

Date : 2023-12-08

CERTIFICATE OF ANALYSIS - GC PROFILING

SAMPLE IDENTIFICATION

**Internal code :** 23L01-PTH01

**Customer Identification :** Organic Helichrysum Italicum - France - H90112R

**Type :** Essential Oil

**Source :** *Helichrysum italicum*

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

**Date :** 2023-12-08

## PHYSICOCHEMICAL DATA

**Refractive index :**  $1.4784 \pm 0.0003$  (20 °C)

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

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

**Date :** 2023-12-01

## 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              |
|---------------------------------------|-------|--------------------|
| Isovaleral                            | tr    | Aliphatic aldehyde |
| 2-Methylbutyral                       | 0.02  | Aliphatic aldehyde |
| 3-Pentanone                           | 0.03  | Aliphatic ketone   |
| 2-Ethylfuran                          | 0.01  | Furan              |
| 2-Methylbutanol                       | 0.01  | Aliphatic alcohol  |
| 2-Methyl-3-pentanone                  | 0.07  | Aliphatic ketone   |
| Unknown                               | 0.01  | Unknown            |
| Unknown                               | 0.03  | Unknown            |
| Hexanal                               | 0.01  | Aliphatic aldehyde |
| Octane                                | 0.02  | Alkane             |
| 2-Methyl-2-heptene                    | 0.13  | Alkene             |
| 4-Methyl-3-hexanone                   | 0.14  | Aliphatic ketone   |
| (3Z)-Hexenol                          | tr    | Aliphatic alcohol  |
| Furfuryl alcohol                      | 0.01  | Furan              |
| Hexanol                               | 0.01  | Aliphatic alcohol  |
| Isoamyl acetate                       | 0.01  | Aliphatic ester    |
| Nonane                                | 0.03  | Alkane             |
| Bornylene                             | 0.04  | Monoterpene        |
| Isobutyl isobutyrate                  | 0.01  | Aliphatic ester    |
| $\alpha$ -Thujene                     | 0.01  | Monoterpene        |
| $\alpha$ -Pinene                      | 14.18 | Monoterpene        |
| $\alpha$ -Fenchene                    | 0.47  | Monoterpene        |
| Camphene                              | 0.18  | Monoterpene        |
| Thuja-2,4(10)-diene                   | 0.01  | Monoterpene        |
| Sabinene                              | tr    | Monoterpene        |
| $\beta$ -Pinene                       | 0.62  | Monoterpene        |
| 6-Methyl-5-hepten-2-one               | 0.02  | Aliphatic ketone   |
| <i>trans</i> -Dehydroxylinalool oxide | 0.04  | Monoterpenic ether |
| Myrcene                               | 0.07  | Monoterpene        |
| 6-Methyl-5-hepten-2-ol                | 0.01  | Aliphatic alcohol  |
| Unknown                               | 0.03  | Monoterpene        |
| $\alpha$ -Phellandrene                | 0.03  | Monoterpene        |
| Isobutyl 2-methylbutyrate             | 0.03  | Aliphatic ester    |
| $\Delta^3$ -Carene                    | tr    | Monoterpene        |
| Isobutyl isovalerate                  | 0.02  | Aliphatic ester    |
| (3Z)-Hexenyl acetate                  | 0.02  | Aliphatic ester    |
| $\alpha$ -Terpinene                   | 0.21  | Monoterpene        |
| <i>para</i> -Methylanisole            | 0.02  | Simple phenolic    |
| <i>para</i> -Cymene                   | 0.21  | Monoterpene        |
| 1,8-Cineole                           | 0.26  | Monoterpenic ether |

|  |      |                       |
|--|------|-----------------------|
| Limonene                               | 3.45 | Monoterpene           |
| (Z)- $\beta$ -Ocimene                  | 0.01 | Monoterpene           |
| (E)- $\beta$ -Ocimene                  | 0.05 | Monoterpene           |
| Isobutyl angelate                      | 0.18 | Aliphatic ester       |
| $\gamma$ -Terpinene                    | 0.56 | Monoterpene           |
| Terpinolene                            | 0.19 | Monoterpene           |
| <i>para</i> -Cymenene                  | 0.01 | Monoterpene           |
| 2-Nonanone                             | 0.03 | Aliphatic ketone      |
| 2,4-Dimethylheptane-3,5-dione          | 0.07 | $\beta$ -Diketone     |
| Linalool                               | 1.07 | Monoterpenic alcohol  |
| 2-Methylbutyl 2-methylbutyrate         | 0.05 | Aliphatic ester       |
| Isoamyl isovalerate                    | 0.01 | Aliphatic ester       |
| Nonanal                                | 0.07 | Aliphatic aldehyde    |
| endo-Fenchol                           | 0.06 | Monoterpenic alcohol  |
| $\alpha$ -Campholenal                  | 0.02 | Monoterpenic aldehyde |
| <i>trans</i> -Pinocarveol              | 0.05 | Monoterpenic alcohol  |
| <i>trans</i> -Verbenol                 | 0.02 | Monoterpenic alcohol  |
| <i>para</i> -Vinylanisole              | 0.05 | Simple phenolic       |
| Isoamyl angelate                       | 0.03 | Aliphatic ester       |
| Nerol oxide                            | 0.09 | Aliphatic ether       |
| 2-Methylbutyl angelate                 | 0.41 | Aliphatic ester       |
| Pinocarvone                            | 0.05 | Monoterpenic ketone   |
| Borneol                                | 0.05 | Monoterpenic alcohol  |
| Unknown                                | 0.01 | Aliphatic ester       |
| Terpinen-4-ol                          | 0.30 | Monoterpenic alcohol  |
| 4,6-Dimethyloctane-3,5-dione epimer I  | 0.16 | $\beta$ -Diketone     |
| 4,6-Dimethyloctane-3,5-dione epimer II | 0.18 | $\beta$ -Diketone     |
| $\alpha$ -Terpineol                    | 0.33 | Monoterpenic alcohol  |
| Myrtenol                               | 0.01 | Monoterpenic alcohol  |
| 2-Methylbutyl tiglate                  | 0.01 | Aliphatic ester       |
| Verbenone                              | tr   | Monoterpenic ketone   |
| Unknown                                | 0.02 | Unknown               |
| Decanal                                | 0.07 | Aliphatic aldehyde    |
| Nerol                                  | 1.59 | Monoterpenic alcohol  |
| Hexyl 2-methylbutyrate                 | 0.02 | Aliphatic ester       |
| Hexyl isovalerate                      | 0.01 | Aliphatic ester       |
| 3-Methylpentyl angelate                | 0.01 | Aliphatic ester       |
| Unknown                                | 0.05 | Aliphatic ester       |
| Linalyl acetate                        | 0.01 | Monoterpenic ester    |
| (3Z)-Hexenyl angelate                  | 0.04 | Aliphatic ester       |
| Hexyl angelate                         | 0.09 | Aliphatic ester       |
| 2-Undecanone                           | 0.02 | Aliphatic ketone      |
| Tridecane                              | 0.08 | Alkane                |
| Hexyl tiglate                          | 0.01 | Aliphatic ester       |
| Bicycloelemene                         | 0.01 | Sesquiterpene         |

|   |       |                      |
|---|-------|----------------------|
| $\alpha$ -Terpinyl acetate                                      | 0.03  | Monoterpenic ester   |
| Cyclosativene I   | 0.03  | Sesquiterpene        |
| Cyclosativene II  | 0.16  | Sesquiterpene        |
| Neryl acetate   | 16.67 | Monoterpenic ester   |
| $\alpha$ -Ylangene  | 0.10  | Sesquiterpene        |
| $\alpha$ -Copaene   | 0.85  | Sesquiterpene        |
| Italicene isomer  | 0.57  | Sesquiterpene        |
| Geranyl acetate   | 0.05  | Monoterpenic ester   |
| Sativene  | 0.01  | Sesquiterpene        |
| Hexyl hexanoate   | 0.03  | Aliphatic ester      |
| Isoitalicene  | 0.11  | Sesquiterpene        |
| Italicene   | 2.13  | Sesquiterpene        |
| Isocaryophyllene  | 0.08  | Sesquiterpene        |
| $\alpha$ -Gurjunene   | 0.05  | Sesquiterpene        |
| $\alpha$ -Cedrene   | 0.04  | Sesquiterpene        |
| <i>cis</i> - $\alpha$ -Bergamotene                              | 0.96  | Sesquiterpene        |
| $\beta$ -Caryophyllene  | 4.36  | Sesquiterpene        |
| $\beta$ -Copaene  | 0.04  | Sesquiterpene        |
| <i>trans</i> - $\alpha$ -Bergamotene                            | 0.94  | Sesquiterpene        |
| Italidione I (4,6,9-Trimethyldec-8-ene-3,5-dione)               | 1.97  | $\beta$ -Diketone    |
| Unknown   | 0.04  | Sesquiterpene        |
| Cadina-4,11-diene   | 0.05  | Sesquiterpene        |
| $\alpha$ -Humulene  | 0.20  | Sesquiterpene        |
| $\alpha$ -Acoradiene  | 0.27  | Sesquiterpene        |
| Neryl propionate  | 2.11  | Monoterpenic ester   |
| ( <i>E</i> )- $\beta$ -Farnesene                                | 0.40  | Sesquiterpene        |
| 4,5-diepi-Aristolochene   | 0.29  | Sesquiterpene        |
| Unknown   | 0.23  | Sesquiterpene        |
| Selina-4,11-diene   | 2.40  | Sesquiterpene        |
| $\alpha$ -Amorphene   | 0.16  | Sesquiterpene        |
| <i>trans</i> -Cadina-1(6),4-diene                               | 0.07  | Sesquiterpene        |
| $\gamma$ -Curcumene   | 9.67  | Sesquiterpene        |
| $\beta$ -Selinene   | 8.95  | Sesquiterpene        |
| Italidione II isomer I (2,4,6,9-Tetramethyldec-8-ene-3,5-dione) | 1.70  | $\beta$ -Diketone    |
| <i>ar</i> -Curcumene  | 1.73  | Sesquiterpene        |
| Valencene   | 0.23  | Sesquiterpene        |
| $\alpha$ -Selinene  | 6.16  | Sesquiterpene        |
| Italidione II isomer II (5,7,10-Trimethylundec-9-ene-4,6-dione) | 1.49  | $\beta$ -Diketone    |
| Italidione II analog  | 0.56  | $\beta$ -Diketone    |
| $\delta$ -Amorphene   | 0.35  | Sesquiterpene        |
| $\beta$ -Bisabolene   | 0.10  | Sesquiterpene        |
| 10-epi-Italicene ether  | 0.06  | Sesquiterpenic ether |

|   |      |                          |
|---|------|--------------------------|
| 7-epi- $\alpha$ -Selinene                     | 0.15 | Sesquiterpene            |
| $\beta$ -Curcumene                            | 0.40 | Sesquiterpene            |
| $\gamma$ -Cadinene                            | 0.17 | Sesquiterpene            |
| Sesquicineole                                 | 0.02 | Sesquiterpenic ether     |
| <i>trans</i> -Calamenene                      | 0.04 | Sesquiterpene            |
| $\delta$ -Cadinene                            | 0.41 | Sesquiterpene            |
| <i>trans</i> -Cadina-1,4-diene                | 0.09 | Sesquiterpene            |
| Italicene ether                               | 0.09 | Sesquiterpenic ether     |
| ( <i>E</i> )- $\gamma$ -Bisabolene            | 0.07 | Sesquiterpene            |
| $\alpha$ -Cadinene                            | 0.04 | Sesquiterpene            |
| Selina-3,7(11)-diene                          | 0.05 | Sesquiterpene            |
| ( <i>E</i> )- $\alpha$ -Bisabolene            | 0.10 | Sesquiterpene            |
| ( <i>E</i> )-Nerolidol                        | 0.06 | Sesquiterpenic alcohol   |
| Italidione III isomer I                       | 0.31 | $\beta$ -Diketone        |
| Italidione III isomer II                      | 0.49 | $\beta$ -Diketone        |
| Italidione III isomer III                     | 0.21 | $\beta$ -Diketone        |
| Guaiol  | 0.13 | Sesquiterpenic alcohol   |
| Copaborneol                                   | 0.13 | Sesquiterpenic alcohol   |
| Eudesm-5-en-11-ol                             | 0.52 | Sesquiterpenic alcohol   |
| Unknown                                       | 0.19 | Oxygenated sesquiterpene |
| Unknown                                       | 0.08 | Oxygenated sesquiterpene |
| Unknown                                       | 0.04 | Unknown                  |
| Neryl angelate?                               | 0.07 | Monoterpenic ester       |
| Eudesmol analog?                              | 0.26 | Sesquiterpenic alcohol   |
| Caryophylladienol I                           | 0.01 | Sesquiterpenic alcohol   |
| $\gamma$ -Eudesmol                            | 0.04 | Sesquiterpenic alcohol   |
| $\tau$ -Cadinol                               | 0.04 | Sesquiterpenic alcohol   |
| $\tau$ -Muurolol                              | 0.02 | Sesquiterpenic alcohol   |
| $\beta$ -Eudesmol                             | 0.08 | Sesquiterpenic alcohol   |
| Selin-11-en-4 $\alpha$ -ol                    | 0.30 | Sesquiterpenic alcohol   |
| $\alpha$ -Eudesmol                            | 0.06 | Sesquiterpenic alcohol   |
| Bulnesol                                      | 0.03 | Sesquiterpenic alcohol   |
| $\beta$ -Bisabolol                            | 0.08 | Sesquiterpenic alcohol   |
| epi- $\alpha$ -Bisabolol                      | 0.01 | Sesquiterpenic alcohol   |
| $\alpha$ -Bisabolol                           | 0.01 | Sesquiterpenic alcohol   |
| Neryl 4-methylvalerate?                       | 0.10 | Monoterpenic ester       |
| Geranyl 4-methylvalerate?                     | 0.03 | Monoterpenic ester       |
| Unknown                                       | 0.14 | Oxygenated sesquiterpene |
| Unknown                                       | 0.01 | Oxygenated sesquiterpene |
| Geranyl hexanoate                             | 0.01 | Monoterpenic ester       |
| Unknown                                       | 0.01 | Oxygenated sesquiterpene |
| Unknown                                       | 0.02 | Oxygenated sesquiterpene |
| Unknown                                       | 0.01 | Oxygenated sesquiterpene |
| Unknown                                       | 0.01 | Oxygenated sesquiterpene |
| <i>trans</i> -Bisabola-1(6),10-diene-2,3-diol | 0.04 | Sesquiterpenic alcohol   |

|                           |              |         |
|---------------------------|--------------|---------|
| Unknown                   | 0.02         | Unknown |
| <b>Consolidated total</b> | <b>98.27</b> |         |

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

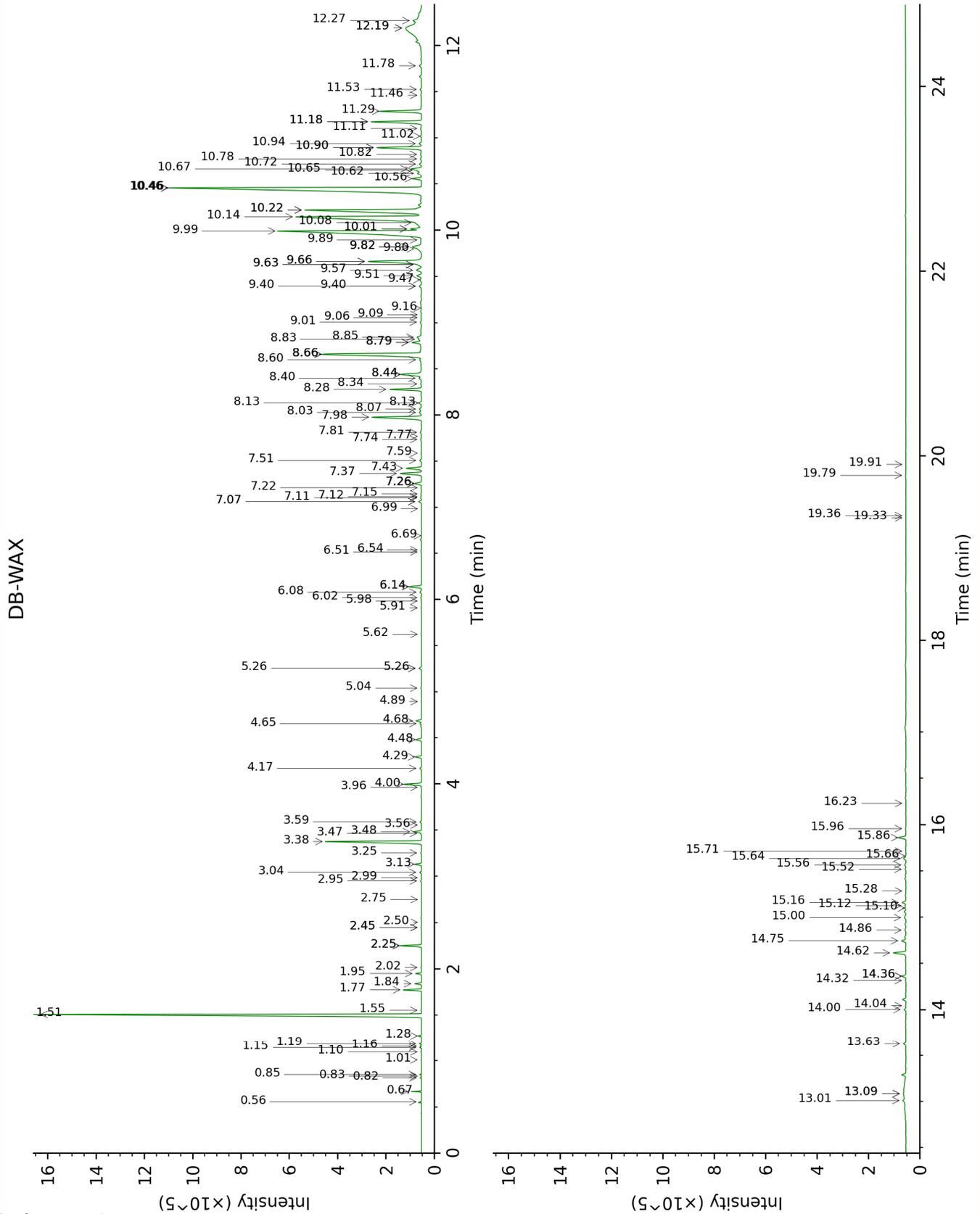
Note: no correction factor was applied

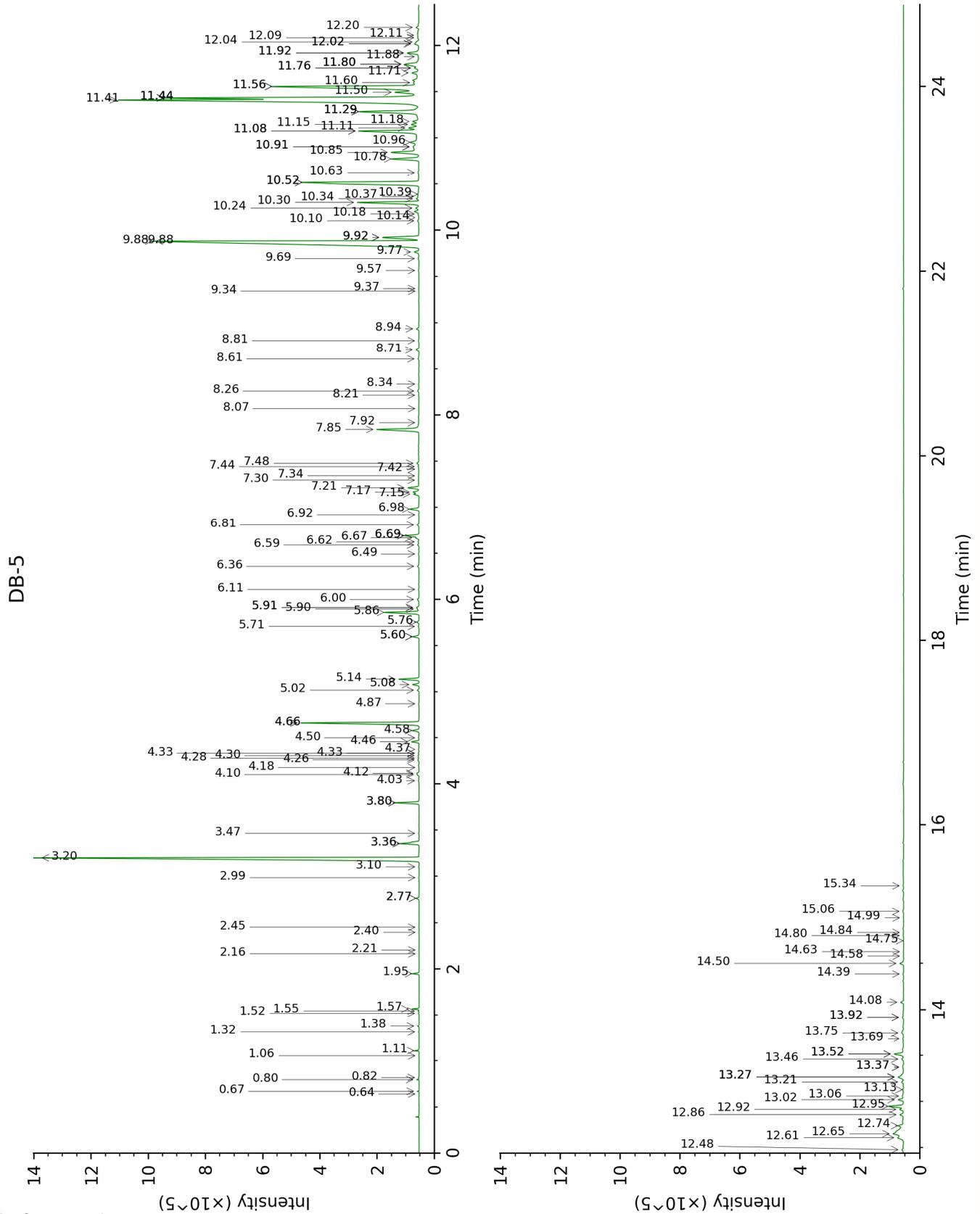
**About "consolidated" data:** The table above presents the breakdown of the sample volatile constituents after applying an algorithm to collapse data acquired from the multi-columns system of PhytoChemia into a single set of consolidated contents. In case of discrepancies between columns, the algorithm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

| Isovaleral   | Column DB-WAX |        |        | Column DB-5 |       |        |
|--|---------------|--------|--------|-------------|-------|--------|
|  | 0.84          | 886.3  | tr     | 0.64        | 640.7 | tr     |
| 2-Methylbutyral  | 0.82          | 880.2  | 0.02   | 0.67        | 650.8 | 0.02   |
| 3-Pentanone  | 1.14          | 940.9  | 0.03   | 0.80        | 693.1 | 0.03   |
| 2-Ethylfuran   | 1.01          | 920.7  | 0.01   | 0.82        | 700.7 | 0.01   |
| 2-Methylbutanol  | 3.56          | 1172.5 | 0.01   | 1.06        | 735.7 | 0.01   |
| 2-Methyl-3-pentanone   | 1.28          | 960.7  | 0.08   | 1.11        | 743.3 | 0.07   |
| Unknown HEIT III<br>[m/z 73, 41 (54),<br>87 (50), 56 (47), 54<br>(29), 55 (25), 100<br>(23)... 115? (6)] | 1.10          | 933.9  | 0.01   | 1.32        | 772.3 | 0.01   |
| Unknown HEIT II<br>[m/z 73, 87 (52),<br>41 (45), 56 (42),<br>100 (29)...]                                | 1.16          | 943.4  | 0.02   | 1.38        | 780.9 | 0.03   |
| Hexanal  | 2.02          | 1045.1 | 0.02   | 1.52        | 799.7 | 0.01   |
| Octane   | 0.56          | 783.3  | 0.01   | 1.55        | 803.1 | 0.02   |
| 2-Methyl-2-heptene   | 0.67          | 831.0  | 0.13   | 1.57        | 805.8 | 0.13   |
| 4-Methyl-3-hexanone  | 1.95          | 1039.0 | 0.14   | 1.95        | 837.1 | 0.14   |
| (3Z)-Hexenol   | 5.98          | 1348.5 | 0.01   | 2.16        | 854.6 | tr     |
| Furfuryl alcohol   | 9.16          | 1585.3 | 0.02   | 2.21        | 858.0 | 0.01   |
| Hexanol  | 5.62          | 1322.8 | 0.01   | 2.40        | 873.7 | 0.01   |
| Isoamyl acetate  | 2.50          | 1091.2 | tr     | 2.45        | 878.2 | 0.01   |
| Nonane   | 0.85          | 892.1  | 0.03   | 2.76*       | 903.9 | [0.08] |
| Bornylene  | 1.19          | 947.3  | 0.04   | 2.76*       | 903.9 | [0.08] |
| Isobutyl isobutyrate   | 2.25*         | 1067.4 | [0.62] | 2.99        | 918.7 | 0.01   |
| α-Thujene  | 1.55          | 1001.5 | 0.01   | 3.10        | 926.4 | 0.01   |
| α-Pinene   | 1.51          | 995.9  | 14.18  | 3.20        | 932.8 | 14.18  |
| α-Fenchene   | 1.78          | 1022.3 | 0.47   | 3.36*       | 943.0 | [0.65] |
| Camphene   | 1.84          | 1028.6 | 0.18   | 3.36*       | 943.0 | [0.65] |
| Thuja-2,4(10)-diene  | 2.45*         | 1085.9 | [0.02] | 3.47        | 950.2 | 0.01   |
| Sabinene   | 2.45*         | 1085.9 | [0.02] | 3.80*       | 972.0 | [0.62] |
| β-Pinene   | 2.25*         | 1067.4 | [0.62] | 3.80*       | 972.0 | [0.62] |
| 6-Methyl-5-hepten-2-one  | 5.26*         | 1295.1 | [0.09] | 4.03        | 987.6 | 0.02   |
| trans-Dehydroxylinalool oxide  | 3.59          | 1175.0 | 0.05   | 4.10        | 992.0 | 0.04   |

|  |       |        |        |       |        |        |
|--|-------|--------|--------|-------|--------|--------|
| Myrcene  | 3.04  | 1133.7 | 0.06   | 4.12  | 992.9  | 0.07   |
| 6-Methyl-5-hepten-2-ol   | 7.12  | 1430.6 | 0.01   | 4.18  | 997.0  | 0.01   |
| Unknown HEIT I<br>[m/z = 123, 43<br>(16), 152 (14), 124<br>(9), 137 (6)] | 2.95  | 1126.6 | 0.03   | 4.26  | 1002.4 | 0.03   |
| $\alpha$ -Phellandrene   | 2.99  | 1129.3 | 0.01   | 4.28  | 1003.6 | 0.03   |
| Isobutyl 2-methylbutyrate  | 3.25  | 1149.6 | 0.03   | 4.30  | 1005.4 | 0.03   |
| $\Delta$ 3-Carene  | 2.75  | 1111.4 | tr     | 4.33* | 1007.1 | [0.02] |
| Isobutyl isovalerate   | 3.47  | 1165.6 | 0.02   | 4.33* | 1007.1 | [0.02] |
| (3Z)-Hexenyl acetate   | 5.04  | 1279.9 | 0.02   | 4.37  | 1009.7 | 0.02   |
| $\alpha$ -Terpinene  | 3.13  | 1140.3 | 0.21   | 4.46  | 1014.8 | 0.21   |
| <i>para</i> -Methylanisole   | 6.51  | 1386.4 | 0.02   | 4.50  | 1017.5 | 0.02   |
| <i>para</i> -Cymene  | 4.29  | 1226.4 | 0.20   | 4.58  | 1022.4 | 0.21   |
| 1,8-Cineole  | 3.48  | 1167.0 | 0.26   | 4.66* | 1027.5 | [3.72] |
| Limonene   | 3.38  | 1158.9 | 3.45   | 4.66* | 1027.5 | [3.72] |
| (Z)- $\beta$ -Ocimene  | 3.96  | 1203.1 | 0.01   | 4.87  | 1040.4 | 0.01   |
| (E)- $\beta$ -Ocimene  | 4.17  | 1217.7 | 0.05   | 5.02  | 1050.1 | 0.05   |
| Isobutyl angelate  | 4.68  | 1254.2 | 0.18   | 5.08  | 1053.9 | 0.18   |
| $\gamma$ -Terpinene  | 4.00  | 1205.5 | 0.59   | 5.14  | 1057.6 | 0.56   |
| Terpinolene  | 4.48  | 1239.7 | 0.19   | 5.60* | 1086.2 | [0.20] |
| <i>para</i> -Cymenene  | 6.54  | 1388.0 | 0.01   | 5.60* | 1086.2 | [0.20] |
| 2-Nonanone   | 6.02  | 1351.2 | 0.02   | 5.71  | 1093.1 | 0.03   |
| 2,4-Dimethylheptane-3,5-dione  | 7.74  | 1476.4 | 0.04   | 5.76  | 1096.1 | 0.07   |
| Linalool   | 8.28  | 1517.1 | 1.07   | 5.86  | 1102.6 | 1.07   |
| 2-Methylbutyl 2-methylbutyrate   | 4.65  | 1252.0 | 0.05   | 5.90  | 1104.9 | 0.05   |
| Isoamyl isovalerate  | 4.89  | 1268.9 | 0.01   | 5.91* | 1105.9 | [0.08] |
| Nonanal  | 6.08  | 1355.3 | 0.07   | 5.91* | 1105.9 | [0.08] |
| endo-Fenchol   | 8.60  | 1541.7 | 0.06   | 6.00  | 1111.5 | 0.06   |
| $\alpha$ -Campholenal  | 7.22  | 1437.8 | 0.02   | 6.11  | 1118.4 | 0.02   |
| <i>trans</i> -Pinocarveol  | 9.40* | 1603.7 | [0.10] | 6.36  | 1134.4 | 0.05   |
| <i>trans</i> -Verbenol   | 9.80  | 1636.0 | 0.15   | 6.49  | 1142.9 | 0.02   |
| <i>para</i> -Vinylanisole  | 9.63* | 1622.5 | [0.11] | 6.59  | 1149.1 | 0.05   |
| Isoamyl angelate   | 6.14* | 1359.6 | [0.44] | 6.62  | 1151.3 | 0.03   |
| Nerol oxide  | 7.06* | 1426.7 | [0.10] | 6.67  | 1154.0 | 0.09   |
| 2-Methylbutyl  | 6.14* | 1359.6 | [0.44] | 6.69* | 1155.5 | [0.46] |

|   |        |        |        |       |        |        |
|---|--------|--------|--------|-------|--------|--------|
| angelate  |        |        |        |       |        |        |
| Pinocarvone   | 8.13*  | 1505.8 | [0.11] | 6.69* | 1155.5 | [0.46] |
| Borneol   | 10.01* | 1653.4 | [0.39] | 6.81  | 1163.0 | 0.05   |
| Unknown HEIT IV<br>[m/z 83, 100 (34),<br>55 (33), 43 (21), 84<br>(21)...]                     | 5.91   | 1343.2 | 0.01   | 6.92  | 1170.3 | 0.01   |
| Terpinen-4-ol   | 8.79*† | 1556.8 | [0.34] | 6.98  | 1174.2 | 0.30   |
| 4,6-<br>Dimethyloctane-<br>3,5-dione epimer I   | 8.83*† | 1559.4 | [0.08] | 7.15  | 1184.5 | 0.16   |
| 4,6-<br>Dimethyloctane-<br>3,5-dione epimer<br>II   | 8.85   | 1561.1 | 0.18   | 7.17  | 1186.0 | 0.18   |
| α-Terpineol   | 10.01* | 1653.4 | [0.39] | 7.22  | 1188.9 | 0.33   |
| Myrtenol  | 11.10  | 1743.5 | 0.06   | 7.30  | 1194.1 | 0.01   |
| 2-Methylbutyl<br>tiglate  | 7.15   | 1432.8 | 0.03   | 7.34  | 1197.2 | 0.01   |
| Verbenone   | 9.82*  | 1637.8 | [0.55] | 7.42  | 1201.7 | tr     |
| Unknown PIMA 7<br>[m/z 95, 93 (32),<br>121 (24), 79 (22),<br>91 (21), 105 (16)...<br>154 (2)] | 11.18* | 1749.6 | [2.03] | 7.44  | 1203.5 | 0.02   |
| Decanal   | 7.51   | 1459.6 | 0.07   | 7.48  | 1205.9 | 0.07   |
| Nerol   | 11.29  | 1759.2 | 1.60   | 7.85  | 1230.3 | 1.59   |
| Hexyl 2-<br>methylbutyrate  | 6.69   | 1398.9 | 0.01   | 7.92  | 1235.2 | 0.02   |
| Hexyl isovalerate   | 6.99   | 1421.0 | tr     | 8.07  | 1245.4 | 0.01   |
| 3-Methylpentyl<br>angelate  | 7.59   | 1465.4 | 0.02   | 8.22  | 1255.0 | 0.01   |
| Unknown HEIT VI<br>[m/z 83, 55 (29),<br>57 (24), 100 (21),<br>104 (13)...]                    | 7.11   | 1429.7 | 0.03   | 8.26  | 1258.1 | 0.05   |
| Linalyl acetate   | 8.34   | 1521.6 | 0.02   | 8.34  | 1263.0 | 0.01   |
| (3Z)-Hexenyl<br>angelate  | 8.44*  | 1529.6 | [0.93] | 8.61  | 1281.3 | 0.04   |
| Hexyl angelate  | 8.07   | 1500.7 | 0.10   | 8.71  | 1287.8 | 0.09   |
| 2-Undecanone  | 8.79*† | 1556.8 | [0.34] | 8.81  | 1294.7 | 0.02   |
| Tridecane   | 5.26*  | 1295.1 | [0.09] | 8.94  | 1303.4 | 0.08   |
| Hexyl tiglate   | 9.09   | 1579.8 | 0.01   | 9.34  | 1331.8 | 0.01   |
| Bicycloelemene  | 7.26*  | 1441.1 | [0.27] | 9.37  | 1333.8 | 0.01   |
| α-Terpinyl acetate  | 9.90   | 1643.8 | 0.02   | 9.57  | 1347.5 | 0.03   |

|   |         |        |         |         |        |         |
|---|---------|--------|---------|---------|--------|---------|
| Cyclosativene I   | 7.06*   | 1426.7 | [0.10]  | 9.69    | 1356.5 | 0.03    |
| Cyclosativene II  | 7.26*   | 1441.1 | [0.27]  | 9.77    | 1361.6 | 0.16    |
| Neryl acetate   | 10.46*  | 1689.1 | [16.93] | 9.88*   | 1369.8 | [16.78] |
| $\alpha$ -Ylangene  | 7.26*   | 1441.1 | [0.27]  | 9.88*   | 1369.8 | [16.78] |
| $\alpha$ -Copaene   | 7.37    | 1449.2 | 0.85    | 9.92*   | 1372.6 | [1.42]  |
| Italicene isomer  | 7.43    | 1453.3 | 0.57    | 9.92*   | 1372.6 | [1.42]  |
| Geranyl acetate   | 10.78   | 1715.8 | 0.04    | 10.10   | 1385.2 | 0.05    |
| Sativene  | 7.77    | 1478.8 | 0.01    | 10.14   | 1387.6 | 0.01    |
| Hexyl hexanoate   | 9.06    | 1577.4 | 0.03    | 10.18   | 1390.4 | 0.03    |
| Isoitalicene  | 8.03    | 1497.9 | 0.10    | 10.24   | 1394.8 | 0.11    |
| Italicene   | 7.98    | 1494.2 | 2.13    | 10.30   | 1399.1 | 2.13    |
| Isocaryophyllene  | 8.40    | 1526.4 | 0.09    | 10.34   | 1402.0 | 0.08    |
| $\alpha$ -Gurjunene   | 7.81    | 1482.0 | 0.05    | 10.36   | 1403.8 | 0.05    |
| $\alpha$ -Cedrene   | 8.13*   | 1505.8 | [0.11]  | 10.39   | 1405.4 | 0.04    |
| <i>cis</i> - $\alpha$ -<br>Bergamotene  | 8.44*   | 1529.6 | [0.93]  | 10.52*  | 1414.9 | [5.32]  |
| $\beta$ -Caryophyllene  | 8.66*   | 1546.3 | [5.35]  | 10.52*  | 1414.9 | [5.32]  |
| $\beta$ -Copaene  | 8.66*   | 1546.3 | [5.35]  | 10.63   | 1423.1 | 0.04    |
| <i>trans</i> - $\alpha$ -<br>Bergamotene  | 8.66*   | 1546.3 | [5.35]  | 10.78   | 1434.3 | 0.94    |
| Italidione I (4,6,9-<br>Trimethyldec-8-<br>ene-3,5-dione)   | 12.19*† | 1836.8 | [3.73]  | 10.85*† | 1439.5 | [1.17]  |
| Unknown BOCA<br>IV [m/z 91, 161<br>(92), 105 (85), 119<br>(63), 133 (53), 79<br>(49), 204 (46)]         | 9.01    | 1573.6 | 0.04    | 10.91*† | 1444.0 | [0.50]  |
| Cadina-4,11-diene   | 9.40*   | 1603.7 | [0.10]  | 10.91*† | 1444.0 | [0.50]  |
| $\alpha$ -Humulene  | 9.51    | 1612.8 | 0.20    | 10.96*† | 1447.7 | [0.60]  |
| $\alpha$ -Acoradiene  | 9.57    | 1617.6 | 0.27    | 11.08*  | 1456.7 | [2.38]  |
| Neryl propionate  | 11.18*  | 1749.6 | [2.03]  | 11.08*  | 1456.7 | [2.38]  |
| ( <i>E</i> )- $\beta$ -Farnesene  | 9.82*   | 1637.8 | [0.55]  | 11.11   | 1459.1 | 0.40    |
| 4,5-diepi-<br>Aristolochene   | 9.63*   | 1622.5 | [0.11]  | 11.15   | 1462.0 | 0.29    |
| Unknown CEDE VI<br>[m/z 119, 91 (85),<br>93 (77), 105 (76),<br>79 (61), 134 (60),<br>94 (49), 204 (46)] | 9.66*   | 1625.2 | [2.63]  | 11.18   | 1464.3 | 0.23    |
| Selina-4,11-diene   | 9.66*   | 1625.2 | [2.63]  | 11.29*  | 1472.3 | [2.63]  |
| $\alpha$ -Amorphene   | 9.82*   | 1637.8 | [0.55]  | 11.29*  | 1472.3 | [2.63]  |
| <i>trans</i> -Cadina-<br>1(6),4-diene   | 9.47    | 1609.2 | 0.07    | 11.29*  | 1472.3 | [2.63]  |
| $\gamma$ -Curcumene   | 9.99    | 1651.6 | 9.67    | 11.41*† | 1481.6 | [13.77] |

|   |         |        |         |         |        |        |
|---|---------|--------|---------|---------|--------|--------|
| β-Selinene  | 10.14   | 1663.9 | 8.95    | 11.44*† | 1483.3 | [7.98] |
| Italidione II isomer I (2,4,6,9-Tetramethyldec-8-ene-3,5-dione) | 12.27*† | 1843.9 | [0.99]  | 11.44*† | 1483.3 | [7.98] |
| ar-Curcumene  | 10.90*  | 1726.1 | [1.81]  | 11.44*† | 1483.3 | [7.98] |
| Valencene   | 10.08   | 1658.8 | 0.23    | 11.50*† | 1487.8 | [0.96] |
| α-Selinene  | 10.22*  | 1669.9 | [6.50]  | 11.56*† | 1492.5 | [6.91] |
| Italidione II isomer II (5,7,10-Trimethylundec-9-ene-4,6-dione) | 12.19*† | 1836.8 | [3.73]  | 11.56*† | 1492.5 | [6.91] |
| Italidione II analog  | 13.01*† | 1909.9 | [0.49]  | 11.60†  | 1495.5 | 0.23   |
| δ-Amorphene   | 10.22*  | 1669.9 | [6.50]  | 11.71   | 1503.4 | 0.35   |
| β-Bisabolene  | 10.46*  | 1689.1 | [16.93] | 11.76*  | 1507.5 | [0.15] |
| 10-epi-Italicene ether  | 11.53   | 1779.1 | 0.06    | 11.76*  | 1507.5 | [0.15] |
| 7-epi-α-Selinene  | 10.65   | 1705.5 | 0.15    | 11.80*  | 1510.7 | [0.72] |
| β-Curcumene   | 10.46*  | 1689.1 | [16.93] | 11.80*  | 1510.7 | [0.72] |
| γ-Cadinene  | 10.62   | 1702.5 | 0.17    | 11.80*  | 1510.7 | [0.72] |
| Sesquicineole   | 10.56   | 1697.2 | 0.32    | 11.88   | 1517.1 | 0.02   |
| trans-Calamenene  | 11.46   | 1773.8 | 0.04    | 11.92*  | 1520.2 | [0.45] |
| δ-Cadinene  | 10.67   | 1706.7 | 0.41    | 11.92*  | 1520.2 | [0.45] |
| trans-Cadina-1,4-diene  | 10.90*  | 1726.1 | [1.81]  | 12.02*  | 1528.0 | [0.18] |
| Italicene ether   | 11.78   | 1800.9 | 0.09    | 12.02*  | 1528.0 | [0.18] |
| (E)-γ-Bisabolene  | 10.72   | 1711.0 | 0.08    | 12.04   | 1529.5 | 0.07   |
| α-Cadinene  | 11.02   | 1736.5 | 0.04    | 12.09   | 1533.1 | 0.04   |
| Selina-3,7(11)-diene  | 10.82   | 1719.9 | 0.04    | 12.11   | 1535.2 | 0.05   |
| (E)-α-Bisabolene  | 10.94   | 1729.7 | 0.09    | 12.20   | 1541.8 | 0.10   |
| (E)-Nerolidol   | 14.00   | 2001.4 | 0.07    | 12.48   | 1564.0 | 0.06   |
| Italidione III isomer I   | 13.09*† | 1916.7 | [0.72]  | 12.61   | 1574.2 | 0.31   |
| Italidione III isomer II  | 13.09*† | 1916.7 | [0.72]  | 12.65   | 1577.6 | 0.49   |
| Italidione III isomer III                                       |         |        |         | 12.74   | 1584.4 | 0.21   |
| Guaiol  | 14.36*  | 2036.0 | [0.15]  | 12.86   | 1593.7 | 0.13   |
| Copaborneol   | 15.16   | 2113.0 | 0.15    | 12.92   | 1598.2 | 0.13   |
| Eudesm-5-en-11-ol   | 14.62   | 2060.1 | 0.50    | 12.95   | 1600.8 | 0.52   |
| Unknown MIAL II [m/z 43, 81 (97),                               | 14.75   | 2072.6 | 0.17    | 13.02   | 1606.5 | 0.19   |

|  |        |        |        |        |        |        |
|--|--------|--------|--------|--------|--------|--------|
| 135 (71), 95 (62),<br>204 (61), 71 (59),<br>207 (56)... 222 (3)]   |        |        |        |        |        |        |
| Unknown MECA V<br>[m/z 179, 161 (66),<br>119 (44), 95 (38),<br>105 (35)... 204<br>(24), 222 (1)]               | 14.86  | 2083.6 | 0.06   | 13.06  | 1609.8 | 0.08   |
| Unknown HEIT VIII<br>[m/z 182, 109 (58),<br>69 (50), 41 (42), 43<br>(40), 139 (31)...<br>235 (17), 250 (1)...] | 14.32  | 2031.5 | 0.03   | 13.13  | 1615.5 | 0.04   |
| Neryl angelate?  |        |        |        | 13.21  | 1622.3 | 0.07   |
| Eudesmol analog?   |        |        |        | 13.27* | 1626.7 | [0.31] |
| Caryophylladienol<br>I   | 16.23  | 2221.0 | 0.01   | 13.27* | 1626.7 | [0.31] |
| γ-Eudesmol   | 15.12  | 2109.5 | 0.04   | 13.27* | 1626.7 | [0.31] |
| τ-Cadinol  | 15.10  | 2107.0 | 0.04   | 13.37* | 1635.5 | [0.06] |
| τ-Muurolol   | 15.28  | 2125.4 | 0.02   | 13.37* | 1635.5 | [0.06] |
| β-Eudesmol   | 15.64  | 2160.6 | 0.11   | 13.46  | 1642.8 | 0.08   |
| Selin-11-en-4α-ol  | 15.86  | 2183.0 | 0.30   | 13.52* | 1647.4 | [0.37] |
| α-Eudesmol   | 15.56  | 2153.5 | 0.06   | 13.52* | 1647.4 | [0.37] |
| Bulnesol   | 15.52  | 2148.9 | 0.04   | 13.69  | 1661.6 | 0.03   |
| β-Bisabolol  | 15.00  | 2096.7 | 0.09   | 13.75  | 1666.7 | 0.08   |
| epi-α-Bisabolol  | 15.71  | 2168.4 | 0.01   | 13.92* | 1680.6 | [0.04] |
| α-Bisabolol  | 15.66  | 2163.1 | 0.01   | 13.92* | 1680.6 | [0.04] |
| Neryl 4-<br>methylvalerate?  | 13.63  | 1966.6 | 0.11   | 14.08  | 1694.0 | 0.10   |
| Geranyl 4-<br>methylvalerate?  | 14.04  | 2005.4 | 0.02   | 14.39  | 1719.9 | 0.03   |
| Unknown HEIT X<br>[m/z 43, 69 (32),<br>198 (29), 41 (27),<br>93 (26)... 202<br>(20)...]                        |        |        |        | 14.50  | 1729.9 | 0.14   |
| Unknown HEIT XI<br>[m/z 82, 125 (40),<br>41 (35), 69 (31), 67<br>(27)... 236? (t)]                             | 15.96  | 2192.7 | 0.04   | 14.58  | 1736.8 | 0.01   |
| Geranyl<br>hexanoate   | 14.36* | 2036.0 | [0.15] | 14.63  | 1740.9 | 0.01   |
| Unknown HEIT XII<br>[m/z 109, 127 (46),<br>138 (45), 81 (27),  | 19.36  | 2563.2 | 0.01   | 14.75  | 1751.1 | 0.01   |

|  |        |        |      |        |        |      |
|--|--------|--------|------|--------|--------|------|
| 123 (25)... 220?<br>(2)]<br>Unknown HEIT<br>XIII [m/z 136, 121<br>(74), 135 (55), 218<br>(36), 148 (33), 40<br>(42)... 236? (1)] |        |        |      | 14.80  | 1756.0 | 0.02 |
| Unknown HEIT<br>XIV [m/z 109, 138<br>(71), 82 (42), 123<br>(41), 127 (38)...]  | 19.33  | 2560.5 | 0.01 | 14.84  | 1758.9 | 0.01 |
| Unknown HEIT<br>XVII [m/z 109, 138<br>(75), 123 (45), 127<br>(42), 81 (30)...]   | 19.91  | 2628.4 | 0.01 | 14.99  | 1772.6 | 0.01 |
| <i>trans</i> -Bisabola-<br>1(6),10-diene-2,3-<br>diol  | 19.79  | 2614.4 | 0.02 | 15.06  | 1778.6 | 0.04 |
| Unknown HEIT<br>XIX [m/z 43, 82<br>(69), 41 (66), 93<br>(62), 96 (55), 55<br>(49), 67 (45), 154<br>(44)...]                      |        |        |      | 15.34  | 1802.5 | 0.02 |
| Total reported   | 97.17% |        |      | 98.01% |        |      |

\*: 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