Date : November 18, 2020

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 20K04-INT01
Customer identification : Baby Magic - Caling Baby Bath - 0204
Type : Aqueous fragrance
Source : Fragrant extract(s) and isolate(s)
Customer : Interne

Analysis

Method: Addition of salt and extraction with dichloromethane 3 times. Addition of an internal standard to estimate concentrations of individual compounds[1]. Concentration of the organic phase. Analysis with PC-MAT-009 - Analysis of the composition of an hydrosol by GC-FID.
Analyst : Alexis St-Gelais, M. Sc., chimiste
Analysis date : November 18, 2020

Checked and approved by :

Alexis St-Gelais, M. Sc., 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Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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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Conclusion

This sample features mostly isolates and/or synthetic single ingredients. Despite the presence of linalool and terpinen-4-ol, the absence of sesquiterpenes and some other key monoterpenols, like lavandulol, do not suggest that either lavender or tea tree oils are present, or in no more than negligible amounts.

Analysis summary

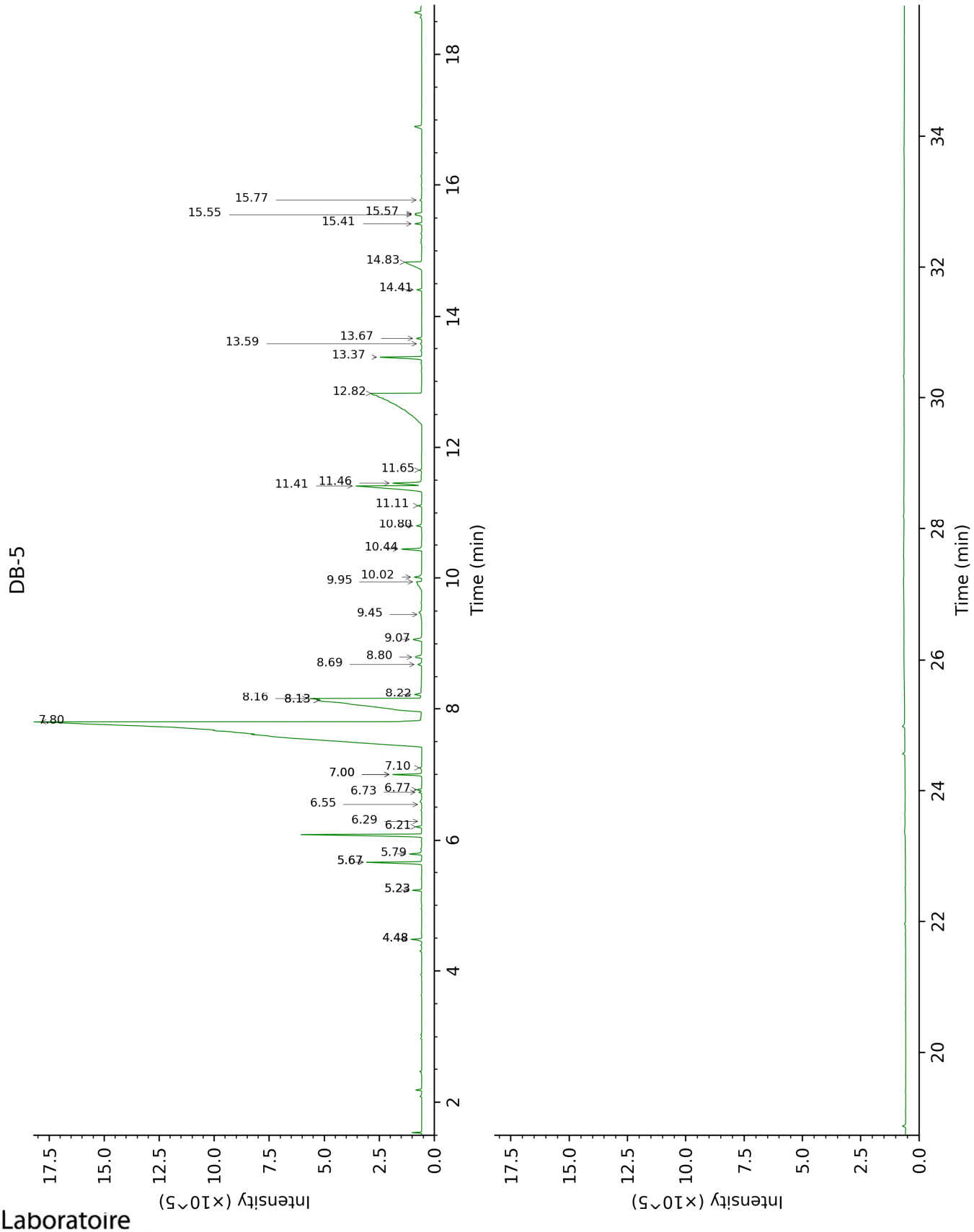
Identification	(mg/L)	% of total volatiles	Classe
Limonene	3.2	0.03	Monoterpene
1,8-Cineole	13.8	0.14	Monoterpenic ether
Dihydromyrcenol	11.4	0.11	Monoterpenic alcohol
cis-Triplal	1.4	0.01	Synthetic
Linalool	93.0	0.92	Monoterpenic alcohol
trans-Triplal	0.5	tr	Synthetic
Phenylethyl alcohol	20.7	0.21	Simple phenolic
Camphor	10.1	0.10	Monoterpenic ketone
Rhodinal (α-citronellal)	0.5	0.01	Synthetic
Benzyl acetate	0.5	0.01	Phenolic ester
Menthol	4.4	0.04	Monoterpenic alcohol
Terpinen-4-ol	7.7	0.08	Monoterpenic alcohol
α-Terpineol	37.3	0.37	Monoterpenic alcohol
Methyl salicylate	9.4	0.09	Phenolic ester
γ-Terpineol	3.7	0.04	Monoterpenic alcohol
2-Phenoxyethanol	6997.5	69.59	Simple phenolic
Geraniol	6.9	0.07	Monoterpenic alcohol
para-Anisaldehyde	17.5	0.17	Simple phenolic
Unknown	1033.4	10.28	Unknown
(*E*)-Cinnamal	10.5	0.10	Phenylpropanoid
Thymol	6.8	0.07	Monoterpenic alcohol
Carvacrol	15.8	0.16	Monoterpenic alcohol
Heliotropin	30.3	0.30	Simple phenolic
Eugenol	3.3	0.03	Phenylpropanoid
Capric acid	34.8	0.35	Aliphatic acid
Vanillin	21.3	0.21	Simple phenolic
Coumarin	45.9	0.46	Coumarin
Ethylvanillin	13.8	0.14	Synthetic
(*E*)-α-Isomethyl-ionone	5.3	0.05	Ionone or analog
Bis(2-ethylhexyl) ether?	206.0	2.05	Synthetic
Mefrosol	61.1	0.61	Synthetic
α-Methyl-ionone	2.9	0.03	Ionone or analog
Lauric acid	857.2	8.53	Aliphatic acid
Methyl *cis*-dihydrojasmonate	95.9	0.95	Jasmonate
Hexyl salicylate	2.5	0.02	Phenolic ester
Methyl *trans*-dihydrojasmonate	10.3	0.10	Jasmonate
(*E*)-Hexylcinnamaldehyde	7.0	0.07	Synthetic
Myristic acid	88.4	0.88	Aliphatic acid
Isopropyl myristate	10.8	0.11	Synthetic

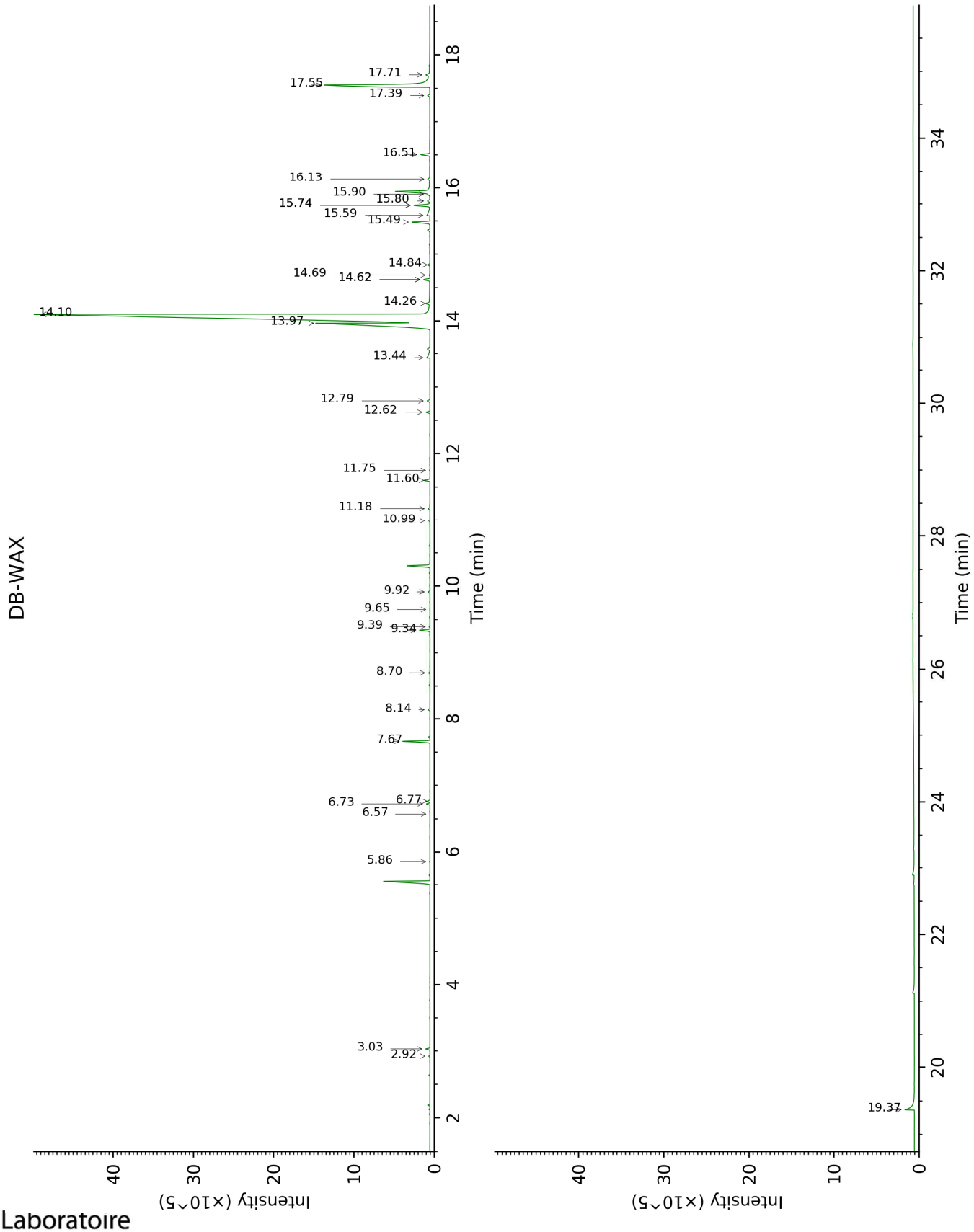
Galaxolide isomer I	9.9	0.10	Synthetic
Galaxolide isomer II	8.4	0.08	Synthetic
Diisobutyl phthalate	4.2	0.04	Synthetic
Consolidated total	**9825.33 mg/L**	**97.72%**	

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
15.77
15.55
15.57
15.41
14.83
14.41
13.59
13.67
13.37
12.82
11.65
11.41
11.46
11.11
10.80
10.44
9.95
10.02
9.45
9.07
8.69
8.80
8.16
8.13
8.22
7.80
7.00
7.10
6.73
6.77
6.55
6.29
6.21
5.79
5.67
5.23
4.48
Time (min)
Intensity (×10^5)
Time (min)
Intensity (×10^5)


DB-WAX
17.71
17.55
17.39
16.51
16.13
15.90
15.80
15.74
15.59
15.49
14.84
14.69
14.62
14.26
14.10
13.97
13.44
12.79
12.62
11.75
11.60
11.18
10.99
9.92
9.65
9.39
9.34
8.70
8.14
7.67
6.73
6.77
6.57
5.86
3.03
2.92
19.37
Time (min)
Intensity (×10^5)

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/L	R.T	R.I	mg/L
Limonene	4.48*	1028	15.2	2.92	1161	3.2
1,8-Cineole	4.48*	1028	[17.2]	3.03	1170	13.8
Dihydromyrcenol	5.23*	1076	12.6	6.73	1445	11.4
cis-Triplal	5.23*	1076	[13.5]	5.86	1381	1.4
Linalool	5.67*	1103	94.2	7.67	1516	93.0
trans-Triplal	5.67*	1103	[98.8]	6.57	1433	0.5
Phenylethyl alcohol	5.79	1112	20.7	11.60	1842	21.5
Camphor	6.21	1138	10.1	6.77	1448	9.8
Rhodinal (α-citronellal)	6.29	1144	0.5			
Benzyl acetate	6.55	1160	0.5	9.65	1674	0.8
Menthol	6.73	1172	4.4	8.70	1597	4.1
Terpinen-4-ol	6.77	1175	7.7	8.14	1552	7.0
α-Terpineol	7.00*	1190	44.7	9.34	1649	37.3
Methyl salicylate	7.00*	1190	[61.7]	9.92	1696	9.4
γ-Terpineol	7.10	1197	3.7	9.39	1653	2.9
2-Phenoxyethanol	7.80	1244	6997.5	14.10	2078	6561.9
Geraniol	8.13*†	1266	1004.2	11.18	1804	6.9
para-Anisaldehyde	8.13*†	1266	[1179.5]	12.62	1936	17.5
Unknown [m/z 55, 97 (66), 43 (29), 115 (20), 69 (18), 41 (18)...]	8.16†	1268	[1155.8]	13.97	2065	1033.4
(*E*)-Cinnamal	8.22	1272	10.5	12.79	1952	12.3
Thymol	8.69	1304	6.8	14.62*	2130	25.6
Carvacrol	8.80	1308	15.8	14.84	2153	7.2
Heliotropin	9.07	1328	30.3	14.62*	2130	[39.2]
Eugenol	9.45	1354	3.3	14.26	2094	14.9
Capric acid	9.94	1390	34.8	15.59	2230	33.1
Vanillin	10.02	1395	21.3	17.71	2464	40.0
Coumarin	10.44	1426	45.9	16.51	2329	44.8
Ethylvanillin	10.80	1453	13.8	17.39	2428	12.8
(*E*)-α-Isomethyl-ionone	11.11	1476	5.3	10.99	1788	5.2
Bis(2-ethylhexyl) ether?	11.41	1499	206.0			
Mefrosol	11.46	1502	61.1	15.74*	2246	63.9
α-Methyl-ionone	11.66	1517	2.9	11.75	1855	2.2
Lauric acid	12.82	1610	857.2	17.55	2447	785.5
Methyl *cis*-dihydrojasmonate	13.37	1656	95.9	15.49	2219	91.1
Hexyl salicylate	13.59	1673	2.5	14.69	2137	2.4
Methyl *trans*-dihydrojasmonate	13.67	1680	10.3	15.90	2264	8.1
(*E*)-Hexylcinnamaldehyde	14.41	1743	7.0	16.13	2288	6.9
Myristic acid	14.83	1780	88.4	19.37	2664	79.2
Isopropyl myristate	15.41	1832	10.8	13.44	2013	27.7
Galaxolide isomer I	15.55	1844	9.9	15.74*	2246	[62.6]

Galaxolide isomer II	15.57	1846	8.4	15.80	2253	9.7
Diisobutyl phthalate	15.77	1865	4.2			

*: 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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