

Date : 2024-07-23

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 24G10-PTH02

**Customer Identification :** Bourbon Geranium - Madagascar - G20110R

**Type :** Essential Oil

**Source :** *Pelargonium graveolens* ct. *Madagascar*

**Customer :** Plant Therapy

Checked and approved by:

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 liquid by FAST GC-FID



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

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

**Date :** 2024-07-19

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.4653 \pm 0.0003$  (20 °C)

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

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

**Date :** 2024-07-11

## 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 |
| 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    |
| Isoamyl formate               | 0.01   | Aliphatic ester    |
| Unknown                       | 0.03   | Unknown            |
| 3-Methylpentanol              | 0.04   | Aliphatic alcohol  |
| (3Z)-Hexenol                  | 0.03   | Aliphatic alcohol  |
| Hexanol                       | 0.01   | Aliphatic alcohol  |
| 3-Acetyl-3-methylcyclopentene | 0.01   | Aliphatic ketone   |
| 3-Methylpentyl formate?       | 0.03   | Aliphatic ester    |
| Hashishene                    | tr     | Monoterpene        |
| Tricyclene                    | 0.02   | Monoterpene        |
| $\alpha$ -Thujene             | tr     | Monoterpene        |
| $\alpha$ -Pinene              | 0.49   | Monoterpene        |
| Unknown                       | 0.02   | Simple phenolic    |
| Camphene                      | 0.03   | Monoterpene        |
| Geranic oxide                 | 0.04   | Monoterpenic ether |
| $\beta$ -Pinene               | 0.05   | Monoterpene        |
| Sabinene                      | 0.01   | Monoterpene        |
| Octen-3-ol                    | 0.04   | Aliphatic alcohol  |
| 6-Methyl-5-hepten-2-one       | 0.07   | Aliphatic ketone   |
| Myrcene                       | 0.16   | Monoterpene        |
| trans-Dehydroxylinalool oxide | 0.05   | Monoterpenic ether |
| 6-Methyl-5-hepten-2-ol        | tr     | Aliphatic alcohol  |
| $\alpha$ -Phellandrene        | 0.09   | Monoterpene        |
| $\Delta^3$ -Carene            | 0.03   | Monoterpene        |
| $\alpha$ -Terpinene           | 0.02   | Monoterpene        |
| para-Cymene                   | 0.10   | Monoterpene        |
| Limonene                      | 0.17   | Monoterpene        |
| 1,8-Cineole                   | [0.18] | Monoterpenic ether |
| Unknown                       | 0.02   | Unknown            |
| $\beta$ -Phellandrene         | [0.18] | Monoterpene        |
| Unknown                       | 0.03   | Unknown            |
| Benzeneacetaldehyde           | 0.01   | Simple phenolic    |
| (Z)- $\beta$ -Ocimene         | 0.13   | Monoterpene        |
| Unknown                       | 0.02   | Unknown            |
| (E)- $\beta$ -Ocimene         | 0.11   | Monoterpene        |

|                                  |       |                           |
|----------------------------------|-------|---------------------------|
| Isobutyl angelate                | 0.02  | Aliphatic ester           |
| $\gamma$ -Terpinene              | 0.01  | Monoterpene               |
| Unknown                          | 0.02  | Oxygenated monoterpene    |
| cis-Linalool oxide (fur.)        | 0.19  | Monoterpenic alcohol      |
| Octanol                          | 0.02  | Aliphatic alcohol         |
| Terpinolene                      | 0.04  | Monoterpene               |
| trans-Linalool oxide (fur.)      | 0.04  | Monoterpenic alcohol      |
| para-Cymenene                    | 0.03  | Monoterpene               |
| Rosefuran                        | 0.03  | Monoterpenic ether        |
| Linalool                         | 4.93  | Monoterpenic alcohol      |
| (Z)-6-Methyl-3,5-heptadien-2-one | 0.03  | Aliphatic ketone          |
| cis-Rose oxide                   | 1.05  | Monoterpenic ether        |
| Phenylethyl alcohol              | 0.03  | Simple phenolic           |
| trans-Rose oxide                 | 0.43  | Monoterpenic ether        |
| trans-Pinocarveol                | 0.02  | Monoterpenic alcohol      |
| Unknown                          | 0.05  | Unknown                   |
| Unknown                          | 0.26  | Oxygenated normonoterpene |
| Menthone                         | 2.20  | Monoterpenic ketone       |
| Citronellal                      | 0.82  | Monoterpenic aldehyde     |
| Isomenthone                      | 5.42  | Monoterpenic ketone       |
| Isoneral                         | 0.02  | Monoterpenic aldehyde     |
| neo-Menthol                      | 0.07  | Monoterpenic alcohol      |
| Terpinen-4-ol                    | 0.04  | Monoterpenic alcohol      |
| Menthol                          | 0.03  | Monoterpenic alcohol      |
| Isomenthol                       | 0.13  | Monoterpenic alcohol      |
| para-Cymen-8-ol                  | 0.03  | Monoterpenic alcohol      |
| $\alpha$ -Terpineol              | 0.37  | Monoterpenic alcohol      |
| Myrtenol                         | 0.04  | Monoterpenic alcohol      |
| Unknown                          | 0.01  | Unknown                   |
| Unknown                          | 0.02  | Oxygenated monoterpene    |
| Nerol                            | 0.55  | Monoterpenic alcohol      |
| Citronellol                      | 21.60 | Monoterpenic alcohol      |
| Neral                            | 0.58  | Monoterpenic aldehyde     |
| Piperitone                       | 0.09  | Monoterpenic ketone       |
| Geraniol                         | 13.71 | Monoterpenic alcohol      |
| Geranal                          | 0.80  | Monoterpenic aldehyde     |
| Citronellyl formate              | 10.23 | Monoterpenic ester        |
| Neryl formate                    | 0.30  | Monoterpenic ester        |
| Geranyl formate                  | 5.84  | Monoterpenic ester        |
| (3Z)-Hexenyl tiglate             | 0.03  | Aliphatic ester           |
| Methyl geranate                  | 0.02  | Monoterpenic ester        |
| $\alpha$ -Cubebene               | 0.09  | Sesquiterpene             |
| Phenylethyl propionate           | 0.06  | Phenolic ester            |
| Citronellyl acetate              | 0.31  | Monoterpenic ester        |
| Neryl acetate                    | 0.02  | Monoterpenic ester        |

|                                      |        |                          |
|--------------------------------------|--------|--------------------------|
| $\alpha$ -Ylangene                   | 0.02   | Sesquiterpene            |
| Geranic acid                         | 0.05   | Aliphatic acid           |
| $\alpha$ -Copaene                    | 0.34   | Sesquiterpene            |
| $\beta$ -Bourbonene                  | 1.01   | Sesquiterpene            |
| Geranyl acetate                      | 0.38   | Monoterpenic ester       |
| $\beta$ -Elemene                     | 0.13   | Sesquiterpene            |
| Phenylethyl isobutyrate              | 0.11   | Phenolic ester           |
| $\alpha$ -Gurjunene                  | 0.02   | Sesquiterpene            |
| $\beta$ -Caryophyllene               | 0.70   | Sesquiterpene            |
| $\beta$ -Ylangene                    | 0.37   | Sesquiterpene            |
| $\beta$ -Copaene                     | 0.10   | Sesquiterpene            |
| Heptyl tiglate                       | 0.01   | Aliphatic ester          |
| $\alpha$ -Guaiene                    | [0.63] | Sesquiterpene            |
| <i>trans</i> - $\alpha$ -Bergamotene | [0.63] | Sesquiterpene            |
| 6,9-Guaiadiene                       | 6.19   | Sesquiterpene            |
| Unknown                              | 0.37   | Sesquiterpene            |
| Citronellyl propionate               | 0.49   | Monoterpenic ester       |
| $\alpha$ -Humulene                   | 0.25   | Sesquiterpene            |
| allo-Aromadendrene                   | 0.17   | Sesquiterpene            |
| <i>trans</i> -Cadina-1(6),4-diene    | 0.25   | Sesquiterpene            |
| $\gamma$ -Murolene                   | 0.10   | Sesquiterpene            |
| Germacrene D                         | 0.78   | Sesquiterpene            |
| Geranyl propionate                   | 0.99   | Monoterpenic ester       |
| $\beta$ -Selinene                    | 0.20   | Sesquiterpene            |
| Phenylethyl isovalerate              | 0.05   | Phenolic ester           |
| $\gamma$ -Amorphene                  | 0.30   | Sesquiterpene            |
| Bicyclogermacrene                    | 0.06   | Sesquiterpene            |
| Viridiflorene                        | 0.08   | Sesquiterpene            |
| 4-epi- <i>cis</i> -Dihydroagarofuran | 0.09   | Sesquiterpenic ether     |
| $\alpha$ -Murolene                   | 0.12   | Sesquiterpene            |
| $\delta$ -Amorphene                  | 0.09   | Sesquiterpene            |
| $\gamma$ -Cadinene                   | 0.01   | Sesquiterpene            |
| Cubebol                              | 0.04   | Sesquiterpenic alcohol   |
| 7-epi- $\alpha$ -Selinene            | 0.22   | Sesquiterpene            |
| Geranyl isobutyrate                  | 0.31   | Monoterpenic ester       |
| <i>trans</i> -Calamenene             | 0.15   | Sesquiterpene            |
| Zonarene                             | 0.28   | Sesquiterpene            |
| $\delta$ -Cadinene                   | 0.36   | Sesquiterpene            |
| Citronellyl butyrate                 | 0.53   | Monoterpenic ester       |
| Phenylethyl angelate?                | 0.05   | Phenolic ester           |
| $\alpha$ -Cadinene                   | 0.04   | Sesquiterpene            |
| $\alpha$ -Agarofuran                 | 0.22   | Sesquiterpenic ether     |
| Europelargone isomer                 | 0.12   | Sesquiterpenic ketone    |
| 1-nor-Bourbonanone                   | 0.04   | Norsesquiterpenic ketone |
| Geranyl butyrate                     | 0.97   | Monoterpenic ester       |

|                              |              |                        |
|------------------------------|--------------|------------------------|
| Caryophyllene oxide          | 0.29         | Sesquiterpenic ether   |
| Caryophyllene oxide isomer   | 0.01         | Sesquiterpenic ether   |
| Globulol                     | 0.05         | Sesquiterpenic alcohol |
| Europelargone A              | 0.52         | Sesquiterpenic ketone  |
| Phenylethyl tiglate          | 0.52         | Phenolic ester         |
| Geranyl 2-methylbutyrate?    | 0.01         | Monoterpenic ester     |
| Geranyl isovalerate          | 0.35         | Monoterpenic ester     |
| 10-epi-γ-Eudesmol            | 0.05         | Sesquiterpenic alcohol |
| 1,10-diepi-Cubenol           | 0.14         | Sesquiterpenic alcohol |
| 1-epi-Cubenol                | 0.02         | Sesquiterpenic alcohol |
| γ-Eudesmol                   | 0.07         | Sesquiterpenic alcohol |
| Citronellyl valerate?        | 0.02         | Monoterpenic ester     |
| Cubenol                      | 0.07         | Sesquiterpenic alcohol |
| τ-Muurolol                   | 0.02         | Sesquiterpenic alcohol |
| τ-Cadinol                    | 0.02         | Sesquiterpenic alcohol |
| β-Eudesmol                   | 0.07         | Sesquiterpenic alcohol |
| α-Cadinol                    | 0.07         | Sesquiterpenic alcohol |
| cis-Calamenen-10-ol          | 0.08         | Sesquiterpenic alcohol |
| Geranyl valerate             | 0.11         | Monoterpenic ester     |
| Citronellyl tiglate          | 0.30         | Monoterpenic ester     |
| Citronellyl 4-methylvalerate | 0.10         | Monoterpenic ester     |
| 3β,4β-Oxidoagarofuran?       | 0.07         | Sesquiterpenic ether   |
| Geranyl tiglate              | 1.29         | Monoterpenic ester     |
| Citronellyl caproate         | 0.04         | Monoterpenic ester     |
| Geranyl 4-methylvalerate?    | 0.12         | Monoterpenic ester     |
| Geranyl caproate             | 0.06         | Monoterpenic ester     |
| Citronellyl heptanoate       | 0.04         | Monoterpenic ester     |
| Phytone                      | 0.03         | Terpenic ketone        |
| Geranyl heptanoate           | 0.05         | Monoterpenic ester     |
| Citronellyl caprylate        | 0.04         | Monoterpenic ester     |
| Geranyl caprylate            | 0.04         | Monoterpenic ester     |
| Unknown                      | 0.46         | Unknown                |
| Unknown                      | 0.61         | Unknown                |
| Unknown                      | 0.21         | Unknown                |
| <b>Consolidated total</b>    | <b>96.49</b> |                        |

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

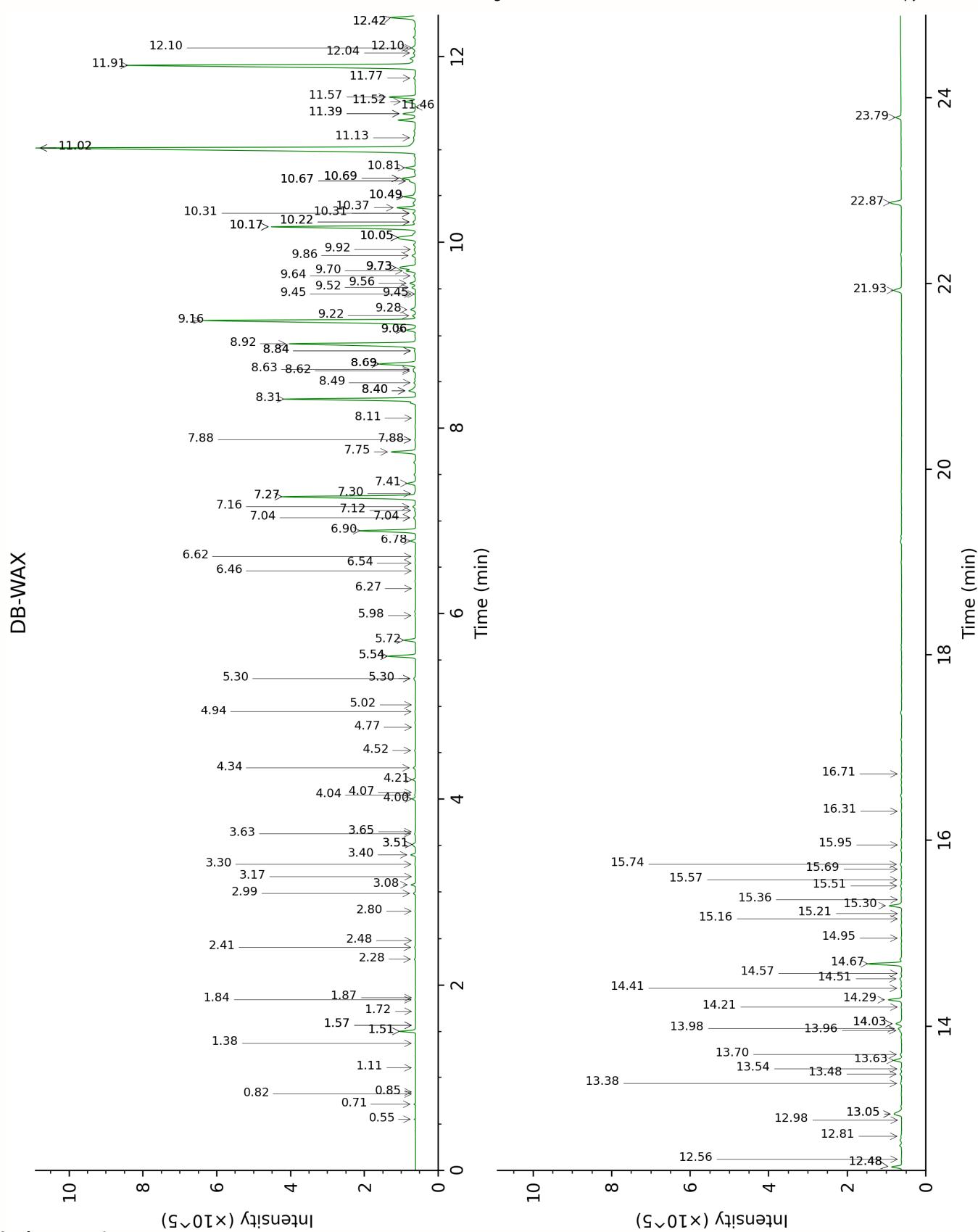
Note: no correction factor was applied

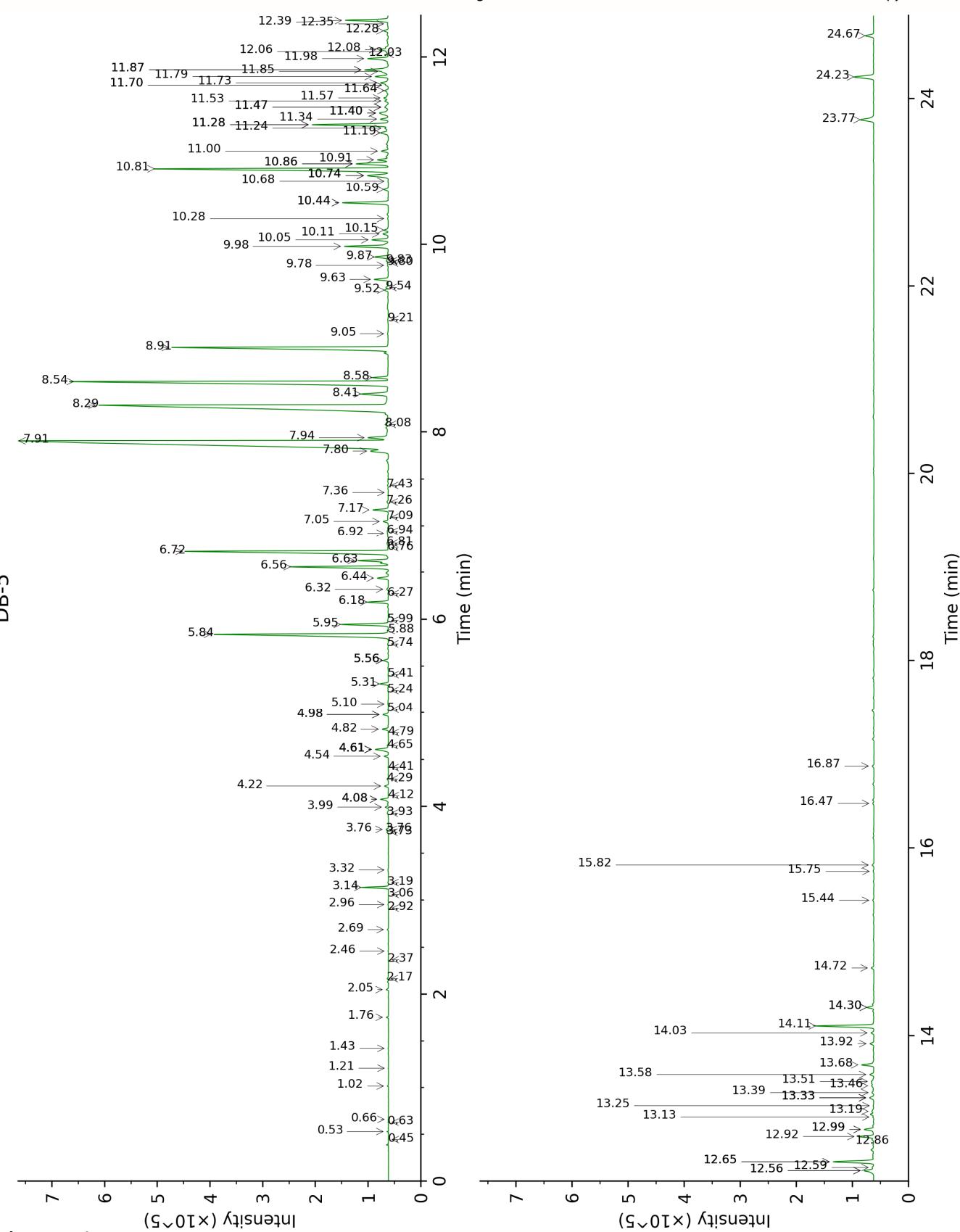
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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

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## FULL ANALYSIS DATA

| <b>Isobutyral</b>                                                                         | <b>Column DB-WAX</b> |        |        | <b>Column DB-5</b> |        |        |
|-------------------------------------------------------------------------------------------|----------------------|--------|--------|--------------------|--------|--------|
|                                                                                           | 0.55                 | 775.5  | 0.02   | 0.44               | 537.3  | tr     |
| 2-Methyl-3-buten-2-ol                                                                     | 1.72                 | 1014.2 | 0.01   | 0.53               | 607.0  | 0.01   |
| Isovaleral                                                                                | 0.85                 | 886.3  | tr     | 0.63               | 641.7  | tr     |
| 2-Methylbutyral                                                                           | 0.82                 | 878.8  | tr     | 0.66               | 652.1  | tr     |
| Isoamyl alcohol                                                                           | 3.65                 | 1177.2 | 0.01   | 1.02               | 733.2  | 0.01   |
| Toluene                                                                                   | 1.57*                | 999.8  | [0.01] | 1.21               | 759.9  | tr     |
| Isoamyl formate                                                                           | 1.84                 | 1026.1 | 0.01   | 1.42               | 790.7  | 0.01   |
| Unknown PEGR III<br>[m/z 81, 69 (80), 41<br>(65), 83 (52), 109 (48),<br>55 (47)...]       | 0.71                 | 840.7  | 0.03   | 1.76               | 823.8  | 0.03   |
| 3-Methylpentanol                                                                          | 5.30*                | 1300.1 | [0.11] | 2.05               | 848.2  | 0.04   |
| (3Z)-Hexenol                                                                              | 5.98                 | 1347.7 | 0.03   | 2.17               | 857.9  | 0.03   |
| Hexanol                                                                                   | 5.54*                | 1317.0 | [1.06] | 2.37               | 874.6  | 0.01   |
| 3-Acetyl-3-methylcyclopentene                                                             | 1.11                 | 930.9  | 0.01   | 2.46               | 882.3  | 0.01   |
| 3-Methylpentyl formate?                                                                   | 3.30                 | 1150.7 | 0.05   | 2.69               | 901.3  | 0.03   |
| Hashishene                                                                                | 1.51*                | 992.8  | [0.49] | 2.92               | 917.1  | tr     |
| Tricyclene                                                                                | 1.38                 | 972.9  | 0.01   | 2.96               | 919.6  | 0.02   |
| $\alpha$ -Thujene                                                                         | 1.57*                | 999.8  | [0.01] | 3.06               | 926.7  | tr     |
| $\alpha$ -Pinene                                                                          | 1.51*                | 992.8  | [0.49] | 3.14               | 931.7  | 0.49   |
| Unknown ACMI I [m/z<br>122, 121 (36), 107<br>(33), 79 (27), 93 (25),<br>77 (25), 43 (20)] | 4.07                 | 1208.1 | 0.02   | 3.19               | 935.1  | 0.02   |
| Camphene                                                                                  | 1.87                 | 1028.3 | 0.01   | 3.32               | 944.0  | 0.03   |
| Geranic oxide                                                                             | 2.41                 | 1079.9 | 0.04   | 3.73               | 970.6  | 0.04   |
| $\beta$ -Pinene                                                                           | 2.28                 | 1067.8 | 0.05   | 3.76*              | 972.6  | [0.05] |
| Sabinene                                                                                  | 2.48                 | 1086.8 | 0.01   | 3.76*              | 972.6  | [0.05] |
| Octen-3-ol                                                                                | 7.04*                | 1423.3 | [0.10] | 3.93               | 984.0  | 0.04   |
| 6-Methyl-5-hepten-2-one                                                                   | 5.30*                | 1300.1 | [0.11] | 3.99               | 988.3  | 0.07   |
| Myrcene                                                                                   | 3.08                 | 1134.1 | 0.16   | 4.08*              | 993.8  | [0.19] |
| <i>trans</i> -Dehydroxylinalool oxide                                                     | 3.63                 | 1175.5 | 0.05   | 4.08*              | 993.8  | [0.19] |
| 6-Methyl-5-hepten-2-ol                                                                    | 7.16                 | 1431.9 | 0.13   | 4.12               | 996.3  | tr     |
| $\alpha$ -Phellandrene                                                                    | 2.99                 | 1127.0 | 0.08   | 4.22               | 1003.1 | 0.09   |
| $\Delta$ 3-Carene                                                                         | 2.80                 | 1112.6 | 0.03   | 4.29               | 1007.9 | 0.03   |
| $\alpha$ -Terpinene                                                                       | 3.17                 | 1140.7 | 0.01   | 4.41               | 1015.5 | 0.02   |

|                                                                                                   |        |        |        |       |        |        |
|---------------------------------------------------------------------------------------------------|--------|--------|--------|-------|--------|--------|
| <i>para</i> -Cymene                                                                               | 4.34   | 1226.6 | 0.09   | 4.54  | 1023.1 | 0.10   |
| Limonene                                                                                          | 3.40   | 1158.4 | 0.17   | 4.61* | 1027.7 | [0.37] |
| 1,8-Cineole                                                                                       | 3.51*  | 1166.9 | [0.18] | 4.61* | 1027.7 | [0.37] |
| Unknown COCI XLIII<br>[m/z 59, 43 (11), 109<br>(10), 41 (10), 127 (8)...]                         | 6.46   | 1381.6 | 0.02   | 4.61* | 1027.7 | [0.37] |
| $\beta$ -Phellandrene                                                                             | 3.51*  | 1166.9 | [0.18] | 4.61* | 1027.7 | [0.37] |
| Unknown COCI XLIV<br>[m/z 59, 43 (12), 109<br>(11), 41 (10), 127 (8)...]                          | 6.62   | 1392.5 | 0.04   | 4.65  | 1030.2 | 0.03   |
| Benzeneacetaldehyde                                                                               | 9.06*  | 1574.4 | [0.37] | 4.79  | 1038.9 | 0.01   |
| (Z)- $\beta$ -Ocimene                                                                             | 4.00   | 1203.2 | 0.13   | 4.82  | 1041.2 | 0.13   |
| Unknown COCI V<br>[m/z 125, 69 (75), 41<br>(34), 55 (25), 93 (22)...<br>140 (3)]                  | 4.94   | 1268.9 | 0.02   | 4.98* | 1051.0 | [0.13] |
| (E)- $\beta$ -Ocimene                                                                             | 4.21   | 1217.7 | 0.11   | 4.98* | 1051.0 | [0.13] |
| Isobutyl angelate                                                                                 | 4.77   | 1257.2 | 0.01   | 5.04  | 1054.6 | 0.02   |
| $\gamma$ -Terpinene                                                                               | 4.04   | 1206.1 | 0.05   | 5.10  | 1058.3 | 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)] | 5.02   | 1274.5 | 0.02   | 5.24  | 1067.4 | 0.02   |
| <i>cis</i> -Linalool oxide<br>(fur.)                                                              | 6.78   | 1404.5 | 0.18   | 5.31  | 1071.9 | 0.19   |
| Octanol                                                                                           | 8.40*  | 1524.1 | [0.39] | 5.41  | 1078.0 | 0.02   |
| Terpinolene                                                                                       | 4.52   | 1239.7 | 0.04   | 5.56* | 1087.6 | [0.13] |
| <i>trans</i> -Linalool oxide<br>(fur.)                                                            | 7.12   | 1429.0 | 0.04   | 5.56* | 1087.6 | [0.13] |
| <i>para</i> -Cymenene                                                                             | 6.54   | 1387.4 | 0.03   | 5.56* | 1087.6 | [0.13] |
| Rosefuran                                                                                         | 6.27   | 1368.2 | 0.03   | 5.74  | 1098.5 | 0.03   |
| Linalool                                                                                          | 8.31   | 1517.3 | 4.90   | 5.84  | 1105.0 | 4.93   |
| (Z)-6-Methyl-3,5-<br>heptadien-2-one                                                              | 8.49   | 1530.8 | 0.07   | 5.88  | 1107.6 | 0.03   |
| <i>cis</i> -Rose oxide                                                                            | 5.54*  | 1317.0 | [1.06] | 5.95  | 1111.7 | 1.05   |
| Phenylethyl alcohol                                                                               | 12.42* | 1852.2 | [1.07] | 5.99  | 1114.5 | 0.03   |
| <i>trans</i> -Rose oxide                                                                          | 5.72   | 1329.1 | 0.43   | 6.18  | 1126.9 | 0.43   |
| <i>trans</i> -Pinocarveol                                                                         | 9.45*  | 1604.4 | [0.03] | 6.27  | 1132.7 | 0.02   |
| Unknown CYFL IV<br>[m/z 95, 67 (86), 41<br>(68), 82 (64), 123<br>(62)...]                         | 7.88*  | 1484.3 | [0.06] | 6.32  | 1135.7 | 0.05   |
| Unknown COCI VIII<br>[m/z 41, 69 (87), 82<br>(66), 67 (55), 109                                   | 9.70   | 1624.2 | 0.35   | 6.44  | 1143.3 | 0.26   |

| (46)... 142 (18)]                                                                                     |        |        |         |       |        |       |
|-------------------------------------------------------------------------------------------------------|--------|--------|---------|-------|--------|-------|
| Menthone                                                                                              | 6.90   | 1413.2 | 2.21    | 6.56  | 1151.0 | 2.20  |
| Citronellal                                                                                           | 7.27*  | 1439.8 | [5.98]  | 6.63† | 1155.2 | 0.67  |
| Isomenthone                                                                                           | 7.27*  | 1439.8 | [5.98]  | 6.72  | 1161.5 | 5.42  |
| Isoneral                                                                                              | 8.11   | 1501.8 | 0.01    | 6.76  | 1164.0 | 0.02  |
| neo-Menthol                                                                                           | 8.84*  | 1557.4 | [0.07]  | 6.81  | 1167.1 | 0.07  |
| Terpinen-4-ol                                                                                         | 8.84*  | 1557.4 | [0.07]  | 6.92  | 1174.2 | 0.04  |
| Menthol                                                                                               | 9.45*  | 1604.4 | [0.03]  | 6.94  | 1175.5 | 0.03  |
| Isomenthol                                                                                            | 9.22   | 1586.2 | 0.12    | 7.05  | 1182.3 | 0.13  |
| para-Cymen-8-ol                                                                                       | 11.77  | 1795.1 | 0.10    | 7.09  | 1185.2 | 0.03  |
| α-Terpineol                                                                                           | 10.05* | 1652.8 | [1.29]  | 7.17  | 1190.2 | 0.37  |
| Myrtenol                                                                                              | 11.13  | 1741.1 | 0.17    | 7.26  | 1195.6 | 0.04  |
| Unknown MEPI V [m/z 43, 99 (84), 81 (46), 986 (43), 126 (36), 71 (28)... 170 (12)]                    |        |        |         | 7.36  | 1202.0 | 0.01  |
| Unknown DRMO II [m/z 123, 81 (40), 67 (29), 79 (29), 93 (26), 121 (25), 41 (24), 55 (18), 69 (15)...] |        |        |         | 7.43  | 1207.0 | 0.02  |
| Nerol                                                                                                 | 11.39* | 1762.8 | [0.54]  | 7.80  | 1231.4 | 0.55  |
| Citronellol                                                                                           | 11.02* | 1731.9 | [21.79] | 7.91  | 1238.7 | 21.60 |
| Neral                                                                                                 | 9.73*  | 1626.9 | [0.91]  | 7.94  | 1241.0 | 0.58  |
| Piperitone                                                                                            | 10.17* | 1661.9 | [6.13]  | 8.08  | 1250.4 | 0.09  |
| Geraniol                                                                                              | 11.91  | 1807.2 | 13.55   | 8.29  | 1264.2 | 13.71 |
| Geranal                                                                                               | 10.37  | 1678.2 | 0.73    | 8.41  | 1272.2 | 0.80  |
| Citronellyl formate                                                                                   | 9.16   | 1582.3 | 10.29   | 8.54  | 1281.0 | 10.23 |
| Neryl formate                                                                                         | 9.73*  | 1626.9 | [0.91]  | 8.58  | 1283.9 | 0.30  |
| Geranyl formate                                                                                       | 10.17* | 1661.9 | [6.13]  | 8.91  | 1305.9 | 5.84  |
| (3Z)-Hexenyl tiglate                                                                                  | 9.64   | 1620.0 | 0.09    | 9.05  | 1316.1 | 0.03  |
| Methyl geranate                                                                                       | 10.05* | 1652.8 | [1.29]  | 9.21  | 1326.8 | 0.02  |
| α-Cubebene                                                                                            | 7.04*  | 1423.3 | [0.10]  | 9.52  | 1348.8 | 0.09  |
| Phenylethyl propionate                                                                                | 12.10* | 1823.5 | [0.23]  | 9.54  | 1350.7 | 0.06  |
| Citronellyl acetate                                                                                   | 9.73*  | 1626.9 | [0.91]  | 9.63  | 1356.8 | 0.31  |
| Neryl acetate                                                                                         | 10.49* | 1687.7 | [0.47]  | 9.78  | 1367.3 | 0.02  |
| α-Ylangene                                                                                            | 7.30   | 1442.2 | 0.05    | 9.80  | 1369.1 | 0.02  |
| Geranic acid                                                                                          |        |        |         | 9.83  | 1370.7 | 0.05  |
| α-Copaene                                                                                             | 7.41   | 1450.2 | 0.34    | 9.87  | 1373.6 | 0.34  |
| β-Bourbonene                                                                                          | 7.75   | 1474.9 | 1.01    | 9.98  | 1381.5 | 1.01  |
| Geranyl acetate                                                                                       | 10.81  | 1714.1 | 0.41    | 10.05 | 1386.4 | 0.38  |
| β-Elemene                                                                                             | 8.63   | 1541.6 | 0.10    | 10.11 | 1390.8 | 0.13  |
| Phenylethyl isobutyrate                                                                               | 12.04  | 1818.7 | 0.11    | 10.15 | 1393.7 | 0.11  |

|                                                                                              |        |        |         |        |        |        |
|----------------------------------------------------------------------------------------------|--------|--------|---------|--------|--------|--------|
| $\alpha$ -Gurjunene                                                                          | 7.88*  | 1484.3 | [0.06]  | 10.28  | 1402.3 | 0.02   |
| $\beta$ -Caryophyllene                                                                       | 8.69*  | 1546.1 | [1.72]  | 10.44* | 1414.7 | [1.07] |
| $\beta$ -Ylangene                                                                            | 8.40*  | 1524.1 | [0.39]  | 10.44* | 1414.7 | [1.07] |
| $\beta$ -Copaene                                                                             | 8.62   | 1540.3 | 0.07    | 10.58  | 1425.3 | 0.10   |
| Heptyl tiglate                                                                               |        |        |         | 10.68  | 1432.3 | 0.01   |
| $\alpha$ -Guaiene                                                                            | 8.69*  | 1546.1 | [1.72]  | 10.74* | 1436.8 | [0.63] |
| <i>trans</i> - $\alpha$ -Bergamotene                                                         | 8.69*  | 1546.1 | [1.72]  | 10.74* | 1436.8 | [0.63] |
| 6,9-Guaadiene                                                                                | 8.92   | 1563.2 | 6.15    | 10.81  | 1442.1 | 6.19   |
| Unknown BOCA IV<br>[m/z 91, 161 (92), 105<br>(85), 119 (63), 133<br>(53), 79 (49), 204 (46)] | 9.06*  | 1574.4 | [0.37]  | 10.86* | 1446.1 | [0.85] |
| Citronellyl propionate                                                                       | 10.49* | 1687.7 | [0.47]  | 10.86* | 1446.1 | [0.85] |
| $\alpha$ -Humulene                                                                           | 9.56   | 1613.6 | 0.25    | 10.91  | 1449.3 | 0.25   |
| allo-Aromadendrene                                                                           | 9.28   | 1591.1 | 0.25    | 11.00  | 1456.2 | 0.17   |
| <i>trans</i> -Cadina-1(6),4-diene                                                            | 9.52   | 1610.0 | 0.15    | 11.19  | 1470.7 | 0.25   |
| $\gamma$ -Murolene                                                                           | 9.86   | 1637.2 | 0.16    | 11.24  | 1474.3 | 0.10   |
| Germacrene D                                                                                 | 10.05* | 1652.8 | [1.29]  | 11.28* | 1477.1 | [1.78] |
| Geranyl propionate                                                                           | 11.57  | 1777.8 | 0.99    | 11.28* | 1477.1 | [1.78] |
| $\beta$ -Selinene                                                                            | 10.17* | 1661.9 | [6.13]  | 11.34  | 1481.5 | 0.20   |
| Phenylethyl isovalerate                                                                      | 13.38  | 1938.3 | 0.05    | 11.40* | 1486.4 | [0.35] |
| $\gamma$ -Amorphene                                                                          | 10.17* | 1661.9 | [6.13]  | 11.40* | 1486.4 | [0.35] |
| Bicyclogermacrene                                                                            | 10.31* | 1673.4 | [0.15]  | 11.47* | 1491.0 | [0.14] |
| Viridiflorene                                                                                | 9.92   | 1642.5 | 0.08    | 11.47* | 1491.0 | [0.14] |
| 4-epi- <i>cis</i> -Dihydroagarofuran                                                         | 10.22* | 1666.0 | [0.13]  | 11.53  | 1495.9 | 0.09   |
| $\alpha$ -Murolene                                                                           | 10.31* | 1673.4 | [0.15]  | 11.57  | 1498.4 | 0.12   |
| $\delta$ -Amorphene                                                                          | 10.22* | 1666.0 | [0.13]  | 11.64  | 1504.1 | 0.09   |
| $\gamma$ -Cadinene                                                                           | 10.67* | 1702.3 | [0.26]  | 11.70* | 1508.8 | [0.06] |
| Cubebol                                                                                      | 12.81  | 1886.3 | 0.04    | 11.70* | 1508.8 | [0.06] |
| 7-epi- $\alpha$ -Selinene                                                                    | 10.69* | 1704.6 | [0.58]  | 11.73  | 1510.6 | 0.22   |
| Geranyl isobutyrate                                                                          | 11.52  | 1773.6 | 0.46    | 11.79  | 1516.0 | 0.31   |
| <i>trans</i> -Calamenene                                                                     | 11.46  | 1769.0 | 0.03    | 11.85  | 1520.2 | 0.15   |
| Zonarene                                                                                     | 10.67* | 1702.3 | [0.26]  | 11.86* | 1521.5 | [0.64] |
| $\delta$ -Cadinene                                                                           | 10.69* | 1704.6 | [0.58]  | 11.86* | 1521.5 | [0.64] |
| Citronellyl butyrate                                                                         | 11.39* | 1762.8 | [0.54]  | 11.98  | 1530.9 | 0.53   |
| Phenylethyl angelate?                                                                        | 14.51  | 2044.5 | 0.09    | 12.03  | 1534.4 | 0.05   |
| $\alpha$ -Cadinene                                                                           | 11.02* | 1731.9 | [21.79] | 12.06  | 1536.8 | 0.04   |
| $\alpha$ -Agarofuran                                                                         | 12.10* | 1823.5 | [0.23]  | 12.08  | 1538.4 | 0.22   |
| Europelargone isomer                                                                         | 13.05* | 1908.1 | [0.51]  | 12.28  | 1554.2 | 0.12   |
| 1-nor-Bourbonanone                                                                           | 13.70  | 1967.5 | 0.06    | 12.35  | 1560.0 | 0.04   |
| Geranyl butyrate                                                                             | 12.42* | 1852.2 | [1.07]  | 12.39  | 1563.0 | 0.97   |

|                                                                                |        |        |        |        |        |        |
|--------------------------------------------------------------------------------|--------|--------|--------|--------|--------|--------|
| Caryophyllene oxide                                                            | 13.05* | 1908.1 | [0.51] | 12.56* | 1575.8 | [0.30] |
| Caryophyllene oxide isomer                                                     | 12.98  | 1902.1 | 0.01   | 12.56* | 1575.8 | [0.30] |
| Globulol                                                                       | 14.21  | 2015.5 | 0.02   | 12.59  | 1578.4 | 0.05   |
| Europelargone A                                                                | 14.29  | 2023.0 | 0.52   | 12.65* | 1583.2 | [1.01] |
| Phenylethyl tiglate                                                            | 15.30  | 2121.0 | 0.52   | 12.65* | 1583.2 | [1.01] |
| Geranyl 2-methylbutyrate?                                                      | 12.48* | 1857.4 | [0.38] | 12.86  | 1599.6 | 0.01   |
| Geranyl isovalerate                                                            | 12.48* | 1857.4 | [0.38] | 12.92  | 1604.4 | 0.35   |
| 10-epi-γ-Eudesmol                                                              | 14.41  | 2034.8 | 0.05   | 13.00* | 1610.6 | [0.25] |
| 1,10-diepi-Cubenol                                                             | 13.98  | 1993.2 | 0.14   | 13.00* | 1610.6 | [0.25] |
| 1-epi-Cubenol                                                                  | 14.03* | 1998.3 | [0.27] | 13.13  | 1621.5 | 0.02   |
| γ-Eudesmol                                                                     | 15.21  | 2112.6 | 0.02   | 13.19  | 1626.5 | 0.07   |
| Citronellyl valerate?                                                          | 12.56  | 1864.6 | 0.03   | 13.25  | 1631.5 | 0.02   |
| Cubenol                                                                        | 13.96  | 1991.2 | 0.07   | 13.33* | 1638.5 | [0.13] |
| τ-Muurolol                                                                     | 15.36  | 2127.5 | 0.02   | 13.33* | 1638.5 | [0.13] |
| τ-Cadinol                                                                      | 15.16  | 2107.0 | 0.02   | 13.33* | 1638.5 | [0.13] |
| β-Eudesmol                                                                     | 15.69  | 2160.1 | 0.03   | 13.39  | 1643.1 | 0.07   |
| α-Cadinol                                                                      | 15.74  | 2165.3 | 0.06   | 13.46  | 1649.1 | 0.07   |
| cis-Calamenen-10-ol                                                            | 16.71  | 2265.3 | 0.02   | 13.51  | 1652.9 | 0.08   |
| Geranyl valerate                                                               | 13.48  | 1947.5 | 0.06   | 13.58  | 1659.0 | 0.11   |
| Citronellyl tiglate                                                            | 13.63  | 1961.0 | 0.33   | 13.68  | 1667.5 | 0.30   |
| Citronellyl 4-methylvalerate                                                   |        |        |        | 13.92  | 1686.8 | 0.10   |
| 3β,4β-Oxidoagarofuran?                                                         | 16.31  | 2223.6 | 0.03   | 14.03  | 1696.3 | 0.07   |
| Geranyl tiglate                                                                | 14.67  | 2060.1 | 1.30   | 14.11  | 1702.5 | 1.29   |
| Citronellyl caproate                                                           | 13.54  | 1952.6 | 0.04   | 14.30* | 1719.5 | [0.16] |
| Geranyl 4-methylvalerate?                                                      | 14.03* | 1998.3 | [0.27] | 14.30* | 1719.5 | [0.16] |
| Geranyl caproate                                                               | 14.57  | 2050.1 | 0.02   | 14.72  | 1755.9 | 0.06   |
| Citronellyl heptanoate                                                         |        |        |        | 15.44  | 1819.1 | 0.04   |
| Phytone                                                                        | 14.95  | 2086.4 | 0.02   | 15.75  | 1847.1 | 0.03   |
| Geranyl heptanoate                                                             | 15.51  | 2142.2 | 0.05   | 15.82  | 1853.2 | 0.05   |
| Citronellyl caprylate                                                          | 15.58  | 2148.7 | 0.03   | 16.47  | 1913.3 | 0.04   |
| Geranyl caprylate                                                              | 15.95  | 2186.1 | 0.01   | 16.87  | 1951.1 | 0.04   |
| Unknown COCl L [m/z 69, 83 (59), 81 (56), 137 (48), 41 (29), 139 (28)...]      | 21.93  | 2876.5 | 0.42   | 23.78  | 2713.7 | 0.46   |
| Unknown UNKN CCXVIII [m/z 69, 81 (86), 137 (48), 83 (29), 95 (29), 41 (19)...] | 22.87  | 3001.4 | 0.60   | 24.23  | 2772.8 | 0.61   |

|                                                                        |        |        |      |        |        |
|------------------------------------------------------------------------|--------|--------|------|--------|--------|
| Unknown UNKN                                                           |        |        |      |        |        |
| CCXIX [m/z 69, 81<br>(66), 95 (31), 41 (19),<br>137 (19), 153 (16...)] | 23.79  | 3129.4 | 0.23 | 24.67  | 2830.6 |
| Total reported                                                         | 95.58% |        |      | 96.55% |        |
|                                                                        |        |        |      |        |        |

\*: 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