**Date :** November 18, 2020

# *Certificate of Analysis – GC Profiling*

## *Sample identification*

**Internal code :** 20J22-INT01
**Customer identification :** P.M.B. - Para mi bebé - Agua de Violetas - Violets Cologne
**Type :** Aqueous fragrance
**Source :** Fragrant 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

*Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia.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 first version issued on October 31, 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 ionone derivatives and benzyl acetate with dipropylene glycol, alongside a few other fragrant isolates. Some minor compounds may remain unidentified (in part obscured by the large dipropylene glycol peaks), but no indication whatsoever of the presence of essential oils, and in particular lavender (no linalool, linalyl acetate, lavandulol, lavandulyl acetate, beta-farnesene or caryophyllene) and tea tree (no terpinene-4-ol, no terpinenes, no viridiflorene, no aromadendrene) were found.

## *Analysis summary*

| Identification | (mg/L) | % of total volatiles | Classe |
|---|---|---|---|
| α-Pinene | 1.1 | 0.02 | Monoterpene |
| 2-Cyclohexenone | [1.6] | [0.02] | Aliphatic ketone |
| β-Pinene | 0.1 | tr | Monoterpene |
| Sabinene | 0.3 | tr | Monoterpene |
| Myrcene | 0.6 | 0.01 | Monoterpene |
| Carbitol | 26.9 | 0.36 | Synthetic |
| Butyl lactate | 2.7 | 0.04 | Aliphatic ester |
| Limonene | 5.8 | 0.08 | Monoterpene |
| Benzyl alcohol | 14.0 | 0.19 | Simple phenolic |
| Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer II | 2001.9 | 27.10 | Synthetic |
| Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer I | [2001.9] | [27.10] | Synthetic |
| Dipropylene glycol II | 1146.8 | 15.52 | Synthetic |
| Dipropylene glycol III | 1340.8 | 18.15 | Synthetic |
| Dipropylene glycol IV, stereoisomer II | 374.2 | 5.06 | Synthetic |
| Citronellal | 0.3 | tr | Monoterpenic aldehyde |
| Benzyl acetate | 508.6 | 6.88 | Phenolic ester |
| Methyl salicylate | 0.2 | tr | Phenolic ester |
| *cis*-Florol | 0.1 | tr | Synthetic |
| Dihydrocitronellol | 0.3 | tr | Synthetic |
| Methyl 2-octynoate | 81.4 | 1.10 | Synthetic |
| *trans*-Piperitol | 0.3 | tr | Monoterpenic alcohol |
| *trans*-Florol | 0.5 | 0.01 | Synthetic |
| Methyl nonanoate | 0.7 | 0.01 | Aliphatic ester |
| Nerol | 0.1 | tr | Monoterpenic alcohol |
| Citronellol | 129.8 | 1.76 | Monoterpenic alcohol |
| (*E*)-Isogeraniol? | 0.6 | 0.01 | Monoterpenic alcohol |
| Benzyl propionate | 0.2 | tr | Phenolic ester |
| Geraniol | 0.2 | tr | Monoterpenic alcohol |
| Octanal diethyl acetal? | 0.2 | tr | Aliphatic acetal |
| Ethyl 2-octynoate | 2.2 | 0.03 | Synthetic |
| 2-Undecanone | 0.1 | tr | Aliphatic ketone |
| α,α-Dimethylphenethyl acetate | 29.1 | 0.39 | Synthetic |
| Heliotropin | 33.4 | 0.45 | Simple phenolic |
| Tripropylene glycol isomer | 4.3 | 0.06 | Synthetic |
| Tripropylene glycol isomer II | 2.2 | 0.03 | Synthetic |

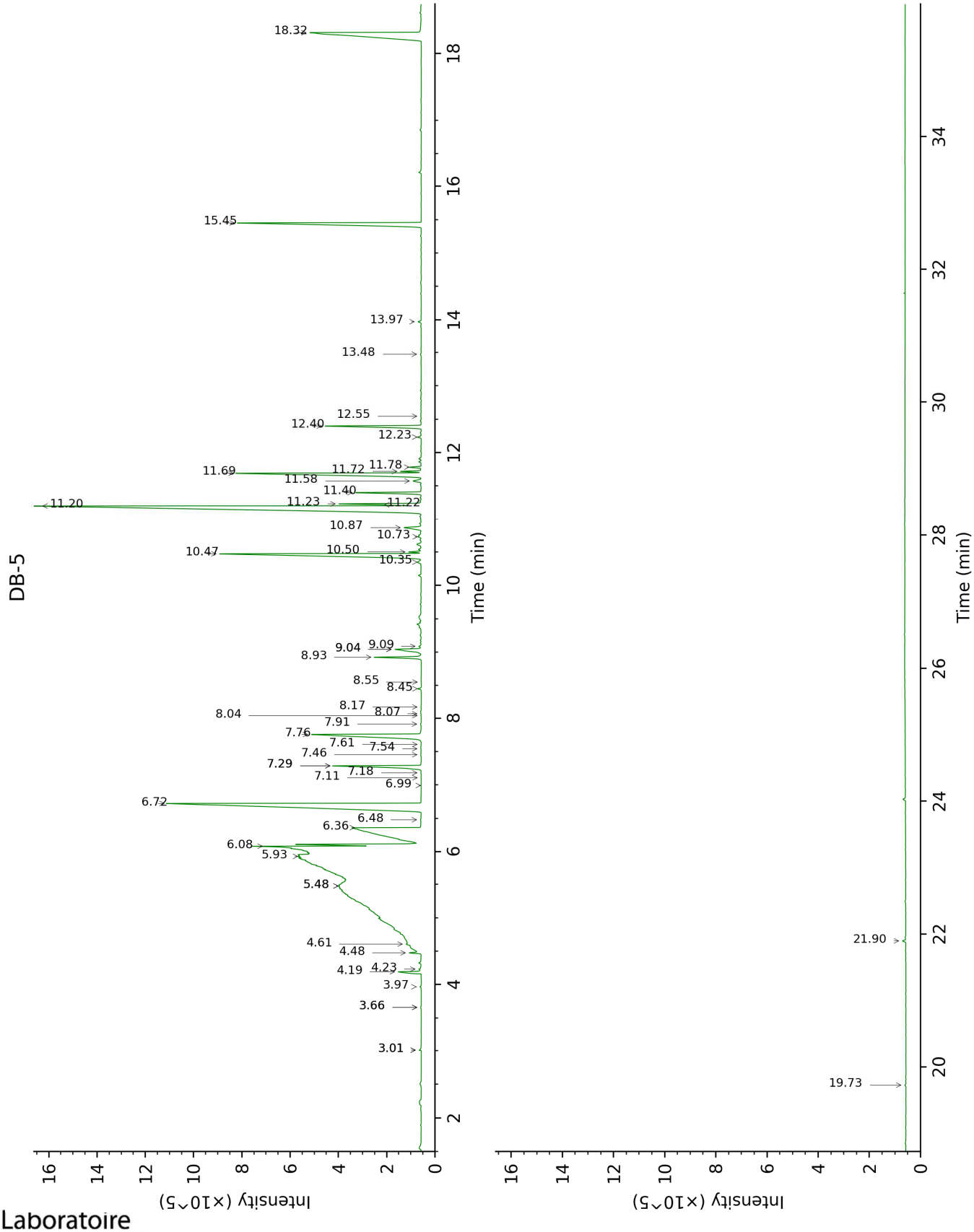
| | | | |
|---|---|---|---|
| Unknown | 4.1 | 0.06 | Unknown |
| (*E*)-α-Ionone | 214.5 | 2.90 | Ionone or analog |
| Unknown | 6.8 | 0.09 | Unknown |
| Unknown | 2.2 | 0.03 | Unknown |
| Cyclamen aldehyde | 13.9 | 0.19 | Synthetic |
| (*E*)-α-Isomethyl-ionone | 564.9 | 7.65 | Ionone or analog |
| Unknown | 10.2 | 0.14 | Unknown |
| (*E*)-β-Ionone | 36.1 | 0.49 | Ionone or analog |
| β-Isomethylionone | 35.2 | 0.48 | Synthetic |
| Unknown | 7.8 | 0.11 | Unknown |
| α-Methyl-ionone | 173.4 | 2.35 | Ionone or analog |
| Unknown | 11.1 | 0.15 | Unknown |
| γ-Methyl-ionone? | 5.9 | 0.08 | Ionone or analog |
| Unknown | 2.6 | 0.04 | Unknown |
| β-Methyl-ionone | 62.7 | 0.85 | Ionone or analog |
| Diethyl phthalate | 0.4 | 0.01 | Synthetic |
| Triethyl citrate | 1.3 | 0.02 | Synthetic |
| Unknown | 2.2 | 0.03 | Unknown |
| Isopropyl myristate | 171.8 | 2.33 | Synthetic |
| 2,4-Dihydroxybenzophenone | 228.3 | 3.09 | Simple phenolic |
| Octyl 4-(dimethylamino)benzoate? | 0.7 | 0.01 | Synthetic |
| Unknown | 2.6 | 0.04 | Unknown |
| **Consolidated total** | **7269.04 mg/L** | **98.39%** | |

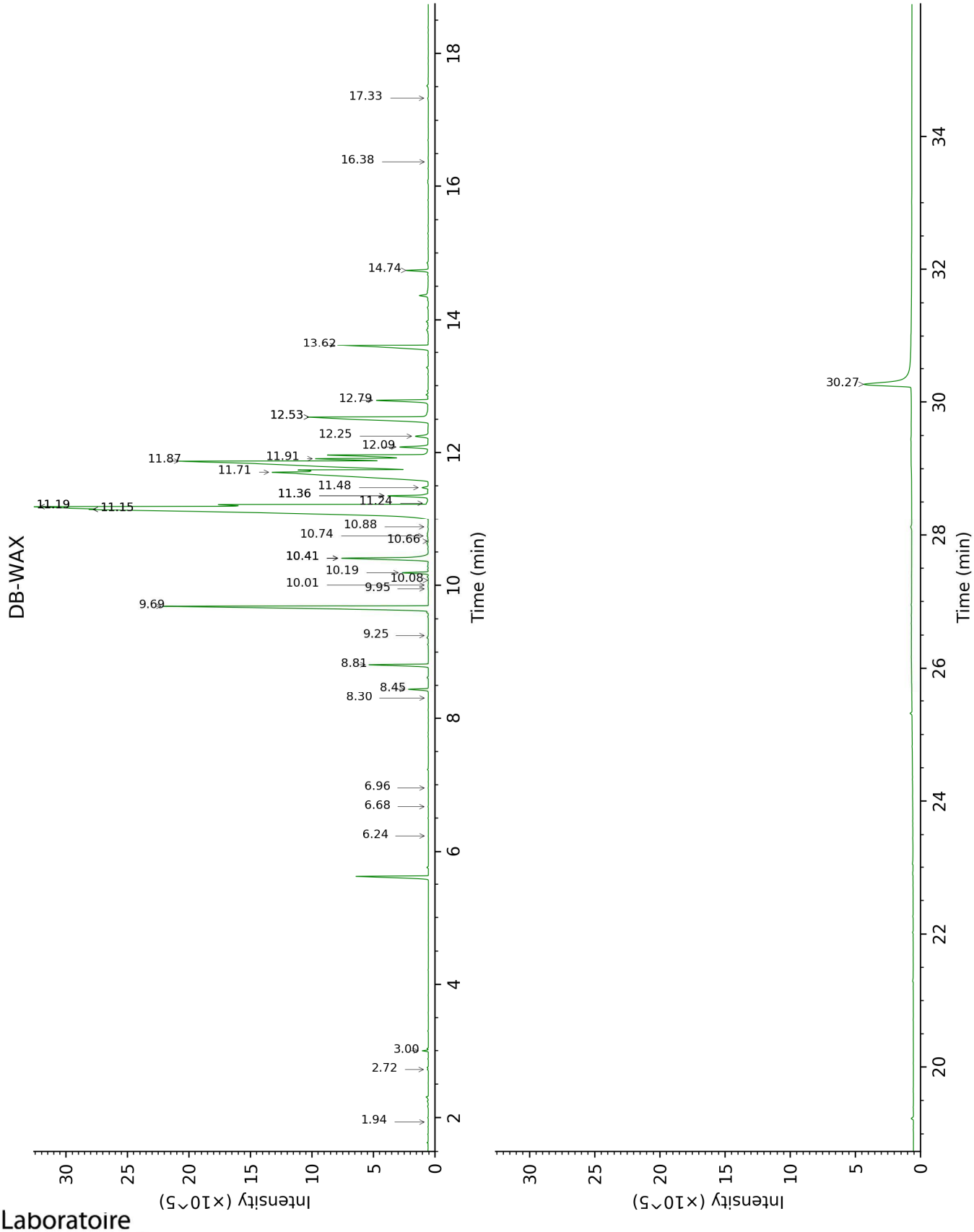
*: Individual compounds concentration could not be found due to overlapping coelutions on columns considered
[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total
tr: < 0.05 mg/L

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
18.32
15.45
13.97
13.48
12.55
12.40
12.23
11.69
11.72
11.78
11.58
11.40
11.20
11.23
11.22
10.87
10.73
10.47
10.50
10.35
9.09
9.04
8.93
8.55
8.45
8.17
8.07
8.04
7.91
7.76
7.61
7.54
7.46
7.29
7.18
7.11
6.99
6.72
6.48
6.36
6.08
5.93
5.48
4.61
4.48
4.23
4.19
3.97
3.66
3.01
21.90
19.73
Time (min)
Intensity (×10^5)


DB-WAX
17.33
16.38
14.74
13.62
12.79
12.53
12.25
12.09
11.91
11.87
11.71
11.48
11.36
11.24
11.19
11.15
10.88
10.74
10.66
10.41
10.19
10.08
10.01
9.95
9.69
9.25
8.81
8.45
8.30
6.96
6.68
6.24
3.00
2.72
1.94
30.27
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 |
| α-Pinene | 3.01* | 930 | 1.1 | | | |
| 2-Cyclohexenone | 3.01* | 930 | [1.6] | | | |
| β-Pinene | 3.66* | 974 | 0.4 | 1.94 | 1070 | 0.1 |
| Sabinene | 3.66* | 974 | [0.4] | | | |
| Myrcene | 3.97 | 995 | 0.6 | 2.72 | 1141 | 0.7 |
| Carbitol | 4.19 | 1010 | 26.9 | 8.45 | 1571 | 31.2 |
| Butyl lactate | 4.23 | 1012 | 2.7 | | | |
| Limonene | 4.48 | 1027 | 5.8 | 3.00 | 1163 | 4.0 |
| Benzyl alcohol | 4.61† | 1036 | 2785.5 | 11.36* | 1814 | 50.0 |
| Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer II | 5.48*† | 1091 | [4512.1] | 11.19*† | 1799 | [3127.7] |
| Dipropylene glycol I (1,1'-oxybis-2-propanol), stereoisomer I | 5.48*† | 1091 | [4512.1] | 11.19*† | 1799 | [3127.7] |
| Dipropylene glycol II | 5.93† | 1120 | [4512.1] | 11.71 | 1845 | 1146.8 |
| Dipropylene glycol III | 6.08† | 1130 | [4512.1] | 11.87 | 1860 | 1340.8 |
| Dipropylene glycol IV, stereoisomer II | 6.36 | 1148 | 374.2 | 12.53* | 1920 | 433.3 |
| Citronellal | 6.48 | 1155 | 0.3 | 6.68 | 1435 | 0.4 |
| Benzyl acetate | 6.72 | 1171 | 508.6 | 9.69 | 1672 | 518.9 |
| Methyl salicylate | 6.99 | 1189 | 0.2 | 10.08 | 1704 | 0.3 |
| *cis*-Florol | 7.11 | 1196 | 0.1 | 9.95 | 1693 | 0.2 |
| Dihydrocitronellol | 7.18 | 1201 | 0.3 | 9.25 | 1636 | 0.2 |
| Methyl 2-octynoate | 7.29* | 1208 | 81.7 | 8.81 | 1600 | 81.4 |
| *trans*-Piperitol | 7.29* | 1208 | [66.8] | 10.01 | 1698 | 0.3 |
| *trans*-Florol | 7.46 | 1219 | 0.5 | 10.41* | 1732 | 152.5 |
| Methyl nonanoate | 7.54 | 1225 | 0.7 | 6.96 | 1456 | 0.4 |
| Nerol | 7.61 | 1230 | 0.1 | 10.66 | 1754 | 0.2 |
| Citronellol | 7.76 | 1240 | 129.8 | 10.41* | 1732 | [133.4] |
| (*E*)-Isogeraniol? | 7.91 | 1250 | 0.6 | 10.88 | 1772 | 0.5 |
| Benzyl propionate | 8.04 | 1259 | 0.2 | 10.41* | 1732 | [148.3] |
| Geraniol | 8.07 | 1261 | 0.2 | 11.24 | 1804 | 3.0 |
| Octanal diethyl acetal? | 8.17 | 1268 | 0.2 | 6.24 | 1402 | 0.2 |
| Ethyl 2-octynoate | 8.45 | 1287 | 2.2 | | | |
| 2-Undecanone | 8.55 | 1294 | 0.1 | 8.30 | 1560 | 0.1 |
| α,α-Dimethylphenethyl acetate | 8.93 | 1317 | 29.1 | 10.19 | 1713 | 26.6 |
| Heliotropin | 9.04* | 1325 | 37.6 | 14.74 | 2132 | 33.4 |
| Tripropylene glycol isomer | 9.04* | 1325 | [38.8] | | | |
| Tripropylene glycol isomer II | 9.09 | 1328 | 2.2 | | | |
| Unknown [m/z 43, 93 (45), 149 (43), 91 (38), 107 (33), 135 (32)...] | 10.35 | 1418 | 4.1 | | | |
| (*E*)-α-Ionone | 10.48 | 1428 | 214.5 | 11.15*† | 1795 | 1916.0 |

| | | | | | | |
|---|---|---|---|---|---|---|
| Unknown [m/z 43, 82 (20), 107 (20), 93 (20), 81 (19), 106 (17)...] | 10.50 | 1430 | 6.8 | 11.48 | 1824 | 7.9 |
| Unknown [m/z 95, 43 (53), 69 (48), 107 (41), 93 (30)...] | 10.73 | 1447 | 2.2 | 10.74 | 1760 | 1.8 |
| Cyclamen aldehyde | 10.87 | 1457 | 13.9 | 12.53* | 1920 | [247.1] |
| (*E*)-α-Isomethyl-ionone | 11.20 | 1482 | 564.9 | 11.15*† | 1795 | [1888.4] |
| Unknown [m/z 135, 43 (80), 163 (79), 123 (78), 177 (65), 107 (57)...] | 11.22 | 1483 | 10.2 | | | |
| (*E*)-β-Ionone | 11.23 | 1484 | 36.1 | 12.09 | 1879 | 36.1 |
| β-Isomethylionone | 11.40 | 1497 | 35.2 | 11.36* | 1814 | [48.9] |
| Unknown [m/z 57, 149 (36), 93 (30), 107 (24), 135 (22), 191 (21), 109 (18), 91 (18)... 206? (4)] | 11.58 | 1510 | 7.8 | | | |
| α-Methyl-ionone | 11.69 | 1520 | 173.4 | 11.91 | 1863 | 162.4 |
| Unknown [m/z 57, 107 (15), 134 (15), 106 (14), 93 (13)... 206 (3)] | 11.72 | 1522 | 11.1 | | | |
| γ-Methyl-ionone? | 11.78 | 1527 | 5.9 | 12.25 | 1893 | 18.2 |
| Unknown [m/z 109, 67 (49), 108 (43), 107 (36), 43 (30), 98 (26), 93 (24), 123 (19)... 206 (9)] | 12.23 | 1562 | 2.6 | | | |
| β-Methyl-ionone | 12.40 | 1575 | 62.7 | 12.78 | 1943 | 64.7 |
| Diethyl phthalate | 12.55 | 1587 | 0.4 | 16.38 | 2301 | 0.1 |
| Triethyl citrate | 13.48 | 1663 | 1.3 | 17.33 | 2405 | 1.6 |
| Unknown [m/z 103, 75 (44), 133 (42), 47 (26), 218 (23), 91 (18), 105 (15)... 248 (3)] | 13.97 | 1704 | 2.2 | | | |
| Isopropyl myristate | 15.45 | 1834 | 171.8 | 13.62 | 2022 | 174.2 |
| 2,4-Dihydroxybenzophenone | 18.32 | 2109 | 228.3 | 30.27 | 3981 | 184.7 |
| Octyl 4-(dimethylamino)benzoate? | 19.73 | 2258 | 0.7 | | | |
| Unknown [m/z 176, 177 (14), 233 (7), 105 (3), 91 (3), 148 (2)...] | 21.90 | 2503 | 2.6 | | | |

*: 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