Date : July 25, 2022

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 22G05-NSO01
Customer identification : Organic CO2 Extract - Black Cumin Total - Lot#291403 - Botanical species: Nigella sativa
Type : CO2 extract
Source : *Nigella sativa*
Customer : Natural Sourcing LLC

Analysis

Method: Extraction of volatile compounds with methanol, 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 : July 25, 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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.

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 viscous liquid
Refractive index: 1.4730 ± 0.0003 (20 °C; method PC-MAT-016)

CONCLUSION

No adulterant, contaminant or diluent has been detected using this method. The detected volatiles sum up to 5.4% of the sample weight.

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ANALYSIS SUMMARY

Identification	(mg/g)	% m/m	Classe
Hexanal	0.02	tr	Aliphatic aldehyde
Butyric acid	0.19	0.02	Aliphatic acid
α-Thujene	4.39	0.44	Monoterpene
α-Pinene	1.02	0.10	Monoterpene
β-Pinene	1.07	0.11	Monoterpene
Sabinene	0.35	0.04	Monoterpene
α-Terpinene	0.08	0.01	Monoterpene
para-Cymene	11.88	1.19	Monoterpene
Limonene	0.72	0.07	Monoterpene
1,8-Cineole	0.11	0.01	Monoterpenic ether
γ-Terpinene	0.01	tr	Monoterpene
cis-Sabinene hydrate	0.02	tr	Monoterpenic alcohol
Terpinolene	0.01	tr	Monoterpene
Methoxythujene I?	0.04	tr	Monoterpenic ether
cis-4-Methoxythujane	0.33	0.03	Monoterpenic ether
Linalool	0.03	tr	Monoterpenic alcohol
trans-4-Methoxythujane	1.84	0.18	Monoterpenic ether
Camphor	0.02	tr	Monoterpenic ketone
Borneol	0.01	tr	Monoterpenic alcohol
Terpinen-4-ol	0.29	0.03	Monoterpenic alcohol
para-Cymen-8-ol	0.05	0.01	Monoterpenic alcohol
Methoxythujane isomer	0.01	tr	Monoterpenic ether
α-Terpinyl methyl ether	0.03	tr	Monoterpenic ether
Thymoquinone	28.62	2.86	Monoterpenic ketone
trans-Ascaridole glycol	0.03	tr	Monoterpenic alcohol
Bornyl acetate	0.06	0.01	Monoterpenic ester
Thymol	0.06	0.01	Monoterpenic alcohol
Carvacrol	0.48	0.05	Monoterpenic alcohol
2,3-Dihydro-3,6-dihydroxyterpinolene	0.05	0.01	Monoterpenic alcohol
α-Longipinene	0.23	0.02	Sesquiterpene
Longifolene	1.08	0.11	Sesquiterpene
β-Caryophyllene	0.03	tr	Sesquiterpene
ar-Curcumene	0.03	tr	Sesquiterpene
β-Bisabolene	0.03	tr	Sesquiterpene
Thymohydroquinone	0.74	0.07	Monoterpenic alcohol
Tetradecanal	0.03	tr	Aliphatic aldehyde
Longibornyl acetate	0.08	0.01	Sesquiterpenic ester
Carvone	0.06	0.01	Monoterpenic ketone
Consolidated total	**54.12 mg/g**	**5.41%**	

tr : < 0.005

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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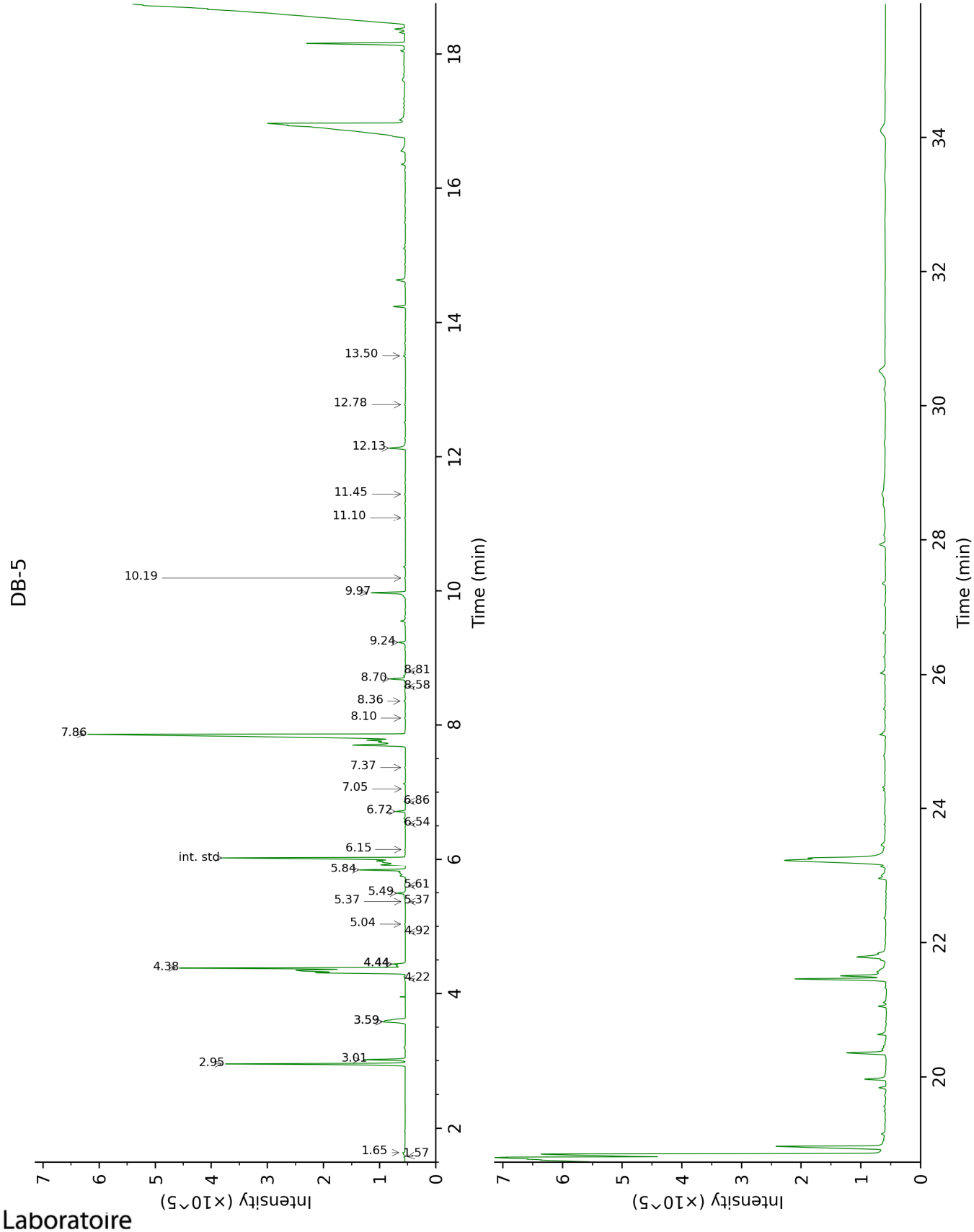
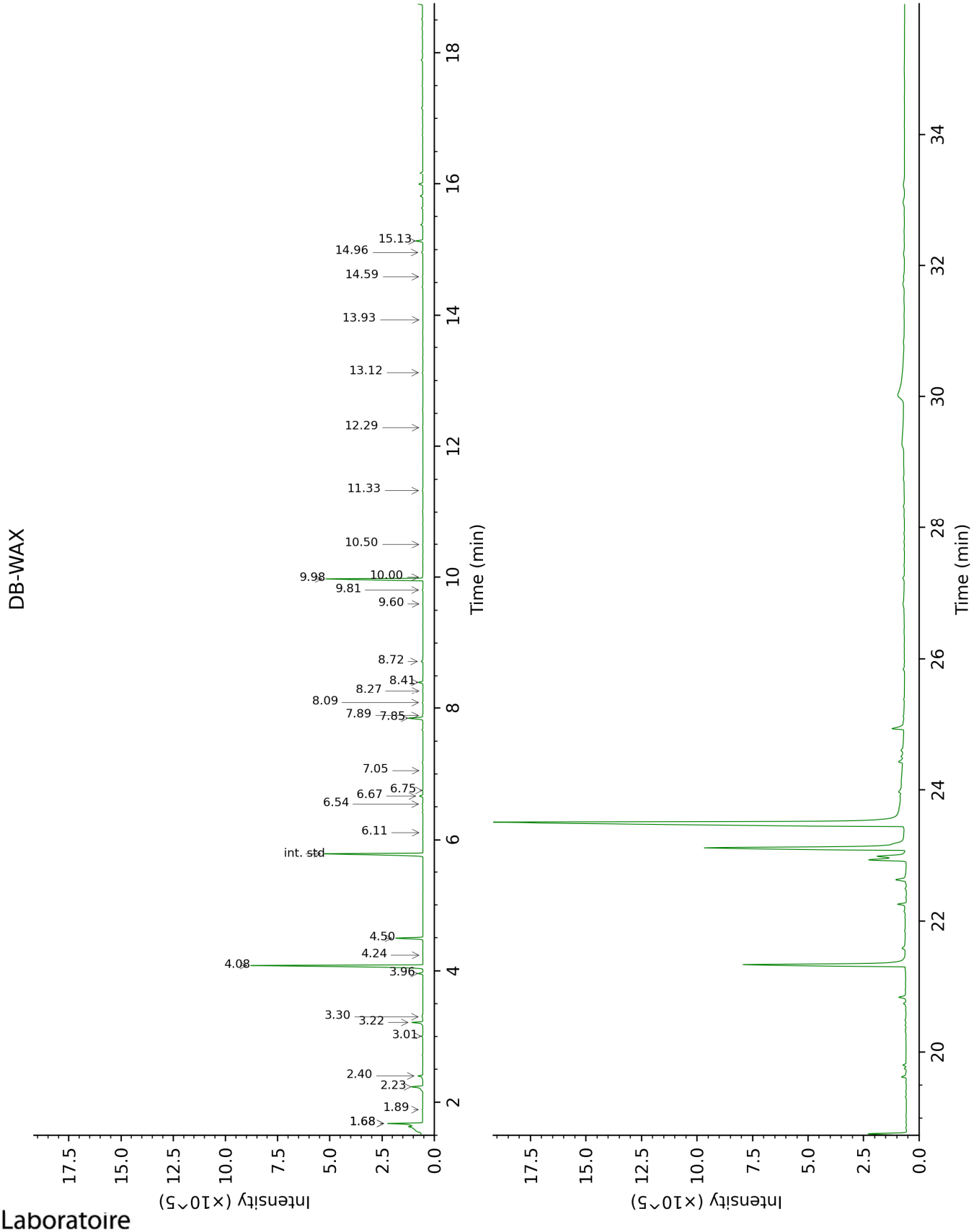

DB-5
Intensity (×10^5)
Time (min)
13.50
12.78
12.13
11.45
11.10
10.19
9.97
9.24
8.81
8.70
8.58
8.36
8.10
7.86
7.37
7.05
6.86
6.72
6.54
6.15
int. std
5.84
5.61
5.49
5.37
5.37
5.04
4.92
4.44
4.38
4.22
3.59
3.01
2.95
1.65
1.57


DB-WAX
Intensity (×10^5)
Time (min)
15.13
14.96
14.59
13.93
13.12
12.29
11.33
10.50
9.98
10.00
9.81
9.60
8.72
8.41
8.27
8.09
7.89
7.85
7.05
6.75
6.67
6.54
6.11
int. std
4.50
4.24
4.08
3.96
3.30
3.22
3.01
2.40
2.23
1.89
1.68

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/g	R.T	R.I	mg/g
Hexanal	1.58	818	0.02	1.89	1052	0.03
Butyric acid	1.64	824	0.19	8.72	1580	0.29
α-Thujene	2.95	930	4.39	1.68*	1031	5.40
α-Pinene	3.01	934	1.02	1.68*	1031	[5.40]
β-Pinene	3.59*	973	1.40	2.23	1087	1.07
Sabinene	3.59*	973	[1.40]	2.40	1103	0.35
α-Terpinene	4.22	1015	0.08	3.01	1152	0.08
para-Cymene	4.38	1025	11.88	4.08	1236	11.91
Limonene	4.44*†	1029	0.66	3.22	1169	0.72
1,8-Cineole	4.44*†	1029	[0.75]	3.30	1176	0.11
γ-Terpinene	4.92	1060	0.01			
cis-Sabinene hydrate	5.04	1067	0.02	6.75	1428	0.03
Terpinolene	5.37*†	1088	0.05	4.24	1248	0.01
Methoxythujene I?	5.37*†	1088	[0.05]			
cis-4-Methoxythujane	5.49	1096	0.33	3.96	1227	0.35
Linalool	5.61	1104	0.03	7.89	1514	0.06
trans-4-Methoxythujane	5.84	1119	1.84	4.50	1268	1.86
Camphor	6.15	1139	0.02	7.05	1451	0.03
Borneol	6.54	1164	0.01	9.60	1650	0.02
Terpinen-4-ol	6.72	1176	0.29	8.41	1555	0.35
para-Cymen-8-ol	6.86	1186	0.05	11.33	1796	0.07
Methoxythujane isomer	7.05	1198	0.01	6.11	1380	0.01
α-Terpinyl methyl ether	7.37	1219	0.03	6.54	1412	0.05
Thymoquinone	7.86	1253	28.62	9.98	1681	9.81
trans-Ascaridole glycol	8.10	1270	0.03	13.93	2036	0.01
Bornyl acetate	8.36	1287	0.06	8.09	1530	0.06
Thymol	8.58	1302	0.06	14.96	2136	0.12
Carvacrol	8.70	1306	0.48	15.13	2154	0.51
2,3-Dihydro-3,6-dihydroxyterpinolene	8.81	1314	0.05	14.59	2099	0.06
α-Longipinene	9.24	1345	0.23	6.67	1422	0.23
Longifolene	9.97	1398	1.08	7.85	1511	1.09
β-Caryophyllene	10.19	1414	0.03	8.27	1544	0.03
ar-Curcumene	11.10	1482	0.03	10.50	1725	0.02
β-Bisabolene	11.45	1508	0.03	10.00	1684	0.05
Thymohydroquinone	12.13	1562	0.74			
Tetradecanal	12.78	1614	0.03	12.28	1882	0.04
Longibornyl acetate	13.50	1674	0.08	13.12	1959	0.06
Carvone				9.81	1668	0.06

*: 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

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