

Date : 2024-01-22

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 24A15-PTH10

**Customer Identification :** Organic Egyptian Geranium - Egypt - GI0110R

**Type :** Essential Oil

**Source :** *Pelargonium graveolens* ct. *Egyptian*

**Customer :** Plant Therapy

Checked and approved by:

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Alexis St-Gelais, Ph. D., Chimiste 2013-174

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## GAS CHROMATOGRAPHIC ANALYSIS

**Method :** PC-MAT-014 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID

**✖ISO**

**Results :** See analysis summary (next page)

**Analyst :** Sylvain Mercier, M. Sc., Chimiste 2014-005

**Date :** 2024-01-18

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.4674 \pm 0.0003$  (20 °C)

**Method :** PC-MAT-016 - Measure of the refractive index of a liquid.

**Analyst :** Cindy Caron B. Sc.

**Date :** 2024-01-16

## CONCLUSION

No adulterant, contaminant or diluent has been detected using this method.

**ANALYSIS SUMMARY - CONSOLIDATED CONTENTS**

New readers of similar reports are encouraged to read table footnotes at least once.

| Identification                        | %    | Class              |
|---------------------------------------|------|--------------------|
| Isobutyral                            | tr   | Aliphatic aldehyde |
| Acetic acid                           | tr   | Aliphatic acid     |
| 2-Methyl-3-buten-2-ol                 | 0.01 | Aliphatic alcohol  |
| Isovaleral                            | tr   | Aliphatic aldehyde |
| 2-Methylbutyral                       | tr   | Aliphatic aldehyde |
| Isoamyl alcohol                       | 0.01 | Aliphatic alcohol  |
| Toluene                               | tr   | Simple phenolic    |
| Isobutyric acid                       | tr   | Aliphatic acid     |
| Prenal                                | 0.01 | Aliphatic aldehyde |
| Isoamyl formate                       | tr   | Aliphatic ester    |
| Hexanal                               | tr   | Aliphatic aldehyde |
| Unknown                               | 0.01 | Unknown            |
| 3-Methylpentanol                      | 0.04 | Aliphatic alcohol  |
| (3Z)-Hexenol                          | 0.01 | Aliphatic alcohol  |
| 3-Acetyl-3-methylcyclopentene         | 0.01 | Aliphatic ketone   |
| 3-Methylpentyl formate?               | 0.02 | Aliphatic ester    |
| $\alpha$ -Pinene                      | 0.46 | Monoterpene        |
| Unknown                               | 0.02 | Unknown            |
| Benzaldehyde                          | 0.02 | Simple phenolic    |
| Geranic oxide                         | 0.05 | Monoterpenic ether |
| $\beta$ -Pinene                       | 0.01 | Monoterpene        |
| Octen-3-ol                            | 0.02 | Aliphatic alcohol  |
| 6-Methyl-5-hepten-2-one               | 0.07 | Aliphatic ketone   |
| <i>trans</i> -Dehydroxylinalool oxide | 0.03 | Monoterpenic ether |
| Myrcene                               | 0.10 | Monoterpene        |
| 6-Methyl-5-hepten-2-ol                | 0.01 | Aliphatic alcohol  |
| $\alpha$ -Phellandrene                | 0.06 | Monoterpene        |
| $\Delta^3$ -Carene                    | 0.03 | Monoterpene        |
| <i>para</i> -Cymene                   | 0.09 | Monoterpene        |
| $\beta$ -Phellandrene                 | 0.06 | Monoterpene        |
| 1,8-Cineole                           | 0.01 | Monoterpenic ether |
| Limonene                              | 0.16 | Monoterpene        |
| Unknown                               | 0.04 | Unknown            |
| Unknown                               | 0.04 | Unknown            |
| Benzeneacetaldehyde                   | 0.01 | Simple phenolic    |
| (Z)- $\beta$ -Ocimene                 | 0.09 | Monoterpene        |
| (E)- $\beta$ -Ocimene                 | 0.10 | Monoterpene        |
| Unknown                               | 0.03 | Unknown            |
| 2,6-Dimethyl-5-heptenal (melonal)     | 0.02 | Aliphatic aldehyde |
| $\gamma$ -Terpinene                   | 0.02 | Monoterpene        |

|   |       |                        |
|---|-------|------------------------|
| <i>cis</i> -Sabinene hydrate              | 0.01  | Monoterpenic alcohol   |
| Unknown                                   | 0.02  | Oxygenated monoterpene |
| <i>cis</i> -Linalool oxide (fur.)         | 0.22  | Monoterpenic alcohol   |
| Octanol                                   | 0.02  | Aliphatic alcohol      |
| Fenchone                                  | 0.02  | Monoterpenic ketone    |
| <i>trans</i> -Linalool oxide (fur.)       | 0.13  | Monoterpenic alcohol   |
| Terpinolene                               | 0.03  | Monoterpene            |
| <i>trans</i> -Sabinene hydrate            | 0.02  | Monoterpenic alcohol   |
| Linalool                                  | 4.23  | Monoterpenic alcohol   |
| ( <i>Z</i> )-6-Methyl-3,5-heptadien-2-one | 0.02  | Aliphatic ketone       |
| <i>cis</i> -Rose oxide                    | 1.04  | Monoterpenic ether     |
| Phenylethyl alcohol                       | 0.02  | Simple phenolic        |
| Myrcenol                                  | 0.01  | Monoterpenic alcohol   |
| <i>trans</i> -Rose oxide                  | 0.43  | Monoterpenic ether     |
| Unknown                                   | 0.05  | Unknown                |
| Isopulegol                                | 0.09  | Monoterpenic alcohol   |
| Menthone                                  | 0.83  | Monoterpenic ketone    |
| Unknown                                   | 0.03  | Unknown                |
| Citronellal                               | 0.05  | Monoterpenic aldehyde  |
| iso-Isopulegol                            | 0.15  | Monoterpenic alcohol   |
| Isomenthone                               | 6.27  | Monoterpenic ketone    |
| Borneol                                   | 0.03  | Monoterpenic alcohol   |
| neo-Menthol                               | 0.07  | Monoterpenic alcohol   |
| Terpinen-4-ol                             | 0.06  | Monoterpenic alcohol   |
| Menthol                                   | 0.02  | Monoterpenic alcohol   |
| Isomenthol                                | 0.18  | Monoterpenic alcohol   |
| <i>para</i> -Cymen-8-ol                   | 0.03  | Monoterpenic alcohol   |
| $\alpha$ -Terpineol                       | 0.33  | Monoterpenic alcohol   |
| Unknown                                   | 0.02  | Unknown                |
| Unknown                                   | 0.03  | Oxygenated monoterpene |
| $\beta$ -Cyclocitral                      | 0.03  | Monoterpenic aldehyde  |
| Nerol                                     | 0.21  | Monoterpenic alcohol   |
| Citronellol                               | 31.64 | Monoterpenic alcohol   |
| Neral                                     | 0.49  | Monoterpenic aldehyde  |
| Piperitone                                | 0.05  | Monoterpenic ketone    |
| Geraniol                                  | 13.63 | Monoterpenic alcohol   |
| Geranial                                  | 0.86  | Monoterpenic aldehyde  |
| Citronellyl formate                       | 6.64  | Monoterpenic ester     |
| Neryl formate                             | 0.07  | Monoterpenic ester     |
| Geranyl formate                           | 2.66  | Monoterpenic ester     |
| (3 <i>Z</i> )-Hexenyl tiglate             | 0.02  | Aliphatic ester        |
| Methyl geranate                           | 0.04  | Monoterpenic ester     |
| Citronellic acid                          | 0.08  | Monoterpenic acid      |
| $\alpha$ -Cubebene                        | 0.23  | Sesquiterpene          |
| Phenylethyl propionate                    | 0.03  | Phenolic ester         |

|                                      |      |                      |
|--------------------------------------|------|----------------------|
| Citronellyl acetate                  | 0.24 | Monoterpenic ester   |
| Neryl acetate                        | 0.02 | Monoterpenic ester   |
| $\alpha$ -Ylangene                   | 0.06 | Sesquiterpene        |
| Geranic acid                         | 0.06 | Aliphatic acid       |
| $\alpha$ -Copaene                    | 0.55 | Sesquiterpene        |
| $\beta$ -Bourbonene                  | 1.12 | Sesquiterpene        |
| 1,5-diepi- $\beta$ -Bourbonene       | 0.07 | Sesquiterpene        |
| $\beta$ -Cubebene                    | 0.03 | Sesquiterpene        |
| Geranyl acetate                      | 0.51 | Monoterpenic ester   |
| Phenylethyl isobutyrate              | 0.08 | Phenolic ester       |
| Isocaryophyllene                     | 0.02 | Sesquiterpene        |
| $\alpha$ -Gurjunene                  | 0.08 | Sesquiterpene        |
| $\beta$ -Caryophyllene               | 1.32 | Sesquiterpene        |
| Thymohydroquinone dimethyl ether     | 0.01 | Monoterpenic ether   |
| $\beta$ -Copaene                     | 0.14 | Sesquiterpene        |
| Heptyl tiglate                       | 0.02 | Aliphatic ester      |
| Aromadendrene                        | 0.06 | Sesquiterpene        |
| Isogermacrene D                      | 0.02 | Sesquiterpene        |
| 6,9-Guaiadiene                       | 0.38 | Sesquiterpene        |
| Unknown                              | 0.39 | Sesquiterpene        |
| Citronellyl propionate               | 0.37 | Monoterpenic ester   |
| $\alpha$ -Humulene                   | 0.30 | Sesquiterpene        |
| allo-Aromadendrene                   | 0.21 | Sesquiterpene        |
| <i>trans</i> -Cadina-1(6),4-diene    | 0.18 | Sesquiterpene        |
| $\gamma$ -Murolene                   | 0.10 | Sesquiterpene        |
| Geranyl propionate                   | 0.67 | Monoterpenic ester   |
| $\alpha$ -Amorphene                  | 0.21 | Sesquiterpene        |
| Germacrene D                         | 1.24 | Sesquiterpene        |
| $\beta$ -Selinene                    | 0.18 | Sesquiterpene        |
| $\gamma$ -Amorphene                  | 0.13 | Sesquiterpene        |
| Phenylethyl isovalerate              | 0.05 | Phenolic ester       |
| 4-epi- <i>cis</i> -Dihydroagarofuran | 0.24 | Sesquiterpenic ether |
| Viridiflorene                        | 0.25 | Sesquiterpene        |
| Bicyclogermacrene                    | 0.27 | Sesquiterpene        |
| $\alpha$ -Selinene                   | 0.20 | Sesquiterpene        |
| $\alpha$ -Murolene                   | 0.33 | Sesquiterpene        |
| $\gamma$ -Cadinene                   | 0.35 | Sesquiterpene        |
| 7-epi- $\alpha$ -Selinene            | 0.09 | Sesquiterpene        |
| Geranyl isobutyrate                  | 0.27 | Monoterpenic ester   |
| <i>trans</i> -Calamenene             | 0.02 | Sesquiterpene        |
| $\delta$ -Cadinene                   | 0.85 | Sesquiterpene        |
| Zonarene                             | 0.18 | Sesquiterpene        |
| Citronellyl butyrate                 | 0.53 | Monoterpenic ester   |
| <i>trans</i> -Cadina-1,4-diene       | 0.09 | Sesquiterpene        |
| Phenylethyl angelate?                | 0.12 | Phenolic ester       |

|  |              |                          |
|--|--------------|--------------------------|
| $\alpha$ -Cadinene                     | 0.01         | Sesquiterpene            |
| $\alpha$ -Agarofuran                   | 0.36         | Sesquiterpenic ether     |
| Geranyl butyrate                       | 1.08         | Monoterpenic ester       |
| 1-nor-Bourbonanone                     | 0.02         | Norsesquiterpenic ketone |
| Spathulenol                            | 0.29         | Sesquiterpenic alcohol   |
| Caryophyllene oxide                    | 0.18         | Sesquiterpenic ether     |
| Globulol                               | 0.11         | Sesquiterpenic alcohol   |
| Phenylethyl tiglate                    | 0.78         | Phenolic ester           |
| Viridiflorol                           | 0.08         | Sesquiterpenic alcohol   |
| Geranyl 2-methylbutyrate?              | 0.10         | Monoterpenic ester       |
| Geranyl isovalerate                    | 0.10         | Monoterpenic ester       |
| 10-epi- $\gamma$ -Eudesmol             | 4.55         | Sesquiterpenic alcohol   |
| 1-epi-Cubenol                          | 0.15         | Sesquiterpenic alcohol   |
| $\gamma$ -Eudesmol                     | 0.20         | Sesquiterpenic alcohol   |
| Citronellyl valerate?                  | 0.04         | Monoterpenic ester       |
| Unknown                                | 0.08         | Oxygenated sesquiterpene |
| $\tau$ -Cadinol                        | 0.02         | Sesquiterpenic alcohol   |
| Agarospinol?                           | 0.13         | Sesquiterpenic alcohol   |
| Cubenol                                | 0.16         | Sesquiterpenic alcohol   |
| $\tau$ -Muurolol                       | 0.05         | Sesquiterpenic alcohol   |
| $\beta$ -Eudesmol                      | 0.28         | Sesquiterpenic alcohol   |
| $\alpha$ -Eudesmol                     | 0.29         | Sesquiterpenic alcohol   |
| $\alpha$ -Cadinol                      | 0.14         | Sesquiterpenic alcohol   |
| Geranyl valerate                       | 0.18         | Monoterpenic ester       |
| Citronellyl tiglate                    | 0.28         | Monoterpenic ester       |
| Citronellyl 4-methylvalerate           | 0.10         | Monoterpenic ester       |
| 3 $\beta$ ,4 $\beta$ -Oxidoagarofuran? | 0.03         | Sesquiterpenic ether     |
| Geranyl tiglate                        | 1.08         | Monoterpenic ester       |
| Geranyl 4-methylvalerate?              | 0.18         | Monoterpenic ester       |
| Citronellyl caproate                   | 0.05         | Monoterpenic ester       |
| Geranyl caproate                       | 0.11         | Monoterpenic ester       |
| Citronellyl heptanoate                 | 0.06         | Monoterpenic ester       |
| Phytone                                | 0.04         | Terpenic ketone          |
| Geranyl heptanoate                     | 0.10         | Monoterpenic ester       |
| Citronellyl caprylate                  | 0.04         | Monoterpenic ester       |
| Geranyl caprylate                      | 0.05         | Monoterpenic ester       |
| Unknown                                | 0.03         | Unknown                  |
| Unknown                                | 0.03         | Unknown                  |
| <b>Consolidated total</b>              | <b>96.99</b> |                          |

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

Note: no correction factor was applied

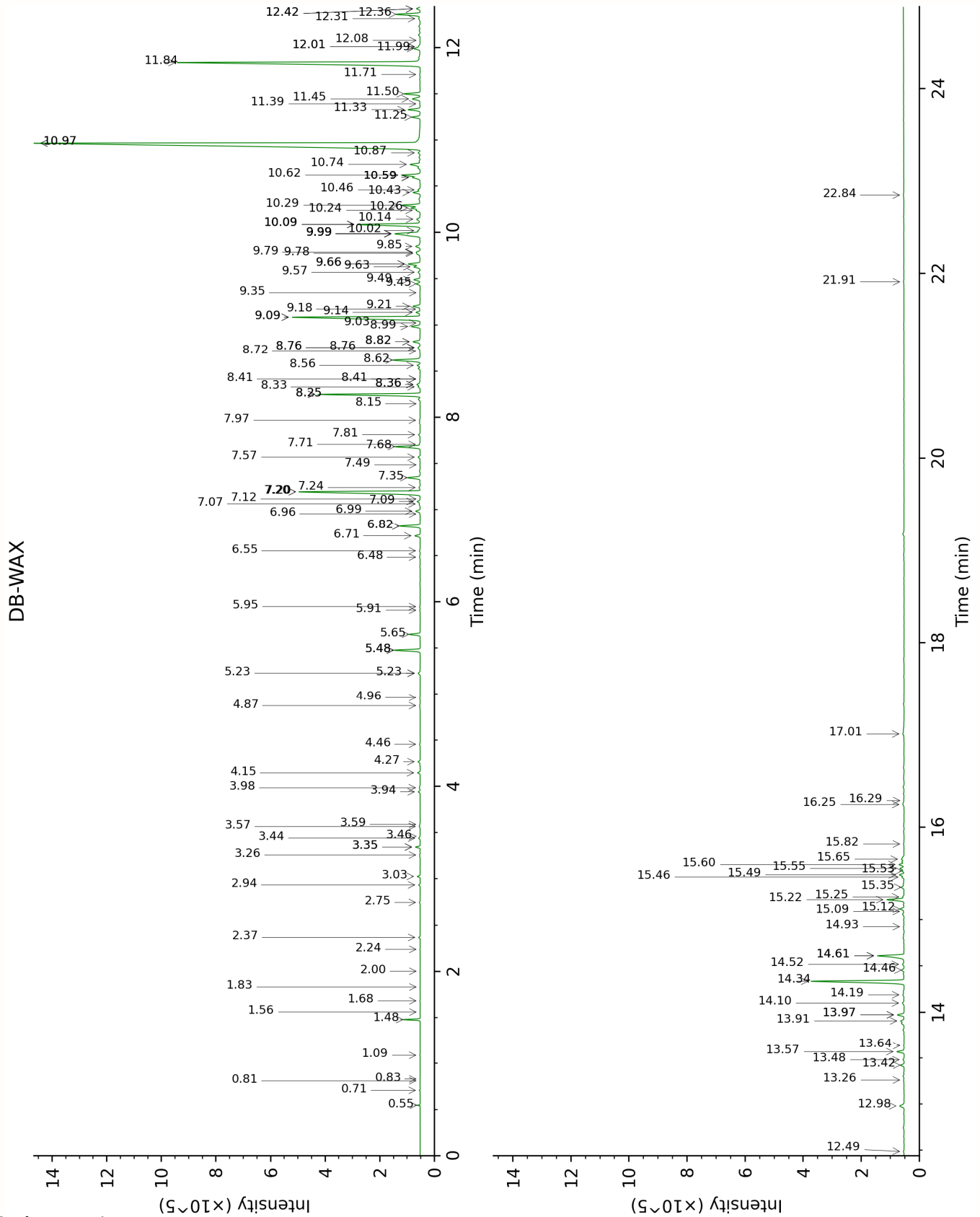
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm 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.

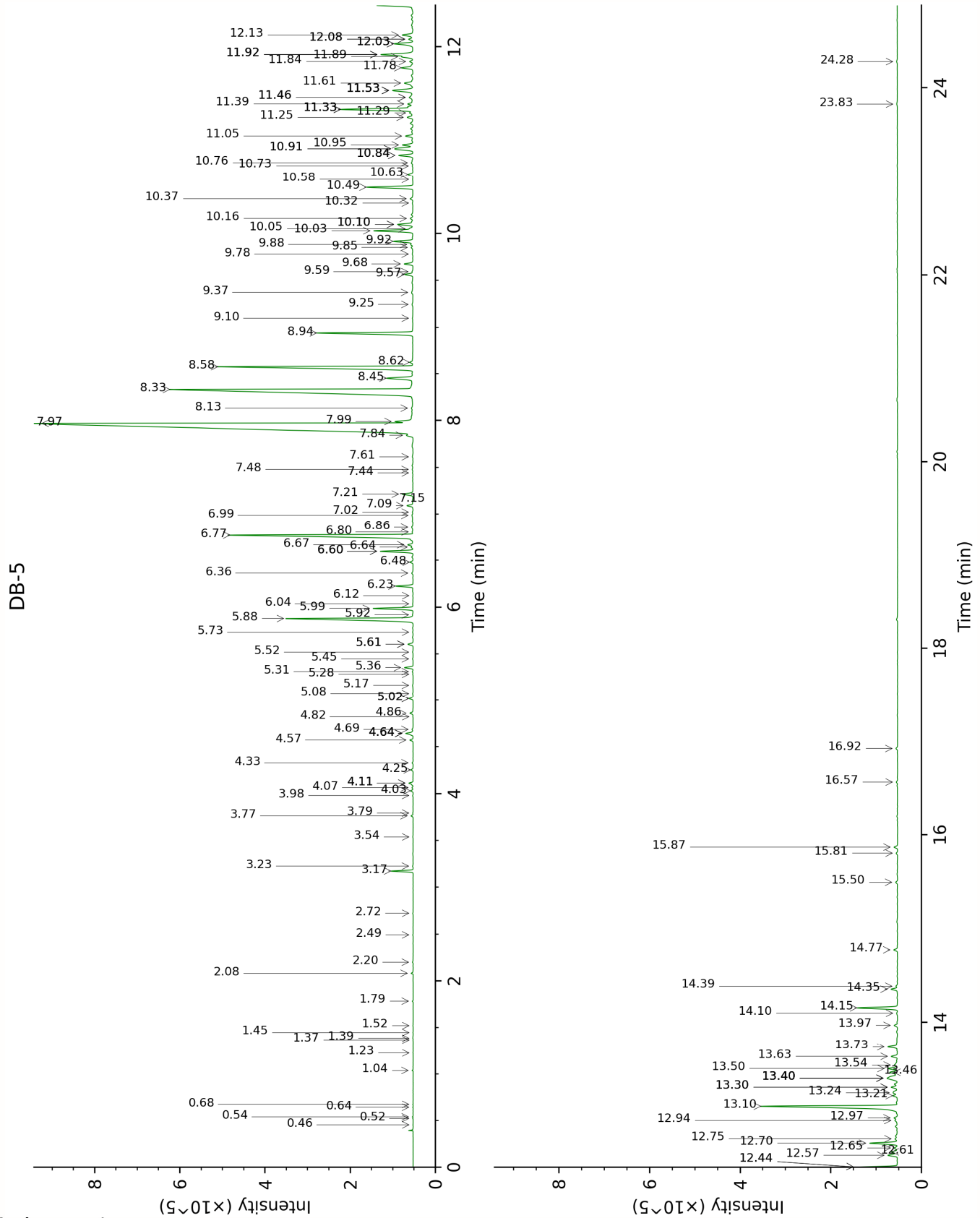
**Unknowns:** Unknown compounds' mass spectral data is presented in the "Full analysis data" table. The occurrence of unknown compounds is to be expected in many samples, and does not denote particular problems unless noted otherwise in the conclusion.

**Bracketed value ([xx]):** A bracketed percent value indicate that two or more compound percentage could not be solved due to coelution.

This page was intentionally left blank. The following pages present the complete data of the analysis.







## FULL ANALYSIS DATA

| Isobutyral   | Column DB-WAX |        |        | Column DB-5 |        |        |
|--|---------------|--------|--------|-------------|--------|--------|
|  | 0.55          | 777.2  | 0.05   | 0.46        | 539.0  | tr     |
| Acetic acid  | 6.82*         | 1408.6 | [0.85] | 0.52        | 595.5  | tr     |
| 2-Methyl-3-buten-2-ol  | 1.68          | 1013.8 | 0.01   | 0.54        | 607.2  | 0.01   |
| Isovaleral   | 0.83          | 885.4  | tr     | 0.64        | 641.6  | tr     |
| 2-Methylbutyral  | 0.81          | 878.8  | tr     | 0.68        | 651.9  | tr     |
| Isoamyl alcohol  | 3.59          | 1175.0 | 0.02   | 1.04        | 733.2  | 0.01   |
| Toluene  | 1.56          | 1002.3 | tr     | 1.23        | 759.1  | tr     |
| Isobutyric acid  | 8.33          | 1521.1 | 0.08   | 1.37        | 778.8  | tr     |
| Prenal   | 3.34*         | 1156.5 | [0.16] | 1.39        | 781.5  | 0.01   |
| Isoamyl formate  | 1.83          | 1027.8 | tr     | 1.45        | 789.8  | tr     |
| Hexanal  | 2.00          | 1043.9 | tr     | 1.52        | 800.0  | tr     |
| Unknown PEGR III<br>[m/z 81, 69 (80), 41<br>(65), 83 (52), 109 (48),<br>55 (47)...]  | 0.71          | 844.3  | 0.02   | 1.79        | 823.6  | 0.01   |
| 3-Methylpentanol   | 5.23*         | 1293.1 | [0.10] | 2.08        | 848.0  | 0.04   |
| (3Z)-Hexenol   | 5.91          | 1343.3 | 0.02   | 2.20        | 857.7  | 0.01   |
| 3-Acetyl-3-methylcyclopentene  | 1.09          | 932.5  | 0.01   | 2.49        | 881.6  | 0.01   |
| 3-Methylpentyl formate?  | 3.26          | 1150.0 | 0.02   | 2.72        | 900.5  | 0.02   |
| $\alpha$ -Pinene   | 1.48          | 991.6  | 0.45   | 3.18        | 931.1  | 0.46   |
| Unknown PEGR IV<br>[m/z 122, 107 (38),<br>121 (35), 79 (28), 77<br>(27), 43 (26)...] |               |        |        | 3.23        | 934.5  | 0.02   |
| Benzaldehyde   | 7.49          | 1458.0 | 0.01   | 3.54        | 955.0  | 0.02   |
| Geranic oxide  | 2.37          | 1078.4 | 0.05   | 3.76        | 969.9  | 0.05   |
| $\beta$ -Pinene  | 2.24          | 1066.2 | 0.01   | 3.79        | 971.8  | 0.01   |
| Octen-3-ol   | 6.96          | 1418.6 | 0.01   | 3.98        | 984.2  | 0.02   |
| 6-Methyl-5-hepten-2-one  | 5.23*         | 1293.1 | [0.10] | 4.03        | 987.4  | 0.07   |
| <i>trans</i> -Dehydroxylinalool oxide  | 3.57          | 1173.3 | 0.04   | 4.07        | 989.7  | 0.03   |
| Myrcene  | 3.03          | 1132.4 | 0.10   | 4.11*       | 992.9  | [0.13] |
| 6-Methyl-5-hepten-2-ol   | 7.12          | 1430.6 | 0.01   | 4.11*       | 992.9  | [0.13] |
| $\alpha$ -Phellandrene   | 2.94          | 1125.4 | 0.06   | 4.26        | 1002.1 | 0.06   |
| $\Delta^3$ -Carene   | 2.75          | 1111.1 | 0.04   | 4.33        | 1007.0 | 0.03   |
| <i>para</i> -Cymene  | 4.27          | 1224.6 | 0.09   | 4.57        | 1022.2 | 0.09   |
| $\beta$ -Phellandrene  | 3.44          | 1163.7 | 0.06   | 4.64*       | 1026.6 | [0.24] |

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|   |       |        |        |       |        |        |
|---|-------|--------|--------|-------|--------|--------|
| 1,8-Cineole   | 3.46  | 1165.3 | 0.01   | 4.64* | 1026.6 | [0.24] |
| Limonene  | 3.34* | 1156.5 | [0.16] | 4.64* | 1026.6 | [0.24] |
| Unknown COCI XLIII<br>[m/z 59, 43 (11), 109<br>(10), 41 (10), 127 (8)...]                         | 6.48  | 1384.2 | 0.04   | 4.64* | 1026.6 | [0.24] |
| Unknown COCI XLIV<br>[m/z 59, 43 (12), 109<br>(11), 41 (10), 127 (8)...]                          | 6.55  | 1389.1 | 0.03   | 4.69  | 1029.3 | 0.04   |
| Benzeneacetaldehyde   | 9.03  | 1574.7 | 0.01   | 4.82  | 1037.8 | 0.01   |
| (Z)- $\beta$ -Ocimene   | 3.94  | 1201.5 | 0.07   | 4.86  | 1040.1 | 0.09   |
| (E)- $\beta$ -Ocimene   | 4.15  | 1216.1 | 0.10   | 5.02* | 1050.0 | [0.12] |
| Unknown COCI V<br>[m/z 125, 69 (75), 41<br>(34), 55 (25), 93 (22)...<br>140 (3)]                  | 4.87  | 1267.8 | 0.03   | 5.02* | 1050.0 | [0.12] |
| 2,6-Dimethyl-5-<br>heptenal (melonal)   | 5.48* | 1312.4 | [1.04] | 5.08  | 1053.6 | 0.02   |
| $\gamma$ -Terpinene   | 3.98  | 1204.6 | 0.03   | 5.16  | 1059.1 | 0.02   |
| <i>cis</i> -Sabinene hydrate  | 7.06  | 1426.7 | 0.06   | 5.28  | 1066.5 | 0.01   |
| Unknown PIMA I [m/z<br>79, 93 (60), 43 (40), 94<br>(35), 137 (33), 77 (26),<br>91 (20), 152 (18)] | 4.96  | 1274.2 | 0.03   | 5.31  | 1068.3 | 0.02   |
| <i>cis</i> -Linalool oxide<br>(fur.)  | 6.72  | 1400.8 | 0.21   | 5.36  | 1071.0 | 0.22   |
| Octanol   | 8.42* | 1527.6 | [0.02] | 5.45  | 1076.9 | 0.02   |
| Fenchone  | 5.95  | 1346.0 | 0.03   | 5.52  | 1081.3 | 0.02   |
| <i>trans</i> -Linalool oxide<br>(fur.)  | 7.09  | 1428.7 | 0.13   | 5.60* | 1086.6 | [0.15] |
| Terpinolene   | 4.46  | 1238.0 | 0.03   | 5.60* | 1086.6 | [0.15] |
| <i>trans</i> -Sabinene<br>hydrate   | 8.15  | 1507.0 | tr     | 5.73  | 1094.7 | 0.02   |
| Linalool  | 8.25* | 1514.9 | [4.12] | 5.88  | 1103.8 | 4.23   |
| (Z)-6-Methyl-3,5-<br>heptadien-2-one  | 8.42* | 1527.6 | [0.02] | 5.92  | 1106.3 | 0.02   |
| <i>cis</i> -Rose oxide  | 5.48* | 1312.4 | [1.04] | 5.99  | 1110.7 | 1.04   |
| Phenylethyl alcohol   | 12.31 | 1847.8 | 0.10   | 6.04  | 1113.7 | 0.02   |
| Myrcenol  | 9.09* | 1579.6 | [6.71] | 6.12  | 1119.3 | 0.01   |
| <i>trans</i> -Rose oxide  | 5.65  | 1324.7 | 0.43   | 6.23  | 1125.9 | 0.43   |
| Unknown CYFL IV<br>[m/z 95, 67 (86), 41<br>(68), 82 (64), 123<br>(62)...]                         | 7.71  | 1474.3 | 0.03   | 6.36  | 1134.7 | 0.05   |
| Isopulegol  | 8.36* | 1523.1 | [0.17] | 6.48  | 1142.1 | 0.09   |
| Menthone  | 6.82* | 1408.6 | [0.85] | 6.60* | 1149.6 | [0.85] |

|   |         |        |         |        |        |         |
|---|---------|--------|---------|--------|--------|---------|
| Unknown PEGR I [m/z<br>43, 141 (51), 55 (36),<br>69 (31), 41 (29)... 156<br>(4)]                                  | 8.72    | 1551.1 | 0.03    | 6.60*  | 1149.6 | [0.85]  |
| Citronellal   | 7.20*   | 1436.4 | [6.34]  | 6.64   | 1152.4 | 0.05    |
| iso-Isopulegol  | 8.25*   | 1514.9 | [4.12]  | 6.67   | 1154.0 | 0.15    |
| Isomenthone   | 7.20*   | 1436.4 | [6.34]  | 6.77   | 1160.6 | 6.27    |
| Borneol   | 9.99*   | 1651.2 | [1.72]  | 6.80   | 1162.8 | 0.03    |
| neo-Menthol   | 8.76*   | 1554.2 | [0.13]  | 6.86   | 1166.0 | 0.07    |
| Terpinen-4-ol   | 8.76*   | 1554.2 | [0.13]  | 6.99   | 1174.4 | 0.06    |
| Menthol   | 9.35    | 1600.0 | 0.02    | 7.02   | 1176.7 | 0.02    |
| Isomenthol  | 9.14    | 1583.6 | 0.17    | 7.09   | 1181.1 | 0.18    |
| <i>para</i> -Cymen-8-ol   | 11.71   | 1794.6 | 0.03    | 7.15   | 1185.1 | 0.03    |
| $\alpha$ -Terpineol   | 9.99*   | 1651.2 | [1.72]  | 7.22   | 1188.9 | 0.33    |
| Unknown MEPI V [m/z<br>43, 99 (84), 81 (46),<br>986 (43), 126 (36), 71<br>(28)... 170 (12)]                       |         |        |         | 7.44   | 1203.4 | 0.02    |
| Unknown DRMO II<br>[m/z 123, 81 (40), 67<br>(29), 79 (29), 93 (26),<br>121 (25), 41 (24), 55<br>(18), 69 (15)...] |         |        |         | 7.48   | 1205.8 | 0.03    |
| $\beta$ -Cyclocitral  | 8.82*   | 1559.2 | [0.32]  | 7.61   | 1214.8 | 0.03    |
| Nerol   | 11.25   | 1755.8 | 0.36    | 7.84   | 1230.2 | 0.21    |
| Citronellol   | 10.97*  | 1732.1 | [31.50] | 7.97*† | 1238.7 | [31.48] |
| Neral   | 9.66*   | 1624.9 | [0.56]  | 7.99*† | 1240.0 | [0.54]  |
| Piperitone  | 10.09*  | 1659.2 | [2.94]  | 8.13   | 1249.5 | 0.05    |
| Geraniol  | 11.84   | 1806.0 | 13.60   | 8.33   | 1262.9 | 13.63   |
| Geranial  | 10.29   | 1676.0 | 0.80    | 8.45   | 1270.9 | 0.86    |
| Citronellyl formate   | 9.09*   | 1579.6 | [6.71]  | 8.58   | 1279.1 | 6.64    |
| Neryl formate   | 9.66*   | 1624.9 | [0.56]  | 8.62   | 1282.3 | 0.07    |
| Geranyl formate   | 10.09*  | 1659.2 | [2.94]  | 8.94   | 1303.7 | 2.66    |
| (3Z)-Hexenyl tiglate  | 9.57    | 1617.8 | 0.11    | 9.10   | 1314.6 | 0.02    |
| Methyl geranate   | 9.99*   | 1651.2 | [1.72]  | 9.25   | 1325.0 | 0.04    |
| Citronellic acid  | 16.24   | 2222.5 | 0.10    | 9.37   | 1334.0 | 0.08    |
| $\alpha$ -Cubebene  | 6.99    | 1420.9 | 0.20    | 9.57   | 1347.5 | 0.23    |
| Phenylethyl<br>propionate   | 12.08   | 1827.0 | 0.02    | 9.59   | 1349.5 | 0.03    |
| Citronellyl acetate   | 9.63    | 1622.5 | 0.30    | 9.68   | 1355.3 | 0.24    |
| Neryl acetate   | 10.43*† | 1687.0 | [0.31]  | 9.78   | 1362.7 | 0.02    |
| $\alpha$ -Ylangene  | 7.24    | 1439.8 | 0.06    | 9.85   | 1367.7 | 0.06    |
| Geranic acid  | 17.01   | 2301.9 | 0.16    | 9.88   | 1369.9 | 0.06    |
| $\alpha$ -Copaene   | 7.35    | 1447.7 | 0.55    | 9.92   | 1372.2 | 0.55    |
| $\beta$ -Bourbonene   | 7.68    | 1472.5 | 1.10    | 10.03  | 1380.2 | 1.12    |

|   |         |        |        |        |        |        |
|---|---------|--------|--------|--------|--------|--------|
| 1,5-diepi- $\beta$ -Bourbonene  | 7.57    | 1464.1 | 0.09   | 10.05  | 1381.6 | 0.07   |
| $\beta$ -Cubebene   | 7.97    | 1493.5 | 0.03   | 10.10* | 1384.9 | [0.46] |
| Geranyl acetate   | 10.74   | 1712.7 | 0.51   | 10.10* | 1384.9 | [0.46] |
| Phenylethyl isobutyrate   | 12.01*  | 1821.0 | [0.07] | 10.16  | 1389.4 | 0.08   |
| Isocaryophyllene  | 8.36*   | 1523.1 | [0.17] | 10.32  | 1401.0 | 0.02   |
| $\alpha$ -Gurjunene   | 7.81    | 1482.0 | 0.08   | 10.37  | 1404.2 | 0.08   |
| $\beta$ -Caryophyllene  | 8.62    | 1543.5 | 1.28   | 10.49  | 1413.3 | 1.32   |
| Thymohydroquinone dimethyl ether  | 12.01*  | 1821.0 | [0.07] | 10.58  | 1419.6 | 0.01   |
| $\beta$ -Copaene  | 8.56    | 1539.0 | 0.13   | 10.64  | 1423.8 | 0.14   |
| Heptyl tiglate  |         |        |        | 10.73  | 1430.6 | 0.02   |
| Aromadendrene   | 8.76*   | 1554.2 | [0.13] | 10.76  | 1433.1 | 0.06   |
| Isogermacrene D   | 9.18    | 1586.2 | 0.02   | 10.84* | 1439.0 | [0.41] |
| 6,9-Guaiadiene  | 8.82*   | 1559.2 | [0.32] | 10.84* | 1439.0 | [0.41] |
| Unknown BOCA IV [m/z 91, 161 (92), 105 (85), 119 (63), 133 (53), 79 (49), 204 (46)] | 8.99    | 1571.8 | 0.39   | 10.91* | 1444.2 | [0.75] |
| Citronellyl propionate  | 10.46*† | 1689.3 | [0.10] | 10.91* | 1444.2 | [0.75] |
| $\alpha$ -Humulene  | 9.49    | 1611.3 | 0.29   | 10.95  | 1447.3 | 0.30   |
| allo-Aromadendrene  | 9.21    | 1588.6 | 0.32   | 11.05  | 1454.4 | 0.21   |
| <i>trans</i> -Cadina-1(6),4-diene   | 9.45    | 1607.7 | 0.17   | 11.25  | 1469.3 | 0.18   |
| $\gamma$ -Murolene  | 9.79*†  | 1635.1 | [0.18] | 11.29  | 1472.7 | 0.10   |
| Geranyl propionate  | 11.50   | 1777.1 | 0.67   | 11.33* | 1475.6 | [2.13] |
| $\alpha$ -Amorphene   | 9.78*†  | 1634.2 | [0.13] | 11.33* | 1475.6 | [2.13] |
| Germacrene D  | 9.99*   | 1651.2 | [1.72] | 11.33* | 1475.6 | [2.13] |
| $\beta$ -Selinene   | 10.02   | 1653.8 | 0.10   | 11.39  | 1479.9 | 0.18   |
| $\gamma$ -Amorphene   | 9.99*   | 1651.2 | [1.72] | 11.46* | 1485.1 | [0.18] |
| Phenylethyl isovalerate   | 13.26   | 1932.9 | 0.05   | 11.46* | 1485.1 | [0.18] |
| 4-epi- <i>cis</i> -Dihydroagarofuran  | 10.09*  | 1659.2 | [2.94] | 11.53* | 1490.6 | [0.78] |
| Viridiflorene   | 9.85    | 1640.2 | 0.25   | 11.53* | 1490.6 | [0.78] |
| Bicyclogermacrene   | 10.26*† | 1673.5 | [0.43] | 11.53* | 1490.6 | [0.78] |
| $\alpha$ -Selinene  | 10.14   | 1663.8 | 0.20   | 11.53* | 1490.6 | [0.78] |
| $\alpha$ -Murolene  | 10.24*† | 1671.5 | [0.17] | 11.61  | 1496.5 | 0.33   |
| $\gamma$ -Cadinene  | 10.59*  | 1700.3 | [0.42] | 11.78  | 1508.8 | 0.35   |
| 7-epi- $\alpha$ -Selinene   | 10.59*  | 1700.3 | [0.42] | 11.84  | 1514.1 | 0.09   |
| Geranyl isobutyrate   | 11.45   | 1772.4 | 0.42   | 11.89  | 1518.1 | 0.27   |
| <i>trans</i> -Calamenene  | 11.39   | 1767.9 | 0.02   | 11.92* | 1519.9 | [1.05] |
| $\delta$ -Cadinene  | 10.62   | 1702.9 | 0.85   | 11.92* | 1519.9 | [1.05] |
| Zonarene  | 10.59*  | 1700.3 | [0.42] | 11.92* | 1519.9 | [1.05] |

|   |        |        |         |        |        |        |
|---|--------|--------|---------|--------|--------|--------|
| Citronellyl butyrate  | 11.33  | 1762.6 | 0.53    | 12.03* | 1529.0 | [0.62] |
| <i>trans</i> -Cadina-1,4-diene  | 10.86  | 1723.3 | 0.09    | 12.03* | 1529.0 | [0.62] |
| Phenylethyl angelate?   | 14.46  | 2044.8 | 0.12    | 12.08* | 1532.7 | [0.12] |
| $\alpha$ -Cadinene  | 10.97* | 1732.1 | [31.50] | 12.08* | 1532.7 | [0.12] |
| $\alpha$ -Agarofuran  | 11.99  | 1819.3 | 0.32    | 12.13  | 1536.3 | 0.36   |
| Geranyl butyrate  | 12.36  | 1852.0 | 1.08    | 12.44* | 1561.2 | [1.13] |
| 1-nor-Bourbonanone  | 13.64  | 1967.4 | 0.02    | 12.44* | 1561.2 | [1.13] |
| Spathulenol   | 14.61* | 2059.7 | [1.37]  | 12.57  | 1571.2 | 0.29   |
| Caryophyllene oxide   | 12.98  | 1907.0 | 0.26    | 12.61  | 1574.0 | 0.18   |
| Globulol  | 14.10  | 2010.7 | 0.10    | 12.65  | 1577.3 | 0.11   |
| Phenylethyl tiglate   | 15.22  | 2118.7 | 0.75    | 12.70  | 1581.3 | 0.78   |
| Viridiflorol  | 14.19  | 2019.3 | 0.07    | 12.75  | 1585.0 | 0.08   |
| Geranyl 2-methylbutyrate?   | 12.42* | 1857.2 | [0.17]  | 12.94  | 1600.4 | 0.10   |
| Geranyl isovalerate   | 12.42* | 1857.2 | [0.17]  | 12.97  | 1602.6 | 0.10   |
| 10-epi- $\gamma$ -Eudesmol  | 14.34  | 2033.3 | 4.27    | 13.10  | 1612.7 | 4.55   |
| 1-epi-Cubenol   | 13.97* | 1998.5 | [0.31]  | 13.21  | 1622.0 | 0.15   |
| $\gamma$ -Eudesmol  | 15.12  | 2108.7 | 0.18    | 13.24  | 1624.6 | 0.20   |
| Citronellyl valerate?   | 12.49  | 1863.0 | 0.04    | 13.30* | 1629.5 | [0.20] |
| Unknown PEGR II<br>[m/z 147, 162 (79), 43<br>(64), 59 (64), 95 (47),<br>91 (44), 105 (43)... 238<br>(13)] | 15.46  | 2143.0 | 0.08    | 13.30* | 1629.5 | [0.20] |
| $\tau$ -Cadinol   | 15.09  | 2106.0 | 0.02    | 13.40* | 1637.5 | [0.58] |
| Agarospinol?  | 15.35  | 2132.1 | 0.13    | 13.40* | 1637.5 | [0.58] |
| Cubenol   | 13.91  | 1992.3 | 0.16    | 13.40* | 1637.5 | [0.58] |
| $\tau$ -Muurolol  | 15.25  | 2121.7 | 0.05    | 13.40* | 1637.5 | [0.58] |
| $\beta$ -Eudesmol   | 15.60  | 2156.6 | 0.23    | 13.46  | 1642.7 | 0.28   |
| $\alpha$ -Eudesmol  | 15.55  | 2152.4 | 0.19    | 13.50  | 1646.1 | 0.29   |
| $\alpha$ -Cadinol   | 15.66  | 2162.4 | 0.12    | 13.54  | 1649.1 | 0.14   |
| Geranyl valerate  | 13.42  | 1947.7 | 0.15    | 13.63  | 1656.8 | 0.18   |
| Citronellyl tiglate   | 13.57  | 1961.2 | 0.32    | 13.73  | 1665.3 | 0.28   |
| Citronellyl 4-methylvalerate  |        |        |         | 13.97  | 1684.6 | 0.10   |
| 3 $\beta$ ,4 $\beta$ -Oxidoagarofuran?  | 16.29  | 2226.9 | 0.03    | 14.10  | 1695.3 | 0.03   |
| Geranyl tiglate   | 14.61* | 2059.7 | [1.37]  | 14.16  | 1700.1 | 1.08   |
| Geranyl 4-methylvalerate?   | 13.97* | 1998.5 | [0.31]  | 14.35  | 1717.1 | 0.18   |
| Citronellyl caproate  | 13.48  | 1953.1 | 0.05    | 14.39  | 1719.9 | 0.05   |
| Geranyl caproate  | 14.52  | 2050.8 | 0.08    | 14.77  | 1753.5 | 0.11   |
| Citronellyl heptanoate  |        |        |         | 15.50  | 1816.6 | 0.06   |

|   |        |        |      |        |        |      |
|---|--------|--------|------|--------|--------|------|
| Phytone   | 14.93  | 2089.8 | 0.03 | 15.81  | 1844.8 | 0.04 |
| Geranyl heptanoate  | 15.49  | 2145.5 | 0.20 | 15.87  | 1850.8 | 0.10 |
| Citronellyl caprylate   | 15.53  | 2149.8 | 0.06 | 16.57  | 1914.3 | 0.04 |
| Geranyl caprylate   | 15.82  | 2178.8 | 0.02 | 16.92  | 1948.3 | 0.05 |
| Unknown COCI L [m/z<br>69, 83 (59), 81 (56),<br>137 (48), 41 (29), 139<br>(28)...]  | 21.91  | 2876.3 | 0.03 | 23.83  | 2708.6 | 0.03 |
| Unknown CYWI III<br>[m/z 69, 81 (84), 137<br>(53), 83 (30), 95 (27),<br>41 (19)...] | 22.84  | 2998.9 | 0.04 | 24.28  | 2767.5 | 0.03 |
| Total reported  | 96.19% |        |      | 97.01% |        |      |

\*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, only the first one is 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.

Note: no correction factor was applied

R.T.: Retention time (minutes)

R.I.: Retention index