
cis-Dihydrocarvone	0.61	0.06	Monoterpenic ketone
Unknown	0.48	0.05	Unknown
trans-Isopiperitenol	0.36	0.04	Monoterpenic alcohol
trans-Dihydrocarvone	1.53	0.15	Monoterpenic ketone
iso-Dihydrocarveol ?	0.13	0.01	Monoterpenic alcohol
trans-Carveol	1.01	0.10	Monoterpenic alcohol
cis-para-Mentha-1(7),8-dien-2-ol	0.25	0.03	Monoterpenic alcohol
cis-Carveol	1.98	0.20	Monoterpenic alcohol
neoiso-Dihydrocarveol	1.17	0.12	Monoterpenic alcohol
Carvone	399.89	39.99	Monoterpenic ketone
(*Z*)-Isogeraniol	0.12	0.01	Monoterpenic alcohol
Isopiperitenone	0.09	0.01	Monoterpenic ketone
Geranial	1.48	0.15	Monoterpenic aldehyde
trans-Carvone oxide	0.37	0.04	Monoterpenic ketone
(*E*)-Anethole	0.40	0.04	Phenylpropanoid
Limonen-10-ol	0.11	0.01	Monoterpenic alcohol
Perilla alcohol	0.14	0.01	Monoterpenic alcohol
Thymol	0.32	0.03	Monoterpenic alcohol
Carvacrol	0.17	0.02	Monoterpenic alcohol
trans-Carvyl acetate	0.92	0.09	Monoterpenic ester
cis-Carvyl acetate	0.51	0.05	Monoterpenic ester
Unknown	0.19	0.02	Unknown
β-Bourbonene	0.13	0.01	Sesquiterpene
β-Elemene	0.27	0.03	Sesquiterpene
Unknown	0.20	0.02	Unknown

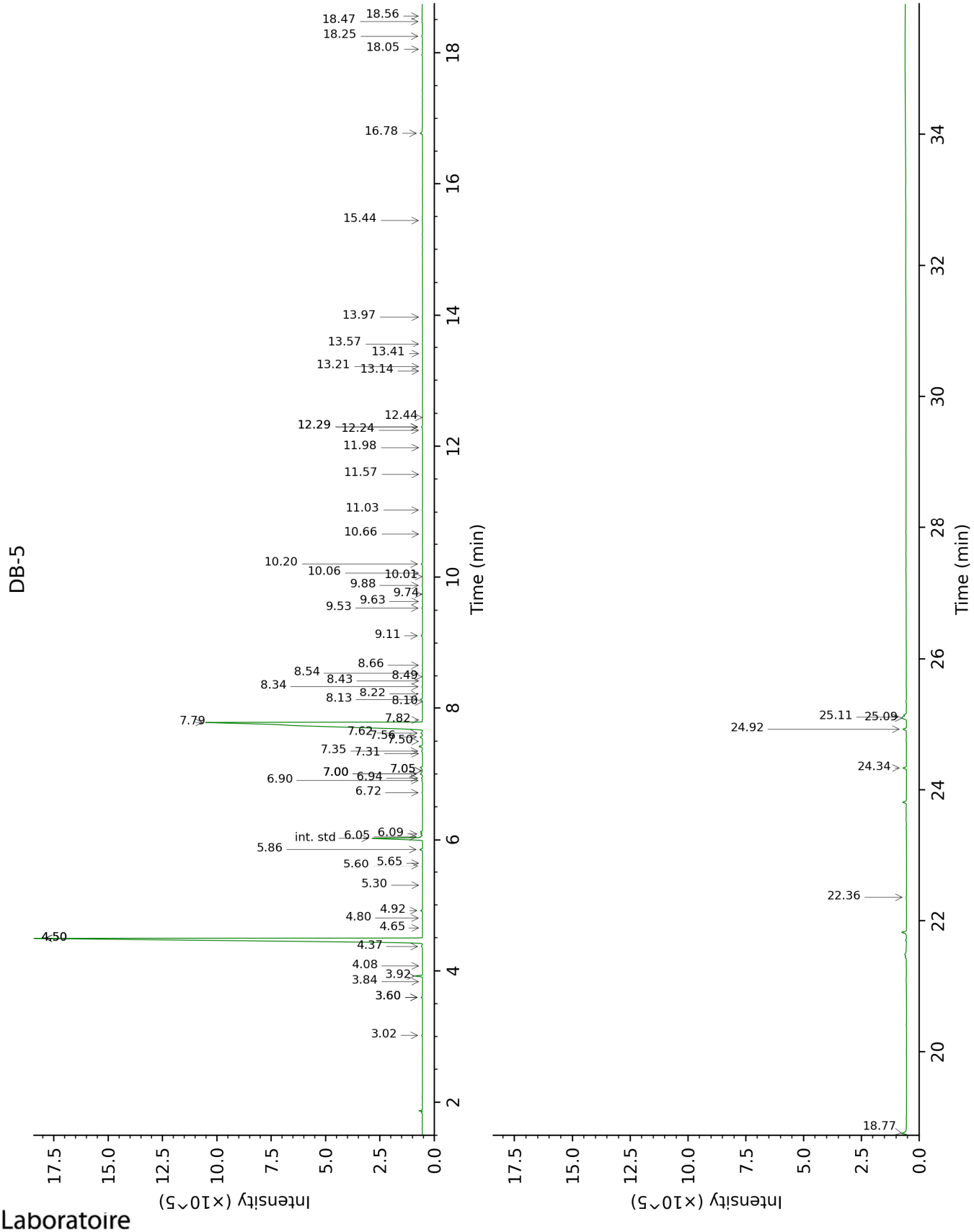
Unknown	0.20	0.02	Unknown
β-Caryophyllene	0.68	0.07	Sesquiterpene
α-Humulene	0.06	0.01	Sesquiterpene
Germacrene D	0.14	0.01	Sesquiterpene
7-epi-α-Selinene	0.11	0.01	Sesquiterpene
Salviadienol?	0.05	0.01	Sesquiterpenic alcohol
Spathulenol	0.17	0.02	Sesquiterpenic alcohol
Caryophyllene oxide isomer	0.10	0.01	Sesquiterpenic ether
Caryophyllene oxide	0.71	0.07	Sesquiterpenic ether
Salvial-4(14)-en-1-one	0.10	0.01	Aliphatic alcohol
Unknown	0.11	0.01	Unknown
Selin-11-en-4α-ol	0.13	0.01	Sesquiterpenic alcohol
(3*Z*)-Caryophylla-3,8(13)-dien-5β-ol	0.10	0.01	Sesquiterpenic alcohol
Germacra-4(15),5,10(14)-trien-1α-ol	0.17	0.02	Sesquiterpenic alcohol
Unknown	0.17	0.02	Oxygenated sesquiterpene
Phytone	0.22	0.02	Terpenic ketone
Palmitic acid	2.14	0.21	Aliphatic acid
Methyl linoleate	0.14	0.01	Aliphatic ester
Phytol	0.46	0.05	Diterpenic alcohol
Linoleic acid	0.54	0.05	Aliphatic acid
cis-Vaccenic acid?	0.15	0.02	Aliphatic acid
Stearic acid	3.63	0.36	Aliphatic acid
Unknown	0.44	0.04	Unknown
Squalene	1.92	0.19	Triterpene
Nonacosane	1.93	0.19	Alkane
Unknown	2.80	0.28	Unknown
Unknown	3.31	0.33	Unknown
Consolidated total	**848.80 mg/g**	**84.88%**	

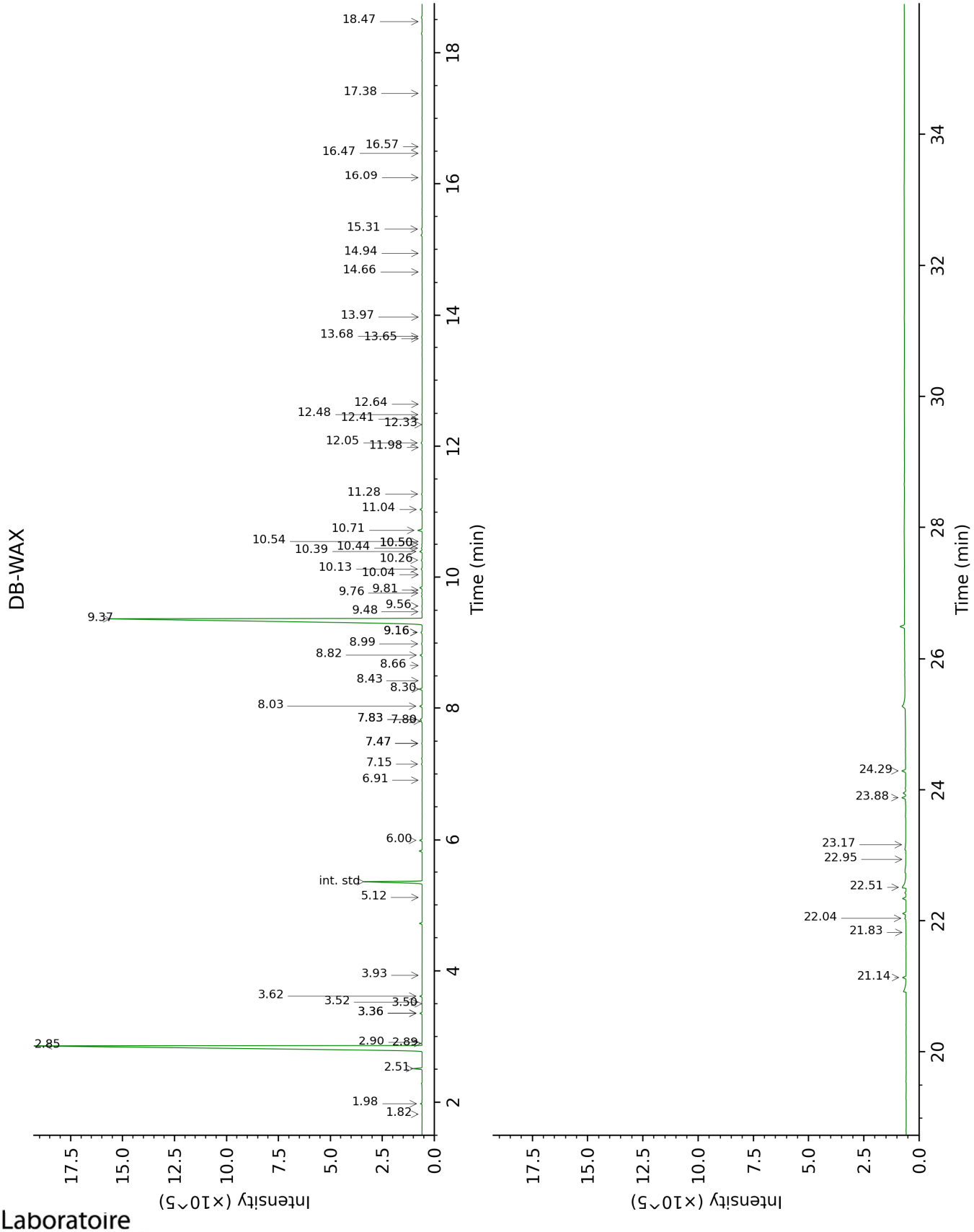
tr: The compound has been detected below 0.005% of total signal.

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.


DB-5
18.47
18.56
18.25
18.05
16.78
15.44
13.97
13.57
13.41
13.21
13.14
12.44
12.29
12.24
11.98
11.57
11.03
10.66
10.20
10.06
10.01
9.88
9.74
9.63
9.53
9.11
8.66
8.54
8.43
8.49
8.34
8.22
8.13
8.10
7.82
7.79
7.62
7.56
7.50
7.35
7.31
7.05
7.00
6.94
6.90
6.72
int. std
6.05
6.09
5.86
5.60
5.65
5.30
4.92
4.80
4.65
4.50
4.37
4.08
3.92
3.84
3.60
3.02
Time (min)
Intensity (×10^5)
25.11
25.09
24.92
24.34
22.36
18.77
Time (min)
Intensity (×10^5)


DB-WAX
18.47
17.38
16.57
16.47
16.09
15.31
14.94
14.66
13.97
13.68
13.65
12.64
12.48
12.41
12.33
12.05
11.98
11.28
11.04
10.71
10.54
10.39
10.44
10.50
10.26
10.13
10.04
9.76
9.81
9.48
9.56
9.37
9.16
8.99
8.82
8.66
8.43
8.30
8.03
7.83
7.80
7.47
7.15
6.91
6.00
int. std
5.12
3.93
3.62
3.52
3.50
3.36
2.85
2.90
2.89
2.51
1.98
1.82
24.29
23.88
23.17
22.95
22.51
22.04
21.83
21.14
Time (min)
Intensity (×10^5)

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g	R.T	R.I	mg/g
α-Pinene	3.02	933	0.39			
β-Pinene	3.60*	972	0.64	1.82	1074	0.06
Sabinene	3.60*	972	[0.64]	1.98	1091	0.59
Octan-3-one	3.84	988	0.04	3.52	1219	0.18
Myrcene	3.92	994	3.26	2.51	1137	3.37
Octanal	4.08	1004	0.10	3.93	1250	0.06
para-Cymene	4.37	1023	0.88	3.62	1226	0.88
1,8-Cineole	4.50*	1031	440.80	2.90	1170	0.06
β-Phellandrene	4.50*	1031	[387.95]	2.89	1169	0.25
Limonene	4.50*	1031	[387.95]	2.85	1166	401.41
(*Z*)-β-Ocimene	4.65	1041	0.08	3.36*	1207	0.98
(*E*)-β-Ocimene	4.80	1051	0.18	3.50	1218	0.04
γ-Terpinene	4.92	1058	0.88	3.36*	1207	[0.98]
Fenchone	5.30	1083	0.03	5.12	1338	0.04
Linalool	5.60	1102	0.28	7.47*	1515	0.27
Unknown [m/z 43, 59 (37), 79 (33), 91 (32), 119 (31)...]	5.65	1105	0.06	8.43	1591	0.06
trans-para-Mentha-2,8-dien-1-ol	5.86	1119	1.68	8.30	1581	1.73
cis-para-Mentha-2,8-dien-1-ol	6.05	1131	1.10	8.82	1623	1.26
trans-Limonene oxide	6.09	1134	1.16	6.00	1403	1.41
Unknown [m/z 69, 84 (62), 41 (30), 123 (26), 97 (24), 109 (23)...]	6.72	1175	0.45	8.99	1637	0.65
trans-Isocarveol	6.90	1188	0.56	10.26	1744	0.58
α-Terpineol	6.94	1190	0.74	9.16*	1652	1.02
Unknown [m/z 121, 79 (61), 93 (55), 94 (40), 91 (39), 84 (37)...]	7.00*	1194	2.19	7.47*	1515	[0.31]
cis-Dihydrocarvone	7.00*	1194	[1.95]	7.83*	1544	1.42
Unknown [m/z 121, 79 (98), 93 (87), 94 (73), 91 (63), 105 (45)...]	7.00*	1194	[2.19]	7.15	1491	0.48
trans-Isopiperitenol	7.05*	1197	0.42	9.76	1701	0.36
trans-Dihydrocarvone	7.05*	1197	[0.42]	8.03	1560	1.53

iso-Dihydrocarveol ?	7.31	1215	0.13	10.13	1732	0.73
trans-Carveol	7.35	1218	1.01	10.71	1783	2.86
cis-para-Mentha-1(7),8-dien-2-ol	7.50	1228	0.25	11.28	1833	0.44
cis-Carveol	7.56	1232	1.98	11.04	1812	1.44
neoiso-Dihydrocarveol	7.62	1236	1.17	10.39	1755	1.56
Carvone	7.78	1248	399.89	9.37	1669	411.44
(*Z*)-Isogeraniol	7.82	1250	0.12	10.54	1768	0.12
Isopiperitenone	8.10	1269	0.09	10.50*	1765	0.32
Geranial	8.13	1272	1.48	9.48	1677	0.30
trans-Carvone oxide	8.22	1278	0.37	10.50*	1765	[0.37]
(*E*)-Anethole	8.34	1286	0.40	10.44	1760	0.48
Limonen-10-ol	8.43	1292	0.11	12.48	1943	0.28
Perilla alcohol	8.49	1296	0.14	12.64	1958	0.09
Thymol	8.54	1300	0.32			
Carvacrol	8.66	1304	0.17	14.66	2156	0.08
trans-Carvyl acetate	9.11	1336	0.92	9.56	1685	0.26
cis-Carvyl acetate	9.53	1366	0.51	10.04	1725	0.09
Unknown [m/z 98, 69 (40), 70 (40), 41 (22), 43 (14), 109 (13)... 166? (t)]	9.63	1373	0.19	16.47	2347	0.27
β-Bourbonene	9.74	1381	0.13	6.91	1472	0.11
β-Elemene	9.88	1390	0.27	7.80	1542	0.63
Unknown [m/z 109, 108 (82), 82 (44), 91 (42), 79 (36), 43 (35)...]	10.01	1400	0.20			
Unknown [m/z 108, 109 (99), 82 (58), 91 (48), 79 (45), 43 (44)...]	10.06	1404	0.20			
β-Caryophyllene	10.20	1414	0.68	7.83*	1544	[1.20]
α-Humulene	10.66	1448	0.06	8.66	1610	0.06
Germacrene D	11.03	1476	0.14	9.16*	1652	[0.88]
7-epi-α-Selinene	11.58	1518	0.11	9.81	1705	0.09
Salviadienol?	11.98	1550	0.05	13.65	2055	0.06
Spathulenol	12.24	1571	0.17	13.68	2058	0.17
Caryophyllene oxide isomer	12.30*	1575	0.75	11.98	1897	0.10

Caryophyllene oxide	12.30*	1575	[0.75]	12.05	1903	0.71
Salvial-4(14)-en-1-one	12.44	1587	0.10	12.41	1937	0.10
Unknown [m/z 123, 43 (86), 81 (75), 95 (73), 82 (68), 161 (64), 105 (63)... 220 (6)]	13.14	1644	0.11	12.33	1929	0.15
Selin-11-en-4α-ol	13.21	1650	0.13	14.94	2185	0.10
(3*Z*)-Caryophylla-3,8(13)-dien-5β-ol	13.41	1666	0.10	16.09	2306	0.23
Germacra-4(15),5,10(14)-trien-1α-ol	13.57	1680	0.17	15.31	2223	0.60
Unknown [m/z 43, 71 (88), 93 (86), 41 (74), 55 (73), 81 (71), 95 (59), 91 (53), 67 (52)... 220 (13)... 236? (t)]	13.97	1714	0.17	16.57	2358	0.11
Phytone	15.44	1844	0.22	13.98	2087	0.03
Palmitic acid	16.78	1970	2.14	21.14	2908	2.48
Methyl linoleate	18.05	2096	0.14	17.38	2449	0.16
Phytol	18.25	2116	0.46	18.47	2575	0.12
Linoleic acid	18.47	2139	0.54	23.17	3187	0.37
cis-Vaccenic acid?	18.56	2148	0.15	22.95	3155	0.12
Stearic acid	18.78	2170	3.63	22.51	3094	7.11
Unknown [m/z 137, 136 (87), 81 (80), 93 (64), 107 (58), 121 (49)...]	22.36	2577	0.44			
Squalene	24.34	2829	1.92	22.04	3029	0.80
Nonacosane	24.92	2909	1.93	21.83	3000	0.08
Unknown [m/z 81, 137 (67), 95 (41), 55 (16), 136 (15)...]	25.09	2932	2.80	23.88	3290	2.99
Unknown [m/z 81, 137 (58), 95 (42), 67 (22), 55 (18), 69 (14)...]	25.11	2934	3.31	24.29	3350	3.03

*: Two or more compounds are coeluting on this column
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
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

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