

**Date :** March 24, 2020

**CERTIFICATE OF ANALYSIS – GC PROFILING**

**SAMPLE IDENTIFICATION**

**Internal code :** 20C11-PSC13

**Customer identification :** Ylang ylang - Ghana - 03032020

**Type :** Essential oil

**Source :** *Cananga odorata* var. *genuina* (Ylang-ylang)

**Customer :** Pacha Soap Co.

**ANALYSIS**

**Method:** PC-MAT-007 - Analysis of the composition of an essential oil or other volatile liquide by FAST GC-FID (in French); identifications validated by GC-MS.

**Analyst :** Sylvain Mercier, M. Sc., Chimiste

**Analysis date :** March 23, 2020

Checked and approved by :

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

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#### PHYSICOCHEMICAL DATA

**Physical aspect:** Clear liquid

**Refractive index:**  $1.4894 \pm 0.0003$  (20 °C)

#### 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              | %     | Classe               |
|-----------------------------|-------|----------------------|
| Ethanol                     | 0.01  | Aliphatic alcohol    |
| Ethyl acetate               | 0.01  | Aliphatic ester      |
| Isovaleral                  | tr    | Aliphatic aldehyde   |
| Isobutyl acetate            | tr    | Aliphatic ester      |
| Octane                      | 0.01  | Alkane               |
| Butyl acetate               | 0.01  | Aliphatic ester      |
| Hexanol                     | 0.01  | Aliphatic alcohol    |
| Isoamyl acetate             | 0.02  | Aliphatic ester      |
| 2-Methylbutyl acetate       | 0.01  | Aliphatic ester      |
| 3-Methyl-3-butenyl acetate  | 0.01  | Aliphatic ester      |
| Isobutyl isobutyrate        | 0.01  | Aliphatic ester      |
| Prenyl acetate              | 0.01  | Aliphatic ester      |
| $\alpha$ -Pinene            | 1.38  | Monoterpene          |
| Camphene                    | 0.03  | Monoterpene          |
| Benzaldehyde                | 0.02  | Simple phenolic      |
| $\beta$ -Pinene             | 0.38  | Monoterpene          |
| Sabinene                    | 0.02  | Monoterpene          |
| 6-Methyl-5-hepten-2-one     | 0.03  | Aliphatic ketone     |
| Myrcene                     | 0.32  | Monoterpene          |
| $\alpha$ -Phellandrene      | 0.01  | Monoterpene          |
| (3Z)-Hexenyl acetate        | 0.08  | Aliphatic ester      |
| para-Methylanisole          | 7.13  | Simple phenolic      |
| $\alpha$ -Terpinene         | 0.01  | Monoterpene          |
| Hexyl acetate               | 0.18  | Aliphatic ester      |
| Limonene                    | 0.10  | Monoterpene          |
| $\beta$ -Phellandrene       | tr    | Monoterpene          |
| 1,8-Cineole                 | 0.73  | Monoterpenic ether   |
| Benzyl alcohol              | 0.42  | Simple phenolic      |
| (Z)- $\beta$ -Ocimene       | 0.06  | Monoterpene          |
| (E)- $\beta$ -Ocimene       | 0.06  | Monoterpene          |
| $\gamma$ -Terpinene         | 0.01  | Monoterpene          |
| cis-Sabinene hydrate        | 0.01  | Monoterpenic alcohol |
| cis-Linalool oxide (fur.)   | 0.03  | Monoterpenic alcohol |
| para-Cresol                 | 0.05  | Simple phenolic      |
| Terpinolene                 | 0.15  | Monoterpene          |
| trans-Linalool oxide (fur.) | 0.07  | Monoterpenic alcohol |
| Methyl benzoate             | 4.36  | Phenolic ester       |
| Linalool                    | 18.87 | Monoterpenic alcohol |
| Nonanal                     | 0.04  | Aliphatic aldehyde   |
| Camphor                     | 0.01  | Monoterpenic ketone  |
| ortho-Dimethoxybenzene      | 0.02  | Simple phenolic      |
| Unknown                     | 0.01  | Phenylpropanoid      |
| Benzyl acetate              | 6.30  | Phenolic ester       |
| para-Cresyl acetate         | 0.13  | Phenolic ester       |
| Ethyl benzoate              | tr    | Phenolic ester       |
| Terpinen-4-ol               | 0.02  | Monoterpenic alcohol |
| $\alpha$ -Terpineol         | 0.44  | Monoterpenic alcohol |

|                                     |       |                        |
|-------------------------------------|-------|------------------------|
| Methylchavicol                      | 0.01  | Phenylpropanoid        |
| Nerol                               | 0.06  | Monoterpenic alcohol   |
| Neral                               | 0.04  | Monoterpenic aldehyde  |
| Phenylethyl acetate                 | 0.03  | Phenolic ester         |
| Geraniol                            | 1.08  | Monoterpenic alcohol   |
| Chavicol                            | 0.03  | Phenylpropanoid        |
| Geranial                            | 0.06  | Monoterpenic aldehyde  |
| (E)-Anethole                        | 0.19  | Phenylpropanoid        |
| 1-Nitro-2-phenylethane              | 0.06  | Simple phenolic        |
| (E)-Cinnamyl alcohol                | 0.06  | Phenylpropanoid        |
| Benzyl butyrate                     | 0.02  | Phenolic ester         |
| $\alpha$ -Cubebene                  | 0.12  | Sesquiterpene          |
| Eugenol                             | 0.15  | Phenylpropanoid        |
| $\alpha$ -Ylangene                  | 0.09  | Sesquiterpene          |
| Neryl acetate                       | 0.05  | Monoterpenic ester     |
| $\alpha$ -Copaene                   | 0.71  | Sesquiterpene          |
| $\beta$ -Bourbonene                 | 0.01  | Sesquiterpene          |
| Geranyl acetate                     | 15.21 | Monoterpenic ester     |
| $\beta$ -Cubebene                   | 0.11  | Sesquiterpene          |
| $\beta$ -Elemene                    | 0.30  | Sesquiterpene          |
| Cyperene                            | 0.03  | Sesquiterpene          |
| Sibirene                            | 0.01  | Sesquiterpene          |
| $\beta$ -Caryophyllene              | 3.04  | Sesquiterpene          |
| $\beta$ -Copaene                    | 0.19  | Sesquiterpene          |
| Caryophylla-4(12),8(13)-diene       | 0.02  | Sesquiterpene          |
| Aromadendrene                       | 0.05  | Sesquiterpene          |
| (E)-Cinnamyl acetate                | 1.72  | Phenylpropanoid ester  |
| (E)-Isoeugenol                      | 0.46  | Phenylpropanoid        |
| $\alpha$ -Humulene                  | 0.95  | Sesquiterpene          |
| <i>cis</i> -Cadina-1(6),4-diene     | 0.06  | Sesquiterpene          |
| <i>cis</i> -Muurolo-4(15),5-diene   | 0.09  | Sesquiterpene          |
| <i>trans</i> -Cadina-1(6),4-diene   | 0.10  | Sesquiterpene          |
| Germacrene D                        | 7.38  | Sesquiterpene          |
| $\gamma$ -Muurolo-4(15),5-diene     | 0.13  | Sesquiterpene          |
| <i>trans</i> -Muurolo-4(15),5-diene | 0.13  | Sesquiterpene          |
| Prenyl benzoate                     | 0.02  | Phenolic ester         |
| epi-Cubebol                         | 0.02  | Sesquiterpenic alcohol |
| Bicyclogermacrene                   | 0.48  | Sesquiterpene          |
| $\alpha$ -Muurolo-4(15),5-diene     | 0.04  | Sesquiterpene          |
| Unknown                             | 0.44  | Sesquiterpene          |
| $\delta$ -Amorphene                 | 0.17  | Sesquiterpene          |
| $\gamma$ -Cadinene                  | 0.38  | Sesquiterpene          |
| Cubebol                             | 0.02  | Sesquiterpenic alcohol |
| (3E,6E)- $\alpha$ -Farnesene        | 14.18 | Sesquiterpene          |
| (Z)- $\gamma$ -Bisabolene           | 0.21  | Sesquiterpene          |
| Zonarene                            | 0.07  | Sesquiterpene          |
| $\delta$ -Cadinene                  | 1.33  | Sesquiterpene          |
| <i>trans</i> -Cadina-1,4-diene      | 0.10  | Sesquiterpene          |
| $\alpha$ -Cadinene                  | 0.15  | Sesquiterpene          |
| <i>cis</i> -Dracunculifolol         | 0.01  | Sesquiterpenic alcohol |
| Isocaryophyllene epoxide B          | 0.02  | Sesquiterpenic ether   |
| Germacrene B                        | 0.05  | Sesquiterpene          |

|                           |               |                          |
|---------------------------|---------------|--------------------------|
| (E)-Nerolidol             | 0.02          | Sesquiterpenic alcohol   |
| β-Calacorene              | 0.01          | Sesquiterpene            |
| (3Z)-Hexenyl benzoate     | 0.02          | Phenolic ester           |
| Spathulenol               | 0.01          | Sesquiterpenic alcohol   |
| Caryophyllene oxide       | 0.04          | Sesquiterpenic ether     |
| Unknown                   | 0.02          | Sesquiterpenic alcohol   |
| Unknown                   | 0.02          | Oxygenated sesquiterpene |
| Viridiflorol              | 0.02          | Sesquiterpenic alcohol   |
| Guaial                    | 0.10          | Sesquiterpenic alcohol   |
| Humulene epoxide II       | 0.01          | Sesquiterpenic ether     |
| 10-epi-Cubenol            | 0.02          | Sesquiterpenic alcohol   |
| (E)-Isoeugenyl acetate    | 0.02          | Phenylpropanoid ester    |
| Junenol                   | 0.07          | Sesquiterpenic alcohol   |
| 1-epi-Cubenol             | 0.07          | Sesquiterpenic alcohol   |
| τ-Muurolol                | 0.21          | Sesquiterpenic alcohol   |
| Cubenol                   | 0.05          | Sesquiterpenic alcohol   |
| τ-Cadinol                 | 0.05          | Sesquiterpenic alcohol   |
| α-Muurolol                | 0.12          | Sesquiterpenic alcohol   |
| Unknown                   | 0.10          | Sesquiterpenic alcohol   |
| α-Cadinol                 | 0.37          | Sesquiterpenic alcohol   |
| Bulnesol                  | 0.05          | Sesquiterpenic alcohol   |
| Unknown                   | 0.04          | Oxygenated sesquiterpene |
| (2E,6Z)-Farnesol          | 0.01          | Sesquiterpenic alcohol   |
| (2E,6E)-Farnesol          | 0.23          | Sesquiterpenic alcohol   |
| (2E,6E)-Farnesal          | 0.01          | Sesquiterpenic aldehyde  |
| Benzyl benzoate           | 2.18          | Phenolic ester           |
| (2E,6E)-Farnesyl acetate  | 0.47          | Sesquiterpenic ester     |
| Benzyl salicylate         | 1.28          | Phenolic ester           |
| Geranyl benzoate          | 0.01          | Phenolic ester           |
| Unknown                   | 0.03          | Unknown                  |
| Unknown                   | 0.01          | Unknown                  |
| <b>Consolidated total</b> | <b>98.60%</b> |                          |

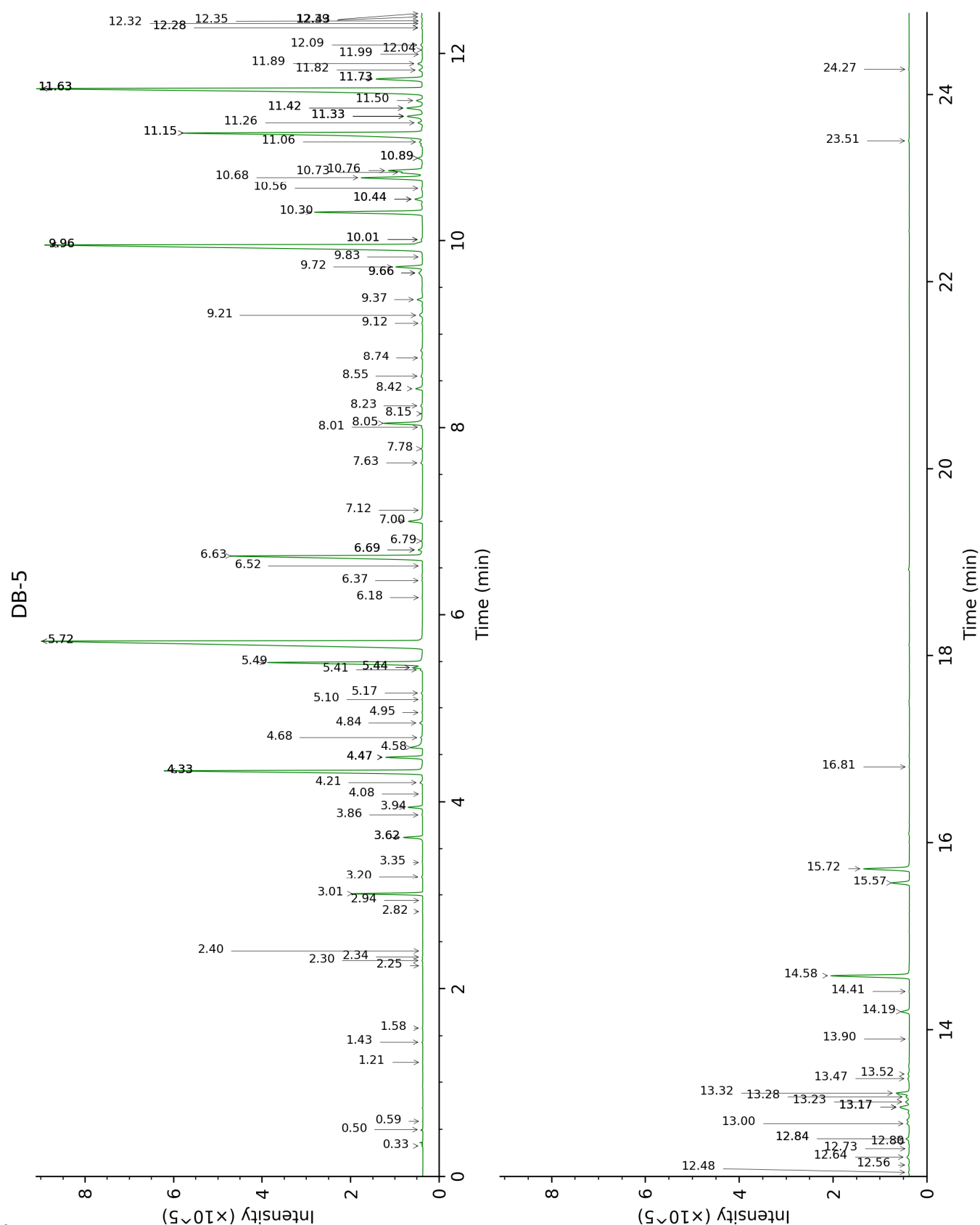
tr: The compound has been detected below 0.005% of total signal.

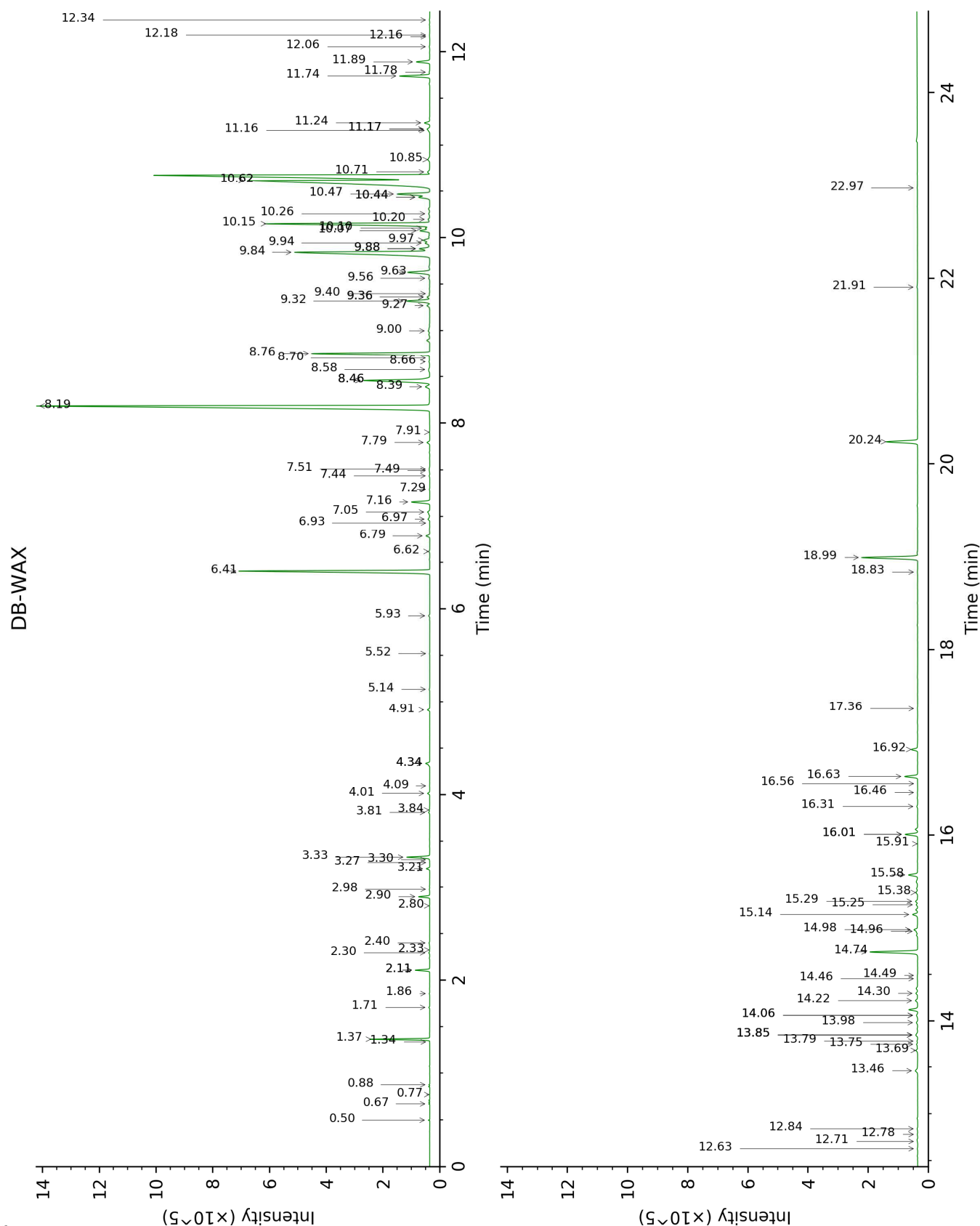
Note: no correction factor was applied

**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.

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





# FULL ANALYSIS DATA

| Identification              | Column DB-5 |      |         | Column DB-WAX |      |        |
|-----------------------------|-------------|------|---------|---------------|------|--------|
|                             | R.T         | R.I  | %       | R.T           | R.I  | %      |
| Ethanol                     | 0.33        | 522  | 0.01    | 0.88          | 911  | 0.01   |
| Ethyl acetate               | 0.50        | 592  | 0.01    | 0.67          | 856  | 0.01   |
| Isovaleral                  | 0.59        | 640  | tr      | 0.77          | 893  | tr     |
| Isobutyl acetate            | 1.21        | 774  | tr      | 1.34          | 988  | tr     |
| Octane                      | 1.43        | 805  | 0.01    | 0.50          | 786  | 0.02   |
| Butyl acetate               | 1.58        | 818  | 0.01    | 1.86          | 1042 | 0.01   |
| Hexanol                     | 2.25        | 873  | 0.01    | 5.52          | 1326 | 0.01   |
| Isoamyl acetate             | 2.30        | 878  | 0.02    | 2.40          | 1095 | 0.02   |
| 2-Methylbutyl acetate       | 2.34        | 881  | 0.01    | 2.33          | 1088 | tr     |
| 3-Methyl-3-butenyl acetate  | 2.40        | 886  | 0.01    | 3.30          | 1165 | 0.01   |
| Isobutyl isobutyrate        | 2.82        | 917  | 0.01    | 2.11*         | 1067 | 0.39   |
| Prenyl acetate              | 2.94        | 925  | 0.01    | 4.09          | 1224 | 0.01   |
| $\alpha$ -Pinene            | 3.01        | 930  | 1.38    | 1.37          | 993  | 1.36   |
| Camphene                    | 3.20        | 942  | 0.03    | 1.71          | 1027 | 0.02   |
| Benzaldehyde                | 3.35        | 952  | 0.02    | 7.44          | 1465 | 0.02   |
| $\beta$ -Pinene             | 3.62*       | 970  | 0.44    | 2.11*         | 1067 | [0.39] |
| Sabinene                    | 3.62*       | 970  | [0.44]  | 2.30          | 1085 | 0.02   |
| 6-Methyl-5-hepten-2-one     | 3.86        | 986  | 0.03    | 5.14          | 1298 | 0.02   |
| Myrcene                     | 3.94        | 991  | 0.32    | 2.90          | 1134 | 0.32   |
| $\alpha$ -Phellandrene      | 4.08        | 1001 | 0.01    | 2.80          | 1126 | 0.01   |
| (3Z)-Hexenyl acetate        | 4.20        | 1008 | 0.08    | 4.91          | 1282 | 0.08   |
| para-Methylanisole          | 4.33*       | 1016 | 7.32    | 6.41          | 1389 | 7.13   |
| $\alpha$ -Terpinene         | 4.33*       | 1016 | [7.32]  | 2.98          | 1140 | 0.01   |
| Hexyl acetate               | 4.33*       | 1016 | [7.32]  | 4.34*†        | 1241 | 0.17   |
| Limonene                    | 4.48*       | 1026 | 0.85    | 3.21          | 1158 | 0.10   |
| $\beta$ -Phellandrene       | 4.48*       | 1026 | [0.85]  | 3.27          | 1162 | tr     |
| 1,8-Cineole                 | 4.48*       | 1026 | [0.85]  | 3.33          | 1167 | 0.73   |
| Benzyl alcohol              | 4.58        | 1032 | 0.42    | 11.89         | 1824 | 0.49   |
| (Z)- $\beta$ -Ocimene       | 4.68        | 1039 | 0.06    | 3.81          | 1203 | 0.04   |
| (E)- $\beta$ -Ocimene       | 4.84        | 1049 | 0.06    | 4.01          | 1218 | 0.07   |
| $\gamma$ -Terpinene         | 4.95        | 1056 | 0.01    | 3.84          | 1205 | 0.02   |
| cis-Sabinene hydrate        | 5.10        | 1065 | 0.01    | 6.93          | 1428 | 0.01   |
| cis-Linalool oxide (fur.)   | 5.17        | 1069 | 0.03    | 6.62          | 1405 | 0.03   |
| para-Cresol                 | 5.41        | 1085 | 0.05    | 13.98         | 2015 | 0.06   |
| Terpinolene                 | 5.44*       | 1087 | 0.21    | 4.34*†        | 1241 | [0.17] |
| trans-Linalool oxide (fur.) | 5.44*       | 1087 | [0.21]  | 6.97          | 1431 | 0.07   |
| Methyl benzoate             | 5.49        | 1090 | 4.36    | 8.76          | 1566 | 4.31   |
| Linalool                    | 5.72*       | 1104 | 18.96   | 8.19          | 1522 | 18.87  |
| Nonanal                     | 5.72*       | 1104 | [18.96] | 5.93          | 1355 | 0.04   |
| Camphor                     | 6.18        | 1135 | 0.01    | 7.29          | 1454 | 0.02   |

|                                                         |        |      |         |         |      |        |
|---------------------------------------------------------|--------|------|---------|---------|------|--------|
| ortho-Dimethoxybenzene                                  | 6.36   | 1147 | 0.02    |         |      |        |
| Unknown [m/z 133, 77 (86), 105 (75), 79 (68), 134 (48)] | 6.52   | 1157 | 0.01    | 12.78   | 1903 | 0.02   |
| Benzyl acetate                                          | 6.63   | 1164 | 6.30    | 10.15   | 1677 | 6.32   |
| para-Cresyl acetate                                     | 6.69*  | 1168 | 0.13    |         |      |        |
| Ethyl benzoate                                          | 6.69*  | 1168 | [0.13]  | 9.36*   | 1613 | 0.09   |
| Terpinen-4-ol                                           | 6.79   | 1174 | 0.02    | 8.66    | 1558 | 0.03   |
| $\alpha$ -Terpineol                                     | 7.00   | 1189 | 0.44    | 9.88*†  | 1655 | [7.96] |
| Methylchavicol                                          | 7.12   | 1196 | 0.01    | 9.40    | 1616 | 0.02   |
| Nerol                                                   | 7.63   | 1231 | 0.06    | 11.16†  | 1761 | 0.15   |
| Neral                                                   | 7.78   | 1241 | 0.04    | 9.56    | 1630 | 0.05   |
| Phenylethyl acetate                                     | 8.01   | 1257 | 0.03    | 11.17*† | 1762 | [0.15] |
| Geraniol                                                | 8.05   | 1260 | 1.08    | 11.74   | 1811 | 1.06   |
| Chavicol                                                | 8.15   | 1267 | 0.03    | 16.56   | 2271 | 0.01   |
| Geranial                                                | 8.23   | 1273 | 0.06    | 10.20   | 1680 | 0.08   |
| (E)-Anethole                                            | 8.42   | 1286 | 0.19    | 11.24   | 1768 | 0.20   |
| 1-Nitro-2-phenylethane                                  | 8.55   | 1295 | 0.06    | 14.30   | 2045 | 0.08   |
| (E)-Cinnamyl alcohol                                    | 8.74   | 1309 | 0.06    | 16.01*  | 2215 | 0.47   |
| Benzyl butyrate                                         | 9.12   | 1336 | 0.02    | 11.78   | 1815 | 0.02   |
| $\alpha$ -Cubebene                                      | 9.21   | 1343 | 0.12    | 6.79    | 1417 | 0.14   |
| Eugenol                                                 | 9.37   | 1355 | 0.15    | 14.98   | 2111 | 0.15   |
| $\alpha$ -Ylangene                                      | 9.66*  | 1368 | 0.20    | 7.05    | 1436 | 0.09   |
| Neryl acetate                                           | 9.66*  | 1368 | [0.20]  | 10.26   | 1685 | 0.05   |
| $\alpha$ -Copaene                                       | 9.72   | 1372 | 0.71    | 7.16    | 1444 | 0.69   |
| $\beta$ -Bourbonene                                     | 9.83   | 1380 | 0.01    | 7.49    | 1469 | 0.02   |
| Geranyl acetate                                         | 9.96*  | 1389 | 15.62   | 10.62*† | 1715 | 29.39  |
| $\beta$ -Cubebene                                       | 9.96*  | 1389 | [15.62] | 7.80    | 1492 | 0.11   |
| $\beta$ -Elemene                                        | 9.96*  | 1389 | [15.62] | 8.46*   | 1543 | 3.03   |
| Cyperene                                                | 10.01* | 1393 | 0.04    | 7.51    | 1470 | 0.03   |
| Sibirene                                                | 10.01* | 1393 | [0.04]  | 7.90    | 1500 | 0.01   |
| $\beta$ -Caryophyllene                                  | 10.30  | 1414 | 3.04    | 8.46*   | 1543 | [3.03] |
| $\beta$ -Copaene                                        | 10.44* | 1424 | 0.21    | 8.39    | 1538 | 0.19   |
| Caryophylla-4(12),8(13)-diene                           | 10.44* | 1424 | [0.21]  | 8.70    | 1562 | 0.02   |
| Aromadendrene                                           | 10.56  | 1433 | 0.05    | 8.58    | 1552 | 0.04   |
| (E)-Cinnamyl acetate                                    | 10.68  | 1442 | 1.72    | 14.74   | 2087 | 1.78   |
| (E)-Isoeugenol                                          | 10.74  | 1446 | 0.46    | 16.63   | 2279 | 0.47   |
| $\alpha$ -Humulene                                      | 10.76  | 1447 | 0.95    | 9.32    | 1610 | 0.93   |
| cis-Cadina-1(6),4-diene                                 | 10.89* | 1457 | 0.15    | 9.00    | 1584 | 0.06   |
| cis-Murola-4(15),5-diene                                | 10.89* | 1457 | [0.15]  | 9.36*   | 1613 | [0.09] |
| trans-Cadina-1(6),4-diene                               | 11.06  | 1470 | 0.10    | 9.27    | 1606 | 0.12   |
| Germacrene D                                            | 11.16* | 1477 | 8.63    | 9.84†   | 1652 | 7.96   |
| $\gamma$ -Murolene                                      | 11.16* | 1477 | [8.63]  | 9.63    | 1635 | 0.94   |

|                                                                                                |        |      |         |         |      |         |
|------------------------------------------------------------------------------------------------|--------|------|---------|---------|------|---------|
| <i>trans</i> -Muurolo-4(15),5-diene                                                            | 11.26  | 1485 | 0.13    | 9.88*†  | 1655 | [7.96]  |
| Prenyl benzoate                                                                                | 11.33* | 1490 | 0.52    | 13.85*  | 2002 | 0.11    |
| epi-Cubebol                                                                                    | 11.33* | 1490 | [0.52]  | 12.06   | 1839 | 0.02    |
| Bicyclogermacrene                                                                              | 11.33* | 1490 | [0.52]  | 10.08†  | 1671 | 0.52    |
| α-Muurolene                                                                                    | 11.42* | 1497 | 0.49    | 10.10†  | 1673 | [0.52]  |
| Unknown [m/z 119, 41 (95), 123 (53), 80 (49), 161 (44), 105 (42)... 204 (2)]                   | 11.42* | 1497 | [0.49]  |         |      |         |
| δ-Amorphene                                                                                    | 11.50  | 1503 | 0.17    | 9.97    | 1662 | 0.29    |
| γ-Cadinene                                                                                     | 11.63* | 1513 | 14.79   | 10.44*  | 1700 | 0.45    |
| Cubebol                                                                                        | 11.63* | 1513 | [14.79] | 12.63   | 1889 | 0.02    |
| (3E,6E)-α-Farnesene                                                                            | 11.63* | 1513 | [14.79] | 10.62*† | 1715 | [29.39] |
| (Z)-γ-Bisabolene                                                                               | 11.63* | 1513 | [14.79] | 9.94    | 1660 | 0.21    |
| Zonarene                                                                                       | 11.73* | 1521 | 1.40    | 10.44*  | 1700 | [0.45]  |
| δ-Cadinene                                                                                     | 11.73* | 1521 | [1.40]  | 10.47   | 1703 | 1.33    |
| <i>trans</i> -Cadina-1,4-diene                                                                 | 11.82  | 1528 | 0.10    | 10.71   | 1724 | 0.11    |
| α-Cadinene                                                                                     | 11.89  | 1534 | 0.15    | 10.84   | 1735 | 0.12    |
| <i>cis</i> -Dracunculifolol                                                                    | 11.99  | 1541 | 0.01    | 12.16   | 1848 | 0.01    |
| Isocaryophyllene epoxide B                                                                     | 12.04  | 1545 | 0.02    | 12.18   | 1850 | 0.01    |
| Germacrene B                                                                                   | 12.09  | 1549 | 0.05    | 11.17*† | 1762 | [0.15]  |
| (E)-Nerolidol                                                                                  | 12.28* | 1564 | 0.03    | 13.85*  | 2002 | [0.11]  |
| β-Calacorene                                                                                   | 12.28* | 1564 | [0.03]  | 12.71   | 1896 | 0.01    |
| (3Z)-Hexenyl benzoate                                                                          | 12.32  | 1567 | 0.02    | 14.46   | 2060 | 0.03    |
| Spathulenol                                                                                    | 12.35  | 1570 | 0.01    | 14.49   | 2063 | 0.01    |
| Caryophyllene oxide                                                                            | 12.39  | 1573 | 0.04    | 12.84   | 1909 | 0.03    |
| Unknown cadinol or muurolo analog [m/z 161, 119 (77), 120 (76), 105 (73), 93 (57)... 204 (36)] | 12.43  | 1576 | 0.02    | 12.34   | 1864 | 0.02    |
| Unknown [m/z 161, 105 (84), 43 (80), 119 (72), 93 (62), 121 (54)... 204 (38), 222 (2)]         | 12.48  | 1580 | 0.02    | 14.06*  | 2022 | 0.07    |
| Viridiflorol                                                                                   | 12.56  | 1586 | 0.02    | 14.06*  | 2022 | [0.07]  |
| Guaiol                                                                                         | 12.64  | 1593 | 0.10    | 14.22   | 2037 | 0.11    |
| Humulene epoxide II                                                                            | 12.73  | 1600 | 0.01    | 13.46   | 1966 | 0.15    |
| 10-epi-Cubenol                                                                                 | 12.80  | 1605 | 0.02    | 13.78   | 1996 | 0.03    |
| (E)-Isoeugenyl acetate                                                                         | 12.84* | 1608 | 0.11    | 17.36   | 2357 | 0.02    |
| Junenol                                                                                        | 12.84* | 1608 | [0.11]  | 13.68   | 1986 | 0.07    |
| 1-epi-Cubenol                                                                                  | 13.00  | 1621 | 0.07    | 13.85*  | 2002 | [0.11]  |
| τ-Muurolo                                                                                      | 13.17* | 1636 | 0.34    | 15.14   | 2127 | 0.21    |
| Cubenol                                                                                        | 13.17* | 1636 | [0.34]  | 13.75   | 1992 | 0.05    |

|                                                                                                         |        |               |        |        |               |        |
|---------------------------------------------------------------------------------------------------------|--------|---------------|--------|--------|---------------|--------|
| τ-Cadinol                                                                                               | 13.17* | 1636          | [0.34] | 14.96  | 2109          | 0.05   |
| α-Muurolol                                                                                              | 13.23  | 1640          | 0.12   | 15.28  | 2141          | 0.10   |
| Unknown cadinol analog II [m/z 95, 121 (73), 43 (57), 79 (43), 161 (43), 109 (40)... 204 (35), 222 (2)] | 13.28  | 1645          | 0.10   | 15.25  | 2138          | 0.06   |
| α-Cadinol                                                                                               | 13.32  | 1648          | 0.37   | 15.58  | 2170          | 0.36   |
| Bulnesol                                                                                                | 13.48  | 1661          | 0.05   | 15.38  | 2151          | 0.09   |
| Unknown [m/z 123, 95 (31), 81 (29), 105 (27)... 222 (5)]                                                | 13.52  | 1665          | 0.04   | 16.31  | 2246          | 0.04   |
| (2E,6Z)-Farnesol                                                                                        | 13.90  | 1696          | 0.01   | 16.46  | 2261          | 0.01   |
| (2E,6E)-Farnesol                                                                                        | 14.19  | 1721          | 0.23   | 16.92  | 2310          | 0.23   |
| (2E,6E)-Farnesal                                                                                        | 14.41  | 1740          | 0.01   | 15.91  | 2204          | 0.01   |
| Benzyl benzoate                                                                                         | 14.58  | 1754          | 2.18   | 18.99  | 2540          | 2.17   |
| (2E,6E)-Farnesyl acetate                                                                                | 15.57  | 1842          | 0.47   | 16.01* | 2215          | [0.47] |
| Benzyl salicylate                                                                                       | 15.72  | 1856          | 1.28   | 20.24  | 2687          | 1.25   |
| Geranyl benzoate                                                                                        | 16.81  | 1958          | 0.01   | 18.83  | 2522          | 0.02   |
| Unknown [m/z 69, 83 (59), 81 (56), 137 (48), 41 (29), 139 (28)...]                                      | 23.51  | 2702          | 0.03   | 21.91  | 2897          | 0.04   |
| Unknown [m/z 69, 81 (42), 147 (26), 119 (25), 93 (25), 41 (24)...]                                      | 24.27  | 2802          | 0.01   | 22.97  | 3038          | 0.01   |
| <b>Total identified</b>                                                                                 |        | <b>98.89%</b> |        |        | <b>97.56%</b> |        |
| <b>Total reported</b>                                                                                   |        | <b>99.12%</b> |        |        | <b>97.75%</b> |        |

\*: 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.

Note: no correction factor was applied  
R.T.: Retention time (minutes)  
R.I.: Retention index