

Date : March 21, 2022

CERTIFICATE OF ANALYSIS – GC PROFILING

SAMPLE IDENTIFICATION

Internal code : 21L21-PTH04


Customer identification : Orange 5 Fold - OR0100

Type : Essential oil

Source : *Citrus sinensis* ct. rectified

Customer : Plant Therapy

ANALYSIS

Method: PC-MAT-014  - Analysis of the composition of an essential oil or other volatile liquid by FAST GC-FID (in French); identifications validated by GC-MS.

Analyst : Seydou Ka, Ph. D.

Analysis date : January 03, 2022

Checked and approved by :



Sylvain Mercier, M. Sc., Chimiste 2014-005

Notes: This report may not be published, including online, without the written consent from Laboratoire PhytoChemia. This report is digitally signed, it is only considered valid if the digital signature is intact. The results only describe the samples that were submitted to the assays.

This report is an update of the version first issued on January 12, 2022 to correct a mistake in the lot number.



PHYSICOCHEMICAL DATA

Physical aspect: Bright orange brownish liquid

Refractive index: 1.4765 ± 0.0003 (20 °C; method PC-MAT-016)

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 |
|---|-------|------------------------|
| Heptanal | 0.01 | Aliphatic aldehyde |
| α -Pinene | 0.06 | Monoterpene |
| Sabinene | 0.11 | Monoterpene |
| β -Pinene | 0.01 | Monoterpene |
| Myrcene | 0.83 | Monoterpene |
| α -Phellandrene | 0.02 | Monoterpene |
| Octanal | 0.17 | Aliphatic aldehyde |
| Δ^3 -Carene | 0.07 | Monoterpene |
| Limonene | 87.33 | Monoterpene |
| β -Phellandrene | 0.23 | Monoterpene |
| (Z)- β -Ocimene | tr | Monoterpene |
| (E)- β -Ocimene | 0.03 | Monoterpene |
| γ -Terpinene | 0.01 | Monoterpene |
| <i>cis</i> -Sabinene hydrate | 0.01 | Monoterpenic alcohol |
| <i>cis</i> -Linalool oxide (fur.) | 0.01 | Monoterpenic alcohol |
| Octanol | 0.05 | Aliphatic alcohol |
| Isoterpinolene | 0.01 | Monoterpene |
| Terpinolene | 0.04 | Monoterpene |
| 6,7-Epoxymyrcene | tr | Monoterpenic ether |
| <i>trans</i> -Sabinene hydrate | tr | Monoterpenic alcohol |
| Linalool | 1.82 | Monoterpenic alcohol |
| Hotrienol | 0.01 | Monoterpenic alcohol |
| Nonanal | 0.10 | Aliphatic aldehyde |
| <i>trans</i> -para-Mentha-2,8-dien-1-ol | 0.10 | Monoterpenic alcohol |
| <i>cis</i> -Limonene oxide | 0.09 | Monoterpenic ether |
| <i>cis</i> -para-Mentha-2,8-dien-1-ol | 0.16 | Monoterpenic alcohol |
| <i>trans</i> -Verbenol | 0.01 | Monoterpenic alcohol |
| Citronellal | 0.22 | Monoterpenic aldehyde |
| Nonanol | 0.01 | Aliphatic alcohol |
| Unknown | 0.04 | Oxygenated monoterpene |
| Cryptone | 0.01 | Normonoterpenic ketone |
| para-Cymen-8-ol | 0.01 | Monoterpenic alcohol |
| α -Terpineol | 0.16 | Monoterpenic alcohol |
| Unknown | 0.05 | Unknown |
| Unknown | 0.06 | Unknown |
| <i>trans</i> -Isopiperitenol | 0.04 | Monoterpenic alcohol |
| Decanal | 1.49 | Aliphatic aldehyde |
| Octyl acetate | 0.04 | Aliphatic ester |
| <i>trans</i> -Carveol | 0.12 | Monoterpenic alcohol |
| <i>cis</i> -Carveol | 0.08 | Monoterpenic alcohol |
| Citronellol | 0.05 | Monoterpenic alcohol |
| Neral | 0.17 | Monoterpenic aldehyde |
| Carvone | 0.08 | Monoterpenic ketone |
| Geraniol | 0.02 | Monoterpenic alcohol |
| (2E)-Decenal | 0.02 | Aliphatic aldehyde |

| | | |
|--|------|--------------------------|
| Perillaldehyde | 0.10 | Monoterpenic aldehyde |
| Geranial | 0.36 | Monoterpenic aldehyde |
| Limonen-10-ol | 0.08 | Monoterpenic alcohol |
| Undecanal | 0.06 | Aliphatic aldehyde |
| <i>cis</i> -para-Mentha-2,8-diene-1-hydroperoxide | tr | Monoterpenic peroxide |
| (2 <i>E</i> ,4 <i>E</i>)-Decadienal | 0.02 | Aliphatic aldehyde |
| para-Mentha-1,8-diene-4-hydroperoxide | 0.04 | Monoterpenic peroxide |
| Limonene <i>trans</i> -glycol | 0.05 | Monoterpenic alcohol |
| Neryl acetate | 0.03 | Monoterpenic ester |
| α -Copaene | 0.11 | Sesquiterpene |
| β -Cubebene | 0.09 | Sesquiterpene |
| Geranyl acetate | 0.13 | Monoterpenic ester |
| Capric acid | tr | Aliphatic acid |
| β -Elemene | 0.08 | Sesquiterpene |
| Dodecanal | 0.27 | Aliphatic aldehyde |
| β -Caryophyllene | 0.09 | Sesquiterpene |
| β -Copaene | 0.17 | Sesquiterpene |
| α -Humulene | 0.04 | Sesquiterpene |
| (<i>E</i>)- β -Farnesene | 0.05 | Sesquiterpene |
| γ -Muurolene | 0.02 | Sesquiterpene |
| Germacrene D | 0.08 | Sesquiterpene |
| Valencene | 0.35 | Sesquiterpene |
| α -Muurolene | 0.05 | Sesquiterpene |
| (3 <i>E</i> ,6 <i>E</i>)- α -Farnesene | 0.05 | Sesquiterpene |
| Cubebol | 0.01 | Sesquiterpenic alcohol |
| γ -Cadinene | 0.04 | Sesquiterpene |
| δ -Cadinene | 0.11 | Sesquiterpene |
| α -Elemol | 0.04 | Sesquiterpenic alcohol |
| (<i>E</i>)-Nerolidol | 0.02 | Sesquiterpenic alcohol |
| Spathulenol | 0.03 | Sesquiterpenic alcohol |
| Caryophyllene oxide isomer | 0.01 | Sesquiterpenic ether |
| Caryophyllene oxide | 0.02 | Sesquiterpenic ether |
| δ -Undecalactone | 0.01 | Aliphatic lactone |
| Tetradecanal | 0.02 | Aliphatic aldehyde |
| Unknown | 0.01 | Oxygenated sesquiterpene |
| β -Sinensal | 0.16 | Sesquiterpenic aldehyde |
| α -Sinensal | 0.10 | Sesquiterpenic aldehyde |
| Nootkatone | 0.06 | Sesquiterpenic ketone |
| Hexadecanal | 0.04 | Aliphatic aldehyde |
| meta-Camphorene | 0.01 | Diterpene |
| Palmitic acid | 0.22 | Aliphatic acid |
| Octadecanal | 0.03 | Aliphatic aldehyde |
| Methyl stearate | 0.02 | Aliphatic ester |
| Linoleic acid | 0.16 | Aliphatic acid |
| Oleic acid | 0.15 | Aliphatic acid |
| <i>cis</i> -Vaccenic acid | 0.15 | Aliphatic acid |
| Stearic acid | 0.26 | Aliphatic acid |
| Pentamethoxyflavone isomer | 0.15 | Flavonoid |
| Tetramethoxyflavone isomer | 0.20 | Flavonoid |
| 3-Methoxynobiletin (3,5,6,7,8,3',4'-heptamethoxyflavone) | 0.35 | Flavonoid |
| Nobiletin | 0.29 | Flavonoid |

| | | |
|---------------------------|---------------|--|
| Consolidated total | 98.95% | |
|---------------------------|---------------|--|

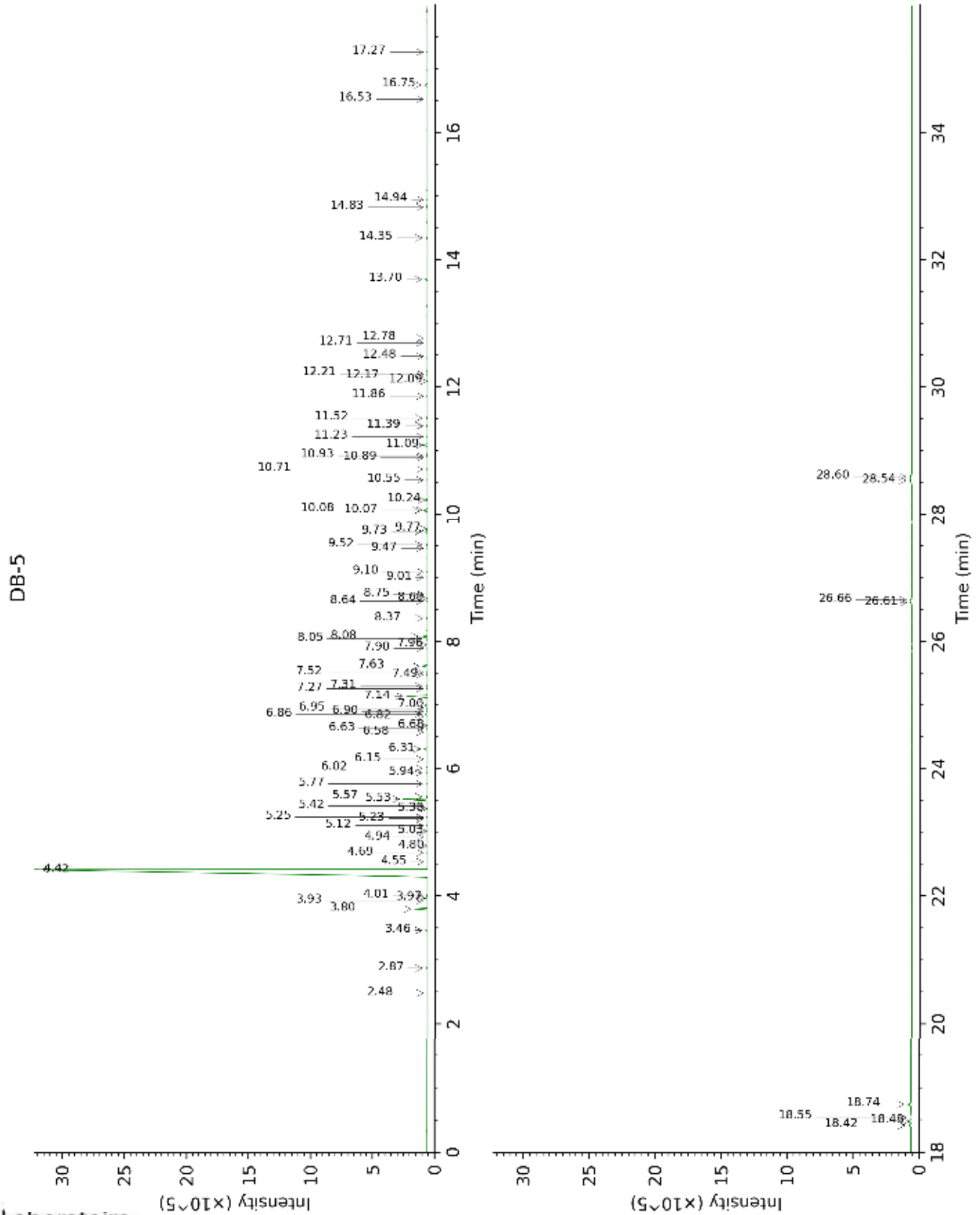
tr: The compound has been detected below 0.005% of total signal.

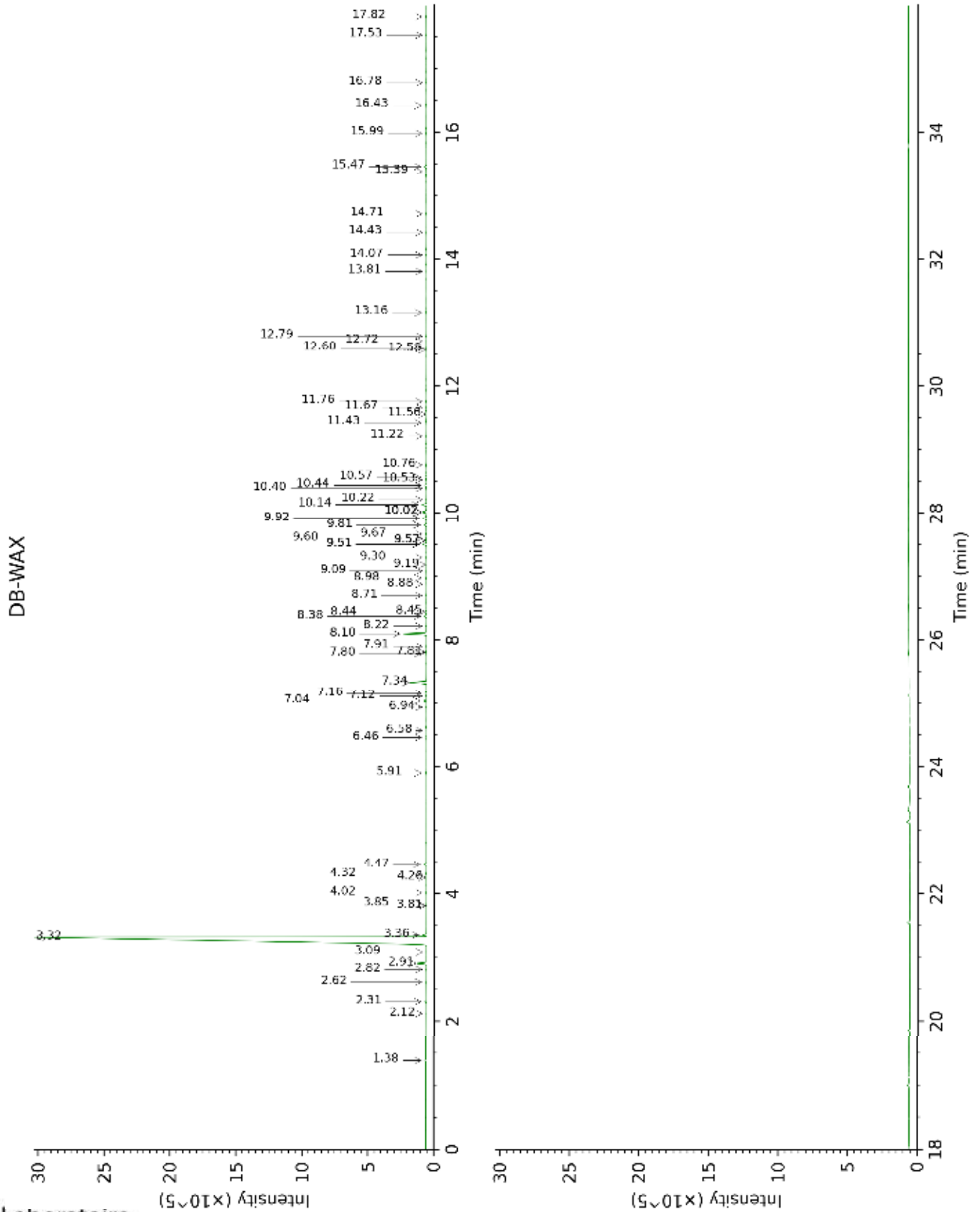
Note: no correction factor was applied

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 | % |
| Heptanal | 2.48 | 903 | 0.01 | 3.09 | 1149 | 0.01 |
| α -Pinene | 2.87 | 930 | 0.06 | 1.38 | 992 | 0.07 |
| Sabinene | 3.46* | 970 | 0.12 | 2.31 | 1085 | 0.11 |
| β -Pinene | 3.46* | 970 | [0.12] | 2.12 | 1067 | 0.01 |
| Myrcene | 3.80 | 993 | 0.83 | 2.91 | 1135 | 0.83 |
| α -Phellandrene | 3.93 | 1002 | 0.02 | 2.82 | 1127 | 0.02 |
| Octanal | 3.97 | 1004 | 0.17 | 4.47 | 1254 | 0.17 |
| Δ^3 -Carene | 4.02 | 1007 | 0.07 | 2.62 | 1112 | 0.07 |
| Limonene | 4.42* | 1033 | 86.65 | 3.32 | 1167 | 87.33 |
| β -Phellandrene | 4.42* | 1033 | [86.65] | 3.36 | 1170 | 0.23 |
| (Z)- β -Ocimene | 4.55 | 1041 | tr | 3.81 | 1206 | 0.01 |
| (E)- β -Ocimene | 4.69 | 1050 | 0.03 | 4.02 | 1221 | 0.03 |
| γ -Terpinene | 4.80 | 1057 | 0.01 | 3.85 | 1208 | 0.01 |
| <i>cis</i> -Sabinene hydrate | 4.94 | 1066 | 0.01 | 6.94 | 1430 | 0.03 |
| <i>cis</i> -Linalool oxide (fur.) | 5.03 | 1072 | 0.01 | 6.58 | 1403 | 0.01 |
| Octanol | 5.12 | 1077 | 0.05 | 8.22 | 1527 | 0.05 |
| Isoterpinolene | 5.23 | 1084 | 0.01 | 4.26 | 1239 | 0.01 |
| Terpinolene | 5.25 | 1086 | 0.04 | 4.32 | 1243 | 0.05 |
| 6,7-Epoxymyrcene | 5.38 | 1094 | tr | | | |
| <i>trans</i> -Sabinene hydrate | 5.42 | 1096 | tr | 7.91 | 1502 | 0.03 |
| Linalool | 5.53 | 1103 | 1.82 | 8.10* | 1518 | 1.85 |
| Hotrienol | 5.57* | 1106 | 0.11 | 8.88 | 1578 | 0.01 |
| Nonanal | 5.57* | 1106 | [0.11] | 5.91 | 1355 | 0.10 |
| <i>trans</i> -para-Mentha-2,8-dien-1-ol | 5.77 | 1119 | 0.10 | 8.98 | 1586 | 0.10 |
| <i>cis</i> -Limonene oxide | 5.94 | 1130 | 0.09 | 6.46 | 1395 | 0.09 |
| <i>cis</i> -para-Mentha-2,8-dien-1-ol | 6.02 | 1135 | 0.16 | 9.51* | 1628 | 0.33 |
| <i>trans</i> -Verbenol | 6.15 | 1143 | 0.01 | 9.60 | 1636 | 0.02 |
| Citronellal | 6.31 | 1154 | 0.22 | 7.04 | 1438 | 0.21 |
| Nonanol | 6.58 | 1171 | 0.01 | 9.51* | 1628 | [0.33] |
| Unknown [m/z 69, 84 (62), 41 (30), 123 (26), 97 (24), 109 (23)...] | 6.63 | 1174 | 0.04 | 9.67 | 1641 | 0.05 |
| Cryptone | 6.68 | 1177 | 0.01 | 9.19 | 1602 | 0.01 |
| para-Cymen-8-ol | 6.82 | 1186 | 0.01 | 11.56 | 1799 | 0.01 |
| α -Terpineol | 6.86 | 1188 | 0.16 | 9.81* | 1653 | 0.23 |
| Unknown [m/z 121, 79 (98), 93 (87), 94 (73), 91 (63), 105 (45)...] | 6.90 | 1192 | 0.05 | 7.81 | 1495 | 0.04 |
| Unknown [m/z 121, 79 (61), 93 (55), 94 (40), 91 (39), 84 (37)...] | 6.95 | 1195 | 0.06 | 8.10* | 1518 | [1.85] |
| <i>trans</i> -Isopiperitenol | 7.00 | 1198 | 0.04 | 10.44* | 1704 | 0.14 |
| Decanal | 7.14 | 1207 | 1.49 | 7.34 | 1460 | 1.42 |
| Octyl acetate | 7.27 | 1216 | 0.04 | 7.12 | 1443 | 0.04 |
| <i>trans</i> -Carveol | 7.31 | 1218 | 0.12 | 11.43 | 1788 | 0.11 |

| | | | | | | |
|--|--------|------|--------|--------|------|--------|
| <i>cis</i> -Carveol | 7.48 | 1230 | 0.08 | 11.76 | 1817 | 0.06 |
| Citronellol | 7.52 | 1233 | 0.05 | 10.76 | 1731 | 0.07 |
| Neral | 7.63* | 1240 | 0.39 | 9.51* | 1628 | [0.33] |
| Carvone | 7.63* | 1240 | [0.39] | 10.02* | 1670 | 0.41 |
| Geraniol | 7.90 | 1258 | 0.02 | 11.67 | 1808 | 0.03 |
| (2 <i>E</i>)-Decenal | 7.96 | 1262 | 0.02 | 9.09 | 1594 | 0.02 |
| Perillaldehyde | 8.05 | 1268 | 0.10 | | | |
| Geranial | 8.08 | 1270 | 0.36 | 10.14 | 1679 | 0.37 |
| Limonen-10-ol | 8.37 | 1290 | 0.08 | 13.16 | 1943 | 0.07 |
| Undecanal | 8.64 | 1308 | 0.06 | 8.71 | 1564 | 0.06 |
| <i>cis</i> -para-Mentha-2,8-diene-1-hydroperoxide | 8.68 | 1311 | tr | | | |
| (2 <i>E</i> ,4 <i>E</i>)-Decadienal | 8.75 | 1316 | 0.02 | 11.22 | 1770 | 0.04 |
| para-Mentha-1,8-diene-4-hydroperoxide | 9.01 | 1334 | 0.04 | | | |
| Limonene <i>trans</i> -glycol | 9.10 | 1340 | 0.05 | 15.99 | 2219 | 0.06 |
| Neryl acetate | 9.47 | 1366 | 0.03 | 10.22 | 1686 | 0.02 |
| α -Copaene | 9.52 | 1370 | 0.11 | 7.16 | 1447 | 0.12 |
| β -Cubebene | 9.73* | 1385 | 0.20 | 7.80 | 1494 | 0.09 |
| Geranyl acetate | 9.73* | 1385 | [0.20] | 10.57 | 1715 | 0.13 |
| Capric acid | 9.73* | 1385 | [0.20] | | | |
| β -Elemene | 9.77 | 1388 | 0.08 | 8.45 | 1545 | 0.06 |
| Dodecanal | 10.07 | 1409 | 0.27 | 10.02* | 1670 | [0.41] |
| β -Caryophyllene | 10.08 | 1410 | 0.09 | 8.44 | 1543 | 0.10 |
| β -Copaene | 10.24 | 1422 | 0.17 | 8.38 | 1539 | 0.17 |
| α -Humulene | 10.55 | 1445 | 0.04 | 9.30 | 1611 | 0.03 |
| (<i>E</i>)- β -Farnesene | 10.71 | 1457 | 0.05 | 9.57* | 1633 | 0.06 |
| γ -Muurolene | 10.90 | 1471 | 0.02 | 9.57* | 1633 | [0.06] |
| Germacrene D | 10.93 | 1473 | 0.08 | 9.81* | 1653 | [0.23] |
| Valencene | 11.09 | 1486 | 0.35 | 9.92 | 1662 | 0.33 |
| α -Muurolene | 11.23 | 1496 | 0.05 | 10.02* | 1670 | [0.41] |
| (3 <i>E</i> ,6 <i>E</i>)- α -Farnesene | 11.39* | 1508 | 0.09 | 10.53 | 1712 | 0.05 |
| Cubebol | 11.39* | 1508 | [0.09] | 12.58 | 1889 | 0.01 |
| γ -Cadinene | 11.39* | 1508 | [0.09] | 10.40 | 1700 | 0.04 |
| δ -Cadinene | 11.52 | 1518 | 0.11 | 10.44* | 1704 | [0.14] |
| α -Elemol | 11.86 | 1545 | 0.04 | 14.07 | 2028 | 0.03 |
| (<i>E</i>)-Nerolidol | 12.09 | 1564 | 0.02 | 13.81 | 2003 | 0.02 |
| Spathulenol | 12.17 | 1569 | 0.03 | 14.42 | 2062 | 0.03 |
| Caryophyllene oxide isomer | 12.21* | 1572 | 0.04 | 12.72 | 1902 | 0.01 |
| Caryophyllene oxide | 12.21* | 1572 | [0.04] | 12.80 | 1909 | 0.02 |
| δ -Undecalactone | 12.48 | 1594 | 0.01 | | | |
| Tetradecanal | 12.71 | 1612 | 0.02 | 12.60 | 1891 | 0.02 |
| Unknown [m/z 161, 43 (74), 105 (57), 121 (45), 81 (43)... 204 (31)...] | 12.78 | 1618 | 0.01 | 14.71* | 2090 | 0.04 |
| β -Sinensal | 13.70 | 1694 | 0.16 | 15.47 | 2165 | 0.17 |
| α -Sinensal | 14.35 | 1750 | 0.10 | 16.43 | 2264 | 0.09 |
| Nootkatone | 14.83 | 1792 | 0.06 | 17.82 | 2414 | 0.06 |
| Hexadecanal | 14.94 | 1802 | 0.04 | 14.71* | 2090 | [0.04] |

| | | | | | | |
|--|--------|---------------|--------|-------|---------------|------|
| meta-Camphorene | 16.53 | 1948 | 0.01 | 15.39 | 2158 | 0.01 |
| Palmitic acid | 16.75 | 1970 | 0.22 | | | |
| Octadecanal | 17.27 | 2019 | 0.03 | 16.78 | 2301 | 0.03 |
| Methyl stearate | 18.42* | 2135 | 0.18 | 17.53 | 2382 | 0.02 |
| Linoleic acid | 18.42* | 2135 | [0.18] | | | |
| Oleic acid | 18.48 | 2142 | 0.15 | | | |
| cis-Vaccenic acid | 18.55 | 2148 | 0.15 | | | |
| Stearic acid | 18.74 | 2169 | 0.26 | | | |
| Pentamethoxyflavone isomer | 26.61 | 3136 | 0.15 | | | |
| Tetramethoxyflavone isomer | 26.66 | 3141 | 0.20 | | | |
| 3-Methoxynobiletin (3,5,6,7,8,3',4'-heptamethoxyflavone) | 28.54 | 3326 | 0.35 | | | |
| Nobiletin | 28.60 | 3331 | 0.29 | | | |
| Total identified | | 98.02% | | | 96.67% | |
| Total reported | | 98.19% | | | 96.76% | |

*: Two or more compounds are coeluting on this column

[xx]: Duplicate percentage due to coelutions, not taken into account in the consolidated total

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