Date : November 18, 2020

Certificate of Analysis – GC Profiling

Sample identification

Internal code : 20J23-INT01
Customer identification : Agua de Violetas - Crusellas
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 : October 31, 2020

Checked and approved by :

Alexis St-Gelais, M. Sc., chimiste 2013-174

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This report is an update of the first version issued on November 2, 2020, to correct some assignations.

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 synthetic compounds, as well as presumably some sweet orange oil terpenes. The presence of linalool and linalyl acetate does not preclude the presence of some lavender oil, but as a very secondary ingredient quantitatively-wise (if indeed present). Similarly, a small amount of terpinen-4-ol has been detected, and could originate from tea tree; there again, if the oil is indeed present, it is in very small amount. In both cases, typical sesquiterpenes of these oils (farnesene and caryophyllene for lavender, and aromadendrenes and viridiflorene for tea tree) were not observed. If they are not entirely absent, they may be obscured by the other ingredients of the product.

Analysis summary

Identification	(mg/L)	% of total volatiles	Classe
α-Thujene	0.9	0.01	Monoterpene
α-Pinene	7.0	0.04	Monoterpene
5-Ethyl-2(5H)-furanone	0.4	tr	Aliphatic lactone
Benzaldehyde	2.4	0.01	Simple phenolic
β-Pinene	0.2	tr	Monoterpene
Sabinene	0.9	0.01	Monoterpene
Unknown	0.2	tr	Unknown
Myrcene	28.8	0.18	Monoterpene
α-Phellandrene	0.3	tr	Monoterpene
Octanal	2.1	0.01	Aliphatic aldehyde
Δ3-Carene	1.8	0.01	Monoterpene
α-Terpinene	0.4	tr	Monoterpene
(2*E*)-Butenylbenzene	1.0	0.01	Simple phenolic
para-Cymene	0.3	tr	Monoterpene
Limonene	1639.3	10.06	Monoterpene
β-Phellandrene	4.2	0.03	Monoterpene
Benzyl alcohol	130.0	0.80	Simple phenolic
Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer I	28.6	0.18	Synthetic
(*Z*)-β-Ocimene	0.3	tr	Monoterpene
Dipropylene glycol II	30.9	0.19	Synthetic
(*E*)-β-Ocimene	1.1	0.01	Monoterpene
γ-Terpinene	4.2	0.03	Monoterpene
Dipropylene glycol III	31.9	0.20	Synthetic
cis-Triplal	1.3	0.01	Synthetic
Dihydromyrcenol	108.0	0.66	Monoterpenic alcohol
meta-Cymenene	0.5	tr	Monoterpene
Terpinolene	1.3	0.01	Monoterpene
para-Cymenene	0.2	tr	Monoterpene
Methyl benzoate	0.6	tr	Phenolic ester
Linalool	155.3	0.95	Monoterpenic alcohol
trans-Triplal	0.7	tr	Synthetic
Nonanal	0.9	0.01	Aliphatic aldehyde
Phenylethyl alcohol	186.7	1.15	Simple phenolic

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Camphor	0.8	tr	Monoterpenic ketone
Unknown	0.3	tr	Unknown
Benzyl acetate	2433.3	14.93	Phenolic ester
Terpinen-4-ol	0.5	tr	Monoterpenic alcohol
α-Terpineol	3.5	0.02	Monoterpenic alcohol
Methylchavicol	0.1	tr	Phenylpropanoid
cis-Patchone	0.7	tr	Synthetic
cis-Florol	18.6	0.11	Synthetic
Decanal	2.3	0.01	Aliphatic aldehyde
trans-Patchone	10.8	0.07	Synthetic
4-tert-Butylcyclohexanone	3.5	0.02	Synthetic
trans-Florol	66.1	0.41	Synthetic
Nerol	127.4	0.78	Monoterpenic alcohol
Citronellol	26.5	0.16	Monoterpenic alcohol
Neral	3.9	0.02	Monoterpenic aldehyde
Carvone	3.5	0.02	Monoterpenic ketone
para-Anisaldehyde	180.8	1.11	Simple phenolic
Linalyl acetate	9.8	0.06	Monoterpenic ester
Geraniol	1037.0	6.36	Monoterpenic alcohol
Geranial	8.3	0.05	Monoterpenic aldehyde
cis-β-Terpinyl acetate	5.8	0.04	Monoterpenic ester
Dicyclopentenyl alcohol?	3.1	0.02	Synthetic
Bornyl acetate	5.6	0.03	Monoterpenic ester
Unknown	1.5	0.01	Unknown
Terpinen-4-yl acetate	0.7	tr	Monoterpenic ester
Hydroxycitronellal	11.7	0.07	Synthetic
Methyl 2-nonynoate	19.4	0.12	Synthetic
α,α-Dimethylphenethyl acetate	490.4	3.01	Synthetic
Unknown	3.6	0.02	Unknown
cis-Woody acetate	632.8	3.88	Synthetic
α-Terpinyl acetate	176.5	1.08	Monoterpenic ester
Limonene *trans*-glycol	17.3	0.11	Monoterpenic alcohol
trans-Woody acetate	1562.1	9.59	Synthetic
Geranyl acetate	2.1	0.01	Monoterpenic ester
Unknown	23.7	0.15	Synthetic
Verdyl acetate, isomer I	700.3	4.30	Synthetic
Verdyl acetate, isomer II	163.8	1.01	Synthetic
(*E*)-α-Ionone	30.2	0.19	Ionone or analog
meta-Floralozone	23.4	0.14	Synthetic
Coumarin	15.7	0.10	Coumarin
para-Floralozone	12.5	0.08	Synthetic
Unknown	24.3	0.15	Synthetic
Unknown	14.4	0.09	Synthetic
Cyclamen aldehyde	19.0	0.12	Synthetic
Jasmal isomer I	4.9	0.03	Synthetic
(*E*)-α-Isomethyl-ionone	1342.9	8.24	Ionone or analog
Unknown	18.5	0.11	Unknown
β-Isomethylionone	101.5	0.62	Synthetic
Unknown	13.2	0.08	Unknown
α-Methyl-ionone	466.2	2.86	Ionone or analog
Unknown	20.8	0.13	Unknown
Isoamyl salicylate	241.8	1.48	Phenolic ester

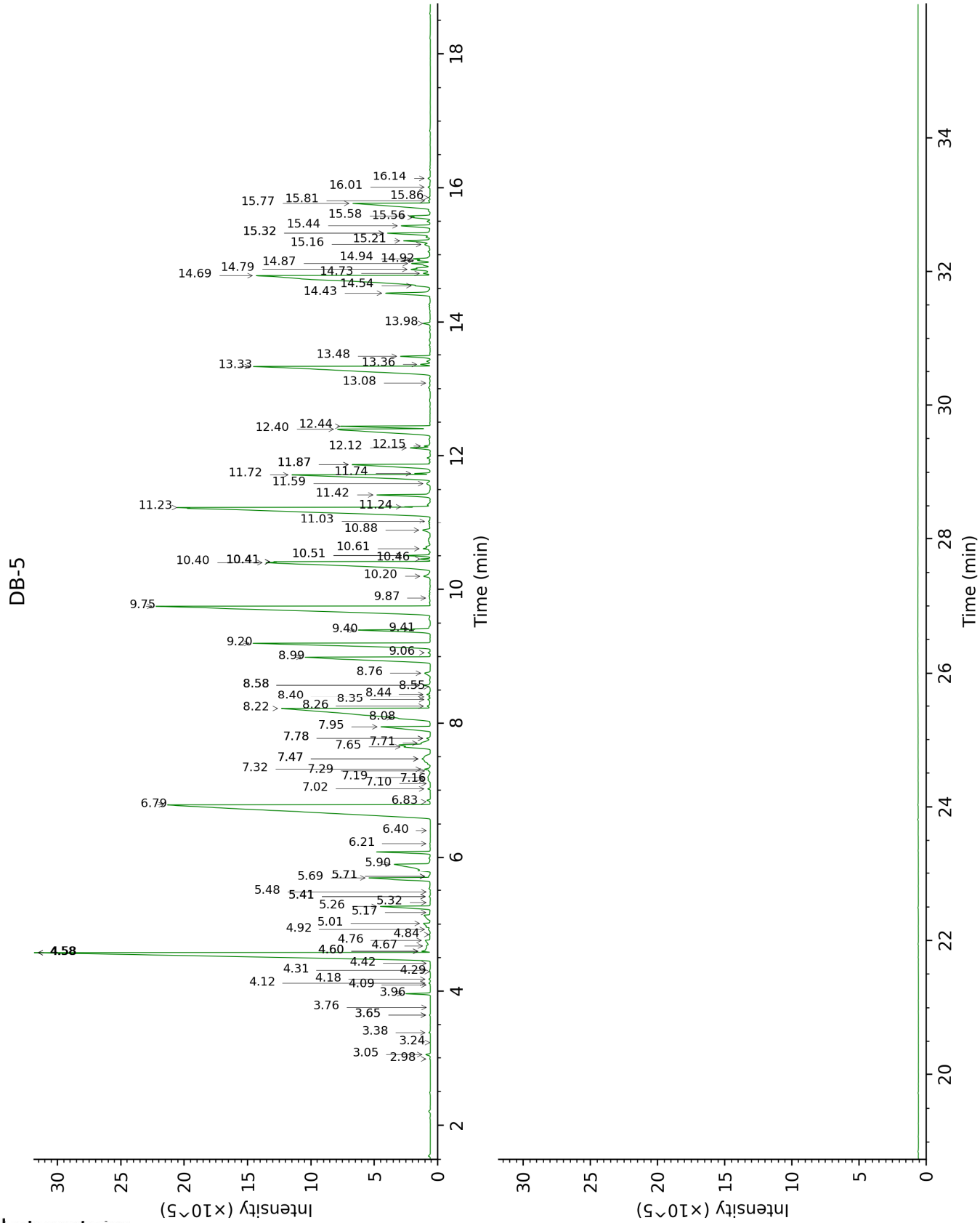
2-methylbutyl salicylate	7.4	0.05	Synthetic
Rose acetate	71.7	0.44	Synthetic
Helional	10.5	0.06	Synthetic
Amyl salicylate	453.2	2.78	Phenolic ester
β-Methyl-ionone	163.3	1.00	Ionone or analog
Galaxolide impurity I	1.3	0.01	Synthetic
(*Z*)-α-Amyl cinnamaldehyde	807.9	4.96	Aliphatic aldehyde
Iso *E* Super isomer I	14.4	0.09	Synthetic
(*E*)-α-Amyl cinnamaldehyde	47.8	0.29	Aliphatic aldehyde
Unknown	15.1	0.09	Unknown
(*E*)-Hexylcinnamaldehyde	101.6	0.62	Synthetic
Cedryl acetate	23.1	0.14	Sesquiterpenic ester
Benzyl benzoate	1077.9	6.62	Phenolic ester
Isobornyl cyclohexanol isomer 4	12.9	0.08	Synthetic
Isobornyl cyclohexanol isomer 5	38.3	0.24	Synthetic
Isobornyl cyclohexanol isomer 6	30.2	0.18	Synthetic
Isobornyl cyclohexanol isomer 7	20.8	0.13	Synthetic
Isobornyl cyclohexanol isomer 8	24.5	0.15	Synthetic
Isobornyl cyclohexanol isomer 10	14.0	0.09	Synthetic
Isobornyl cyclohexanol isomer 1	50.7	0.31	Synthetic
Isobornyl cyclohexanol isomer 3	86.2	0.53	Synthetic
Isobornyl cyclohexanol isomer 2	[86.2]	[0.53]	Synthetic
Isopropyl myristate	61.0	0.37	Synthetic
Galaxolide isomer I	29.2	0.18	Synthetic
Galaxolide isomer II	29.0	0.18	Synthetic
Benzyl salicylate	303.8	1.86	Phenolic ester
Galaxolide isomer III	3.3	0.02	Synthetic
Galaxolide isomer IV	2.6	0.02	Synthetic
Galaxolide isomer V	4.2	0.03	Synthetic
Galaxolide isomer VI	3.9	0.02	Synthetic
Dipropylene glycol IV, stereoisomer II	24.0	0.15	Synthetic
Consolidated total	**16013.41 mg/L**	**98.28%**	

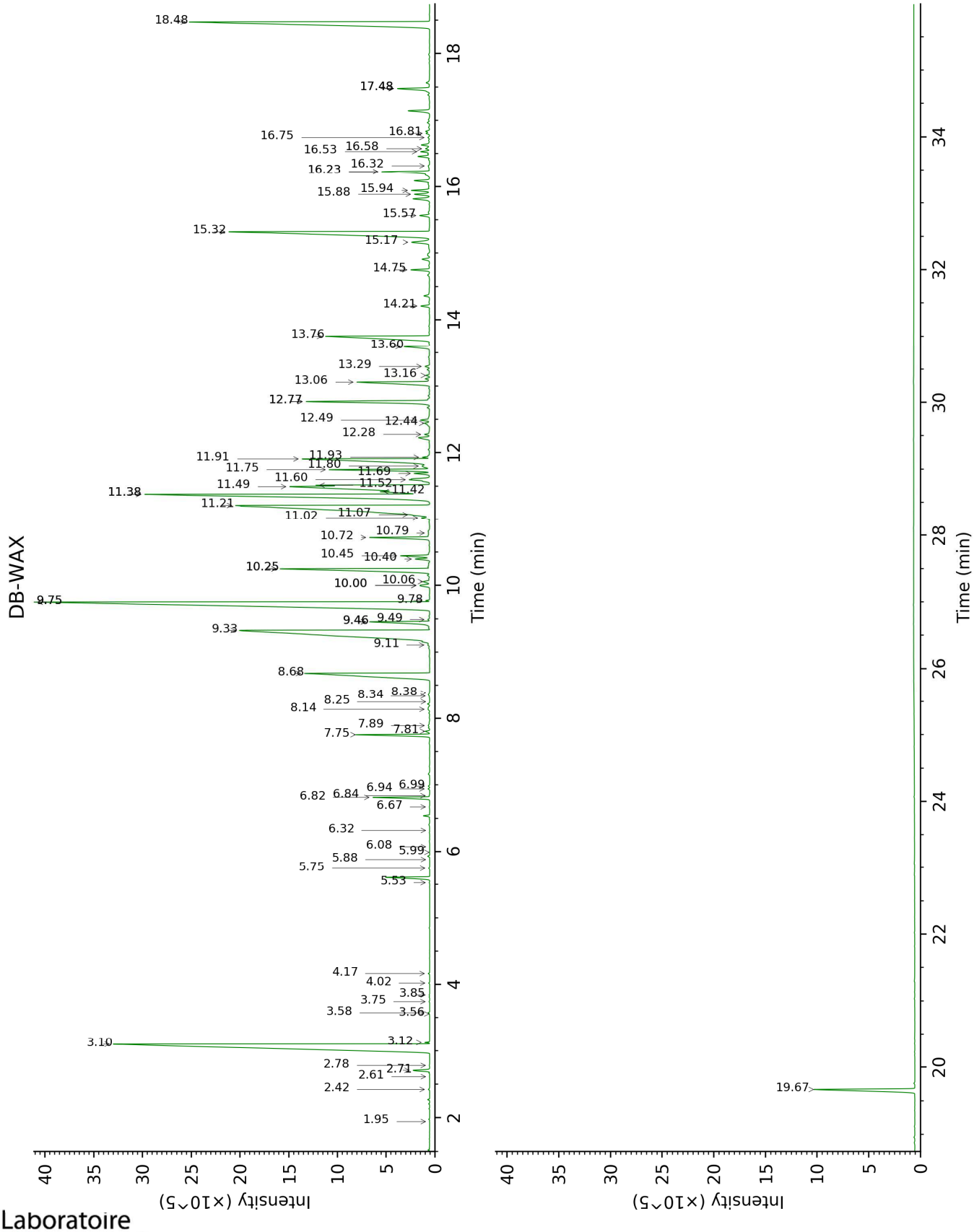
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: < 0.05 mg/L

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
Time (min)
Intensity (×10^5)
Time (min)
Intensity (×10^5)


DB-WAX
Time (min)
Intensity (×10^5)
18.48
17.48
16.75
16.81
16.53
16.58
16.23
16.32
15.88
15.94
15.57
15.32
15.17
14.75
14.21
13.76
13.60
13.29
13.16
13.06
12.77
12.49
12.44
12.28
11.91
11.93
11.75
11.80
11.69
11.60
11.49
11.52
11.42
11.38
11.21
11.02
11.07
10.72
10.79
10.45
10.40
10.25
10.00
10.06
9.75
9.78
9.46
9.49
9.33
9.11
8.68
8.34
8.38
8.25
8.14
7.89
7.81
7.75
6.94
6.99
6.82
6.84
6.67
6.32
6.08
5.99
5.88
5.75
5.53
4.17
4.02
3.85
3.75
3.58
3.56
3.10
3.12
2.78
2.71
2.61
2.42
1.95
19.67

FULL ANALYSIS DATA

Identification	Column DB-5			Column DB-WAX		
	R.T	R.I	mg/L	R.T	R.I	mg/L
α-Thujene	2.98	929	0.9			
α-Pinene	3.05	933	7.0			
5-Ethyl-2(5H)-furanone	3.24	946	0.4			
Benzaldehyde	3.38	956	2.4	6.98	1459	2.5
β-Pinene	3.65*	973	1.0	1.95	1071	0.2
Sabinene	3.65*	973	[1.0]			
Unknown [m/z 111, 93 (44), 91 (29), 83 (28), 77 (20), 108 (17)...]	3.76	981	0.2	6.32	1409	0.7
Myrcene	3.96	995	28.8	2.71	1140	30.0
α-Phellandrene	4.10	1003	0.3	2.61	1132	0.3
Octanal	4.12	1005	2.1	4.17	1254	2.1
Δ3-Carene	4.18	1009	1.8	2.42	1117	1.5
α-Terpinene	4.29	1016	0.4	2.78	1146	0.7
(2*E*)-Butenylbenzene	4.31	1017	1.0			
para-Cymene	4.42	1024	0.3	3.84	1230	0.6
Limonene	4.58*	1034	1640.1	3.10	1172	1639.3
β-Phellandrene	4.58*	1034	[1640.1]	3.12	1174	4.2
Benzyl alcohol	4.60*†	1035	37.7	11.42	1819	130.0
Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer I	4.60*†	1035	[61.0]	11.02	1784	28.6
(*Z*)-β-Ocimene	4.68†	1040	[33.5]	3.56	1209	0.3
Dipropylene glycol II	4.76	1045	30.9	11.60	1835	45.1
(*E*)-β-Ocimene	4.84	1051	1.1	3.74	1223	0.8
γ-Terpinene	4.92	1056	4.2	3.58	1210	2.1
Dipropylene glycol III	5.01	1061	31.9	11.69	1844	46.2
cis-Triplal	5.17	1072	1.3	5.99	1384	0.3
Dihydromyrcenol	5.26	1077	108.0	6.82	1446	102.7
meta-Cymenene	5.32	1081	0.5	5.88	1376	0.3
Terpinolene	5.41*	1086	1.5	4.02	1244	1.3
para-Cymenene	5.41*	1086	[1.4]	6.08	1390	0.2
Methyl benzoate	5.48	1091	0.6	8.34	1563	1.4
Linalool	5.69	1104	155.3	7.76	1517	141.4
trans-Triplal	5.71*	1106	3.6	6.67	1435	0.7
Nonanal	5.71*	1106	[3.5]	5.53	1351	0.9
Phenylethyl alcohol	5.90	1118	186.7	11.75	1849	196.4
Camphor	6.21	1138	0.8	6.84	1448	1.1
Unknown [m/z 167, 43 (8), 81 (86), 71 (83), 139 (72), 93 (70)...]	6.40	1150	0.3			
Benzyl acetate	6.79	1175	2433.3	9.75*	1677	2408.1
Terpinen-4-ol	6.83	1178	0.5	8.25	1556	0.3
α-Terpineol	7.02	1191	3.5	9.49	1655	3.4
Methylchavicol	7.10	1196	0.1			

cis-Patchone	7.16†	1199	17.0	9.46*	1653	144.7
cis-Florol	7.19†	1202	[19.4]	10.00*	1697	31.0
Decanal	7.29	1208	2.3	6.94	1455	2.6
trans-Patchone	7.32	1210	10.8	10.00*	1697	[27.1]
4-tert-Butylcyclohexanone	7.47*†	1220	62.4			
trans-Florol	7.47*†	1220	[70.0]	10.45	1735	66.1
Nerol	7.65	1232	127.4	10.72	1759	122.0
Citronellol	7.70	1236	26.5	10.40	1731	28.4
Neral	7.78*	1241	7.2	9.11	1624	3.9
Carvone	7.78*	1241	[7.4]	9.75*	1677	[2229.4]
para-Anisaldehyde	7.95	1253	180.8	12.77*	1942	379.7
Linalyl acetate	8.08†	1262	1201.1	7.81	1521	9.8
Geraniol	8.22†	1271	[1090.0]	11.38*	1816	1141.9
Geranial	8.26	1274	8.3	9.78	1679	5.3
cis-β-Terpinyl acetate	8.35	1280	5.8	8.14	1547	4.8
Dicyclopentenyl alcohol?	8.40	1283	3.1			
Bornyl acetate	8.44	1286	5.6	7.89	1528	4.6
Unknown [m/z 103, 69 (85), 41 (37), 75 (31), 47 (28), 157 (24)...]	8.55	1294	1.5	5.75	1366	1.9
Terpinen-4-yl acetate	8.58*	1296	13.6	8.38	1566	0.7
Hydroxycitronellal	8.58*	1296	[13.8]	12.28	1896	11.7
Methyl 2-nonynoate	8.76	1305	19.4	10.06	1702	19.7
α,α-Dimethylphenethyl acetate	8.99	1321	490.4	10.25*	1718	484.2
Unknown [m/z 85, 111 (32), 55 (29), 69 (27), 56 (25)... 212? (3)]	9.06	1326	3.6			
cis-Woody acetate	9.20	1336	632.8	8.68	1590	620.1
α-Terpinyl acetate	9.40	1350	176.5	9.46*	1653	[162.7]
Limonene *trans*-glycol	9.41	1351	17.3	15.57	2216	23.9
trans-Woody acetate	9.75	1375	1562.1	9.33	1642	1535.2
Geranyl acetate	9.87	1384	2.1	10.25*	1718	[514.3]
Unknown [m/z 117, 66 (77), 132 (57), 43 (51), 67 (37), 91 (32)... 192 (6)]	10.20	1407	23.7			
Verdyl acetate, isomer I	10.40†	1422	970.3	11.49	1826	700.3
Verdyl acetate, isomer II	10.41*†	1423	[970.3]	11.52	1828	163.8
(*E*)-α-Ionone	10.41*†	1423	[831.0]	11.07	1788	30.2
meta-Floralozone	10.41*†	1423	[773.7]	11.80	1853	23.4
Coumarin	10.46	1426	15.7	16.74	2341	4.3
para-Floralozone	10.51*	1430	31.7	11.93	1865	12.5
Unknown [m/z 82, 124 (49), 66 (47), 43	10.51*	1430	[40.0]			

(43), 83 (42), 67 (24)... 192 (7)]						
Unknown [m/z 132, 117 (84), 43 (79), 150 (57), 91 (53), 79 (45)... 192 (2)]	10.61	1438	14.4			
Cyclamen aldehyde	10.88	1458	19.0	12.49	1916	19.3
Jasmal isomer I	11.03	1469	4.9			
(*E*)-α-Isomethyl-ionone	11.23	1484	1342.9	11.21	1801	1257.6
Unknown [m/z 135, 43 (80), 163 (79), 123 (78), 177 (65), 107 (57)...]	11.24	1485	18.5			
β-Isomethylionone	11.42	1498	101.5	11.38*	1816	[1104.2]
Unknown [m/z 57, 149 (36), 93 (30), 107 (24), 135 (22), 191 (21), 109 (18), 91 (18)... 206? (4)]	11.59	1511	13.2			
α-Methyl-ionone	11.72	1522	466.2	11.91	1863	459.5
Unknown [m/z 57, 107 (15), 134 (15), 106 (14), 93 (13)... 206 (3)]	11.74	1523	20.8			
Isoamyl salicylate	11.87*	1534	268.5	13.06	1969	241.8
2-methylbutyl salicylate	11.87*	1534	[268.5]	13.16	1978	7.4
Rose acetate	12.12	1553	71.7	14.75	2133	70.8
Helional	12.15	1555	10.5			
Amyl salicylate	12.40	1575	453.2	13.76	2035	440.4
β-Methyl-ionone	12.44	1579	163.3	12.77*	1942	[312.5]
Galaxolide impurity I	13.08	1631	1.3	10.79	1764	2.6
(*Z*)-α-Amyl cinnamaldehyde	13.33	1651	807.9	15.32	2190	787.5
Iso *E* Super isomer I	13.36	1654	14.4	13.30	1991	9.2
(*E*)-α-Amyl cinnamaldehyde	13.48	1664	47.8	15.17	2175	49.9
Unknown [m/z 103, 75 (44), 133 (42), 47 (26), 218 (23), 91 (18), 105 (15)... 248 (3)]	13.98	1705	15.1			
(*E*)-Hexylcinnamaldehyde	14.43	1744	101.6	16.23*	2285	99.5
Cedryl acetate	14.54	1754	23.1	14.21	2079	18.2
Benzyl benzoate	14.69	1767	1077.9	18.48	2535	1005.5
Isobornyl cyclohexanol isomer 4	14.73	1770	12.9			
Isobornyl cyclohexanol isomer 5	14.79	1775	38.3			
Isobornyl cyclohexanol isomer 6	14.87	1783	30.2			

Isobornyl cyclohexanol isomer 7	14.92	1787	20.8	16.53	2318	16.3
Isobornyl cyclohexanol isomer 8	14.94	1789	24.5			
Isobornyl cyclohexanol isomer 10	15.16	1808	14.0			
Isobornyl cyclohexanol isomer 1	15.21	1813	50.7			
Isobornyl cyclohexanol isomer 3	15.32*	1823	86.2	17.48*	2422	71.1
Isobornyl cyclohexanol isomer 2	15.32*	1823	[86.2]	17.48*	2422	[71.1]
Isopropyl myristate	15.44	1833	61.0	13.60	2019	58.9
Galaxolide isomer I	15.56	1844	29.2	15.88	2249	30.7
Galaxolide isomer II	15.58	1846	29.0	15.94	2255	33.0
Benzyl salicylate	15.77	1863	303.8	19.67	2677	287.7
Galaxolide isomer III	15.81	1867	3.3	16.23*	2285	[97.6]
Galaxolide isomer IV	15.86	1871	2.6	16.32	2295	2.5
Galaxolide isomer V	16.01	1885	4.2	16.58	2323	9.2
Galaxolide isomer VI	16.14	1897	3.9	16.81	2348	6.5
Dipropylene glycol IV, stereoisomer II				12.44	1911	24.0

*: 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