*plants*

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# Chemical variability of the essential oils from two Portuguese Apiaceae: *Coriandrum sativum* L. and *Foeniculum vulgare* Mill.

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**Table S1.** Percentage composition of the EOs isolated by hydrodistillation, from *Coriandrum sativum* fruits and vegetative aerial parts accessions grown at the experimental field of Escola Superior Agrária de Elvas. For samples codes, see Table 1.

| Components | RI | Accessions | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Fruits | | | Vegetative aerial parts | | | | | | | |
| | | Cs21_fr1 2021 | Cs21_fr2 2021 | Cs21_fr3 2021 | Cs22_lv1 2022 | Cs22_lv2 2022 | Cs22_lv3 2022 | ROMA 2022 | SANTO 2022 | Cs22_lv4 2022 | Cs22_lv5 2022 | Cs22_lv6 2022 |
| *n*-Octane | 800 | | | | t | t | t | t | t | t | t | t |
| 2-*trans*-Hexenal | 866 | | | | 0.1 | 0.2 | 0.1 | 0.1 | 0.1 | 0.1 | t | 0.2 |
| *cis*-2-Hexen-1-ol | 882 | | | | t | t | t | t | t | t | t | t |
| *n*-Hexanol | 883 | | | | t | t | t | t | t | t | t | t |
| *n*-Heptanal | 897 | t | 0.1 | 0.1 | t | t | t | t | t | t | t | t |
| 1-Nonene | 899 | | | | t | t | t | t | t | t | t | t |
| *n*-Nonane | 900 | t | t | t | 2.1 | 2.9 | 2.8 | 3.1 | 1.9 | 0.3 | 0.7 | 1.8 |
| *trans*-3-Nonene * | 901 | | | | t | t | t | t | t | t | t | t |
| Tricyclene | 921 | t | t | t | | | | | | | | |
| α-Thujene | 924 | t | t | 0.1 | | | | | | | | |
| α-Pinene | 930 | 1.7 | 4.3 | 3.6 | t | t | 0.1 | 0.1 | 0.1 | t | t | 0.3 |
| Camphene | 938 | 0.1 | 0.4 | 0.3 | | | | | | | | |
| *n*-Heptanol | 952 | t | t | t | t | t | t | t | t | t | t | t |
| Sabinene | 958 | 0.2 | 0.4 | 0.4 | t | t | t | t | t | t | t | t |
| β-Pinene | 963 | 0.3 | 0.5 | 0.5 | t | t | t | t | t | t | t | t |
| 3-Methyl nonane * | 970 | | | | t | t | t | t | t | t | t | t |
| 2-Pentyl furan | 973 | t | t | t | | | | | | | | |
| *n*-Octanal | 973 | 0.1 | t | 0.1 | 1.1 | 1.1 | 1.2 | 1.2 | 1.2 | 1.1 | 0.7 | 0.8 |
| β-Myrcene | 975 | 0.7 | 1.1 | 0.9 | 0.4 | 0.4 | 0.5 | 0.7 | 0.7 | 0.5 | 0.5 | 0.5 |
| α-Phellandrene | 995 | t | t | t | | | | | | | | |
| *n*-Decane | 1000 | t | t | t | 0.1 | 0.2 | 0.2 | 0.2 | 0.1 | t | 0.1 | 0.1 |
| Phenylacetaldehyde (Benzene acetaldehyde) | 1002 | | | | t | t | t | t | t | t | t | t |
| α-Terpinene | 1002 | 0.1 | 0.1 | 0.1 | | | | | | | | |
| *p*-Cymene | 1003 | 1.6 | 1.4 | 2.1 | t | t | t | t | t | t | t | t |
| 1,8-Cineole | 1005 | t | t | t | t | t | t | t | t | 0.1 | 0.1 | t |

| Components | RI | Accessions | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Fruits | | | Vegetative aerial parts | | | | | | | |
| | | Cs21_fr1 2021 | Cs21_fr2 2021 | Cs21_fr3 2021 | Cs22_lv1 2022 | Cs22_lv2 2022 | Cs22_lv3 2022 | ROMA 2022 | SANTO 2022 | Cs22_lv4 2022 | Cs22_lv5 2022 | Cs22_lv6 2022 |
| β-Phellandrene | 1005 | 0.1 | 0.1 | 0.1 | | | | | | | | |
| Limonene | 1009 | 1.2 | 1.8 | 1.4 | 0.2 | 0.3 | 0.4 | 0.3 | 0.1 | 0.3 | 0.3 | 0.1 |
| *cis*-β-Ocimene | 1017 | t | t | t | | | | | | | | |
| *trans*-β-Ocimene | 1027 | 0.1 | t | 0.1 | t | t | t | t | t | t | t | 0.1 |
| γ-Terpinene | 1035 | 10.4 | 8.1 | 12.0 | t | t | t | t | t | t | t | 0.3 |
| *trans*-Sabinene hydrate | 1037 | t | t | t | | | | | | | | |
| *n*-Octanol | 1045 | 0.2 | t | 0.1 | t | t | t | t | t | t | 0.1 | t |
| Terpinolene | 1064 | 0.4 | 0.4 | 0.4 | t | t | t | t | t | t | t | t |
| *n*-Nonanal | 1073 | 1.1 | 0.4 | 0.4 | 0.6 | 0.7 | 1.0 | 0.6 | 0.6 | 0.4 | 0.6 | 0.5 |
| Linalool | 1074 | **64.0** | **72.6** | **59.6** | 0.1 | 0.2 | 0.1 | 0.1 | 0.1 | t | t | 0.4 |
| *n*-Undecane | 1100 | | | | t | t | t | 0.1 | t | t | t | t |
| Camphor | 1102 | 1.3 | 2.1 | 0.9 | t | t | t | t | t | t | t | t |
| Isopulegol | 1121 | 0.1 | 0.1 | t | | | | | | | | |
| 2-*trans*-Nonen-1-al | 1124 | | | | t | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | t | t |
| Borneol | 1134 | t | t | t | | | | | | | | |
| *n*-Nonanol | 1148 | | | | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | t | t | t |
| Terpinen-4-ol | 1148 | 0.2 | 0.2 | 0.1 | | | | | | | | |
| α-Terpineol | 1159 | 0.1 | 0.2 | 0.1 | | | | | | | | |
| 4-*cis*-Decenal | 1163 | | | | 0.7 | 1.1 | 1.0 | 1.1 | 1.1 | 1.0 | 1.1 | 0.6 |
| *n*-Decanal | 1180 | 1.9 | 0.7 | 1.6 | **30.2** | **28.1** | **26.2** | **29.4** | **29.3** | **13.2** | **19.3** | **23.5** |
| Pulegone | 1207 | | | | t | t | t | t | t | t | t | t |
| Citronellol | 1211 | 0.2 | 0.1 | 0.1 | | | | | | | | |
| Geraniol | 1236 | 0.8 | t | 0.9 | | | | | | | | |
| 2-*trans*-Decenal | 1236 | 3.3 | 1.9 | 1.4 | **40.1** | **40.7** | **39.2** | **36.7** | **38.0** | **63.3** | **49.3** | **39.1** |
| 2-*trans*-Decen-1-ol * | 1256 | | | | 1.0 | 1.2 | 1.7 | 1.8 | 1.7 | 0.6 | 0.7 | 0.5 |
| *n*-Decanol | 1259 | 0.2 | 0.1 | 0.4 | 1.3 | 1.3 | 1.7 | 1.7 | 1.8 | 0.6 | 0.5 | 0.3 |
| *p*-Cymen-7-ol | 1265 | 0.1 | t | t | | | | | | | | |
| 4-Vinylguaiacol | 1285 | | | | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | t | t | 0.1 |

| Components | RI | Accessions | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Fruits | | | Vegetative aerial parts | | | | | | | |
| | | Cs21_fr1 2021 | Cs21_fr2 2021 | Cs21_fr3 2021 | Cs22_lv1 2022 | Cs22_lv2 2022 | Cs22_lv3 2022 | ROMA 2022 | SANTO 2022 | Cs22_lv4 2022 | Cs22_lv5 2022 | Cs22_lv6 2022 |
| *n*-Undecanal | 1288 | 0.7 | 0.3 | 0.5 | 1.6 | 2.0 | 2.2 | 1.7 | 1.6 | 0.6 | 1.7 | 1.9 |
| Myrtenyl acetate | 1290 | t | t | 0.1 | | | | | | | | |
| 2-*trans*-Undecenal | 1334 | 0.1 | t | 0.1 | 3.7 | 4.0 | 5.0 | 2.6 | 3.0 | 4.4 | 6.2 | 6.0 |
| *trans*-2-Undecen-1-ol | 1355 | | | | 0.1 | 0.2 | 0.3 | 0.2 | 0.2 | t | 0.1 | t |
| 1-Undecanol | 1366 | | | | 0.7 | 0.1 | 0.2 | 0.2 | 0.2 | t | 0.1 | t |
| Geranyl acetate | 1370 | 1.7 | 1.4 | 4.5 | | | | | | | | |
| *n*-Dodecanal | 1397 | 0.3 | 0.1 | 0.2 | 1.6 | 1.4 | 1.7 | 1.9 | 1.8 | 1.4 | 1.9 | 2.4 |
| β-Caryophyllene | 1414 | 0.1 | t | t | | | | | | | | |
| 2-*trans*-Dodecenal | 1446 | 1.0 | 0.3 | 0.6 | 7.0 | 6.8 | 6.3 | 6.8 | 7.4 | 6.0 | 8.2 | 11.8 |
| 2-*trans*-Dodecen-1-ol | 1448 | | | | 0.1 | 0.1 | 0.2 | 0.2 | 0.2 | 0.1 | 0.1 | 0.1 |
| 1-Dodecanol | 1468 | | | | t | t | t | t | t | t | t | t |
| α-Amorphene | 1476 | | | | t | t | t | t | t | t | t | t |
| *n*-Tridecanal | 1499 | 0.1 | t | t | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.2 | 0.2 |
| *trans*-Nerolidol | 1549 | t | t | 0.1 | | | | | | | | |
| 2-*trans*-Tridecen-1-al | 1550 | | | | 0.3 | 0.3 | 0.5 | 0.4 | 0.4 | 0.2 | 0.3 | 0.6 |
| β-Caryophyllene oxide | 1561 | 0.3 | t | t | t | t | t | t | t | t | t | t |
| *n*-Tetradecanal | 1596 | t | t | t | 0.3 | 0.2 | 0.3 | 0.3 | 0.3 | 0.4 | 0.4 | 0.5 |
| T-Cadinol | 1616 | | | | t | 0.1 | 0.1 | 0.1 | 0.1 | t | t | t |
| α-Cadinol | 1630 | | | | t | t | t | t | t | t | t | t |
| 2-*trans*-Tetradecenal* | 1643 | 0.2 | 0.1 | 0.2 | 3.2 | 2.5 | 3.0 | 4.1 | 4.0 | 2.5 | 2.8 | 3.7 |
| Pentadecanal | 1688 | | | | t | t | t | t | t | t | t | t |
| Tetradecanoic acid (Myristic acid) | 1723 | 2.2 | 0.1 | 1.6 | | | | | | | | |
| 11-Pentadecenal * | 1735 | | | | 0.3 | 0.3 | 0.2 | 0.4 | 0.4 | 0.2 | 0.3 | 0.4 |
| Pentadecanoic acid * | 1776 | 0.1 | t | 0.1 | | | | | | | | |
| Palmitic acid (Hexadecanoic acid) | 1908 | 1.5 | 0.3 | 2.3 | | | | | | | | |
| Phytol acetate 2 | 2101 | | | | 0.2 | 0.2 | 0.3 | 0.2 | 0.2 | 0.4 | 0.4 | 0.3 |
| *n*-Nonadecanal * | 2102 | | | | 0.2 | 0.2 | 0.3 | 0.2 | 0.2 | 0.4 | 0.4 | 0.3 |
| Linoleic acid | 2108 | t | t | 0.2 | | | | | | | | |

| Components | RI | Accessions | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Fruits | | | Vegetative aerial parts | | | | | | | |
| | | Cs21_fr1 2021 | Cs21_fr2 2021 | Cs21_fr3 2021 | Cs22_lv1 2022 | Cs22_lv2 2022 | Cs22_lv3 2022 | ROMA 2022 | SANTO 2022 | Cs22_lv4 2022 | Cs22_lv5 2022 | Cs22_lv6 2022 |
| Petroselinic acid | 2128 | 0.1 | t | 0.6 | | | | | | | | |
| Eicosanal | 2200 | | | | t | t | t | t | t | t | t | t |
| **% Identification** | | 98.9 | 99.7 | 98.9 | 97.6 | 97.2 | 97.2 | 96.9 | 97.2 | 98.3 | 97.1 | 97.4 |
| **Grouped components** | | | | | | | | | | | | |
| Monoterpene hydrocarbons | | 16.9 | 18.6 | 22.0 | 0.6 | 0.7 | 1.0 | 1.1 | 0.9 | 0.8 | 0.8 | 1.3 |
| Oxygen-containing monoterpenes | | 68.8 | 76.8 | 66.5 | 0.2 | 0.3 | 0.2 | 0.2 | 0.2 | 0.1 | 0.1 | 0.5 |
| Sesquiterpene hydrocarbons | | 0.1 | t | t | t | t | t | t | t | t | t | t |
| Oxygen-containing sesquiterpenes | | 0.3 | t | 0.1 | t | 0.1 | 0.1 | 0.1 | 0.1 | t | t | t |
| Oxygen-containing diterpenes | | | | | 0.2 | 0.2 | 0.3 | 0.2 | 0.2 | 0.4 | 0.4 | 0.3 |
| Fatty acids | | 3.9 | 0.4 | 4.8 | | | | | | | | |
| Other fatty acid derivatives | | | | | 94.3 | 92.6 | 92.5 | 91.8 | 93.7 | 96.6 | 95.0 | 93.2 |
| Others | | 8.9 | 3.9 | 5.5 | 2.3 | 3.3 | 3.1 | 3.5 | 2.1 | 0.4 | 0.8 | 2.1 |

RI: In-lab calculated retention index relative to $C_8$-$C_{23}$ *n*-alkanes on the DB-1 column. t: traces (t < 0.05%). * Identification based on mass spectrum only. Bold: dominant compounds relevant for each cluster.

**Table S2.** Percentage composition of the EOs isolated by hydrodistillation, from *Foeniculum vulgare* fruit accessions grown at the experimental field of Banco Português de Germoplasma Vegetal. For samples codes, see Table 1.

| Components | RI | Accessions | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | **Fv20 _P1 2020** | **Fv20 _P2 2020** | **Fv20 _B 2020** | **Fv20 _VR1 2020** | **Fv20 _VR2 2020** | **Fv20 _VR3 2020** | **Fv20 _VC1 2020** | **Fv20 _VC2 2020** | **Fv20 _VC3 2020** | **Fv20 _CB 2020** | **Fv21 _VR1 2021** | **Fv21 _VR2 2021** | **Fv21 _VR3 2021** | **Fv21 _VR4 2021** | **Fv21 _VR5 2021** | **Fv21 _VC1 2021** | **Fv21 _VC2 2021** | **Fv21 _VC3 2021** | **Fv21 _VC4 2021** |
| α-Thujene | 924 | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t |
| α-Pinene | 930 | 0.7 | 0.6 | 0.7 | 0.9 | 0.8 | 1.6 | 0.4 | 0.4 | 0.7 | 0.9 | 2.7 | 1.3 | 1.0 | 1.2 | 1.1 | 2.1 | 1.1 | 0.5 | 1.1 |
| Camphene | 938 | 0.3 | 0.3 | 0.2 | 0.3 | 0.1 | 0.3 | 0.2 | 0.1 | 0.1 | 0.3 | 0.1 | 0.2 | 0.2 | 0.4 | 0.3 | 0.3 | 0.3 | 0.2 | 0.3 |
| Sabinene | 958 | 0.3 | 0.2 | 0.3 | 0.2 | 0.1 | 0.5 | 0.2 | 0.2 | 0.1 | 0.4 | 0.3 | 0.5 | 0.6 | 0.6 | 0.6 | 0.4 | 0.4 | 0.6 | 0.3 |
| β-Pinene | 963 | 0.1 | 0.1 | 0.1 | 0.2 | 0.1 | 0.2 | 0.5 | t | 0.1 | 0.1 | 0.4 | t | 0.5 | 0.1 | 0.1 | 0.3 | 0.3 | 0.4 | 0.2 |
| β-Myrcene | 975 | 0.9 | 1.3 | 0.7 | 1.0 | 1.1 | 1.5 | 1.0 | 0.6 | 0.4 | 1.3 | 0.6 | 0.9 | 0.8 | 1.2 | 1.4 | 1.2 | 0.9 | 1.5 | 1.0 |
| α-Phellandrene | 995 | 0.3 | 0.2 | 0.4 | 0.4 | 0.3 | 0.3 | 0.4 | 0.3 | 0.2 | 0.3 | 0.4 | 0.6 | 0.4 | 0.8 | 0.5 | 0.8 | 0.5 | 1.2 | 0.6 |
| α-Terpinene | 1002 | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t |
| *p*-Cymene | 1003 | 0.1 | t | 0.1 | 0.2 | t | 0.1 | 0.1 | 0.1 | 0.1 | 0.2 | 0.1 | t | 0.2 | t | 0.2 | 0.1 | t | 0.1 | 0.1 |
| 1,8-Cineole | 1005 | 0.8 | 0.3 | 0.7 | 0.7 | 1.0 | 1.6 | 0.5 | 0.8 | 0.3 | 1.2 | 0.6 | 1.1 | 1.0 | 2.0 | 1.6 | t | 1.1 | 1.3 | 1.0 |
| β-Phellandrene | 1005 | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | 1.1 | t | t | t |
| Limonene | 1009 | 3.6 | 4.9 | 3.1 | 3.4 | 3.5 | 3.3 | 2.8 | 1.4 | 1.9 | 2.5 | 1.3 | 2.1 | 7.1 | 5.1 | 2.6 | 2.2 | 2.7 | 3.8 | 2.2 |
| *cis*-β-Ocimene | 1017 | t | t | t | 0.1 | t | 0.1 | t | t | t | 0.1 | t | t | t | t | t | t | t | t | t |
| *trans*-β-Ocimene | 1027 | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t |
| γ-Terpinene | 1035 | 1.0 | 0.4 | 0.9 | 1.1 | 0.3 | 1.0 | 1.1 | 0.3 | 0.4 | 1.6 | 0.8 | 0.5 | 2.2 | 0.3 | 2.4 | 0.7 | 0.6 | 1.3 | 0.9 |
| *trans*-Sabinene hydrate | 1037 | 0.2 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | t | 0.1 | 0.2 | 0.1 | 0.2 | 0.1 | t | t | 0.1 |
| Fenchone | 1050 | **32.1** | **34.1** | **21.0** | **22.5** | **29.6** | **22.5** | **26.2** | **17.5** | **17.3** | **25.9** | **15.8** | **26.8** | **23.1** | **28.9** | **24.4** | **17.8** | **19.2** | **13.6** | **27.3** |
| 6,7-Myrcene epoxide | 1064 | | | | | | | | | | | t | t | t | t | t | t | t | t | t |
| Terpinolene | 1064 | 0.2 | 0.3 | 0.1 | 0.1 | 0.1 | 0.2 | 0.3 | 0.1 | 0.1 | 0.2 | t | 0.1 | 0.2 | 0.2 | 0.2 | 0.1 | 0.1 | t | 0.2 |
| *cis*-Sabinene hydrate | 1066 | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t |
| Linalool | 1074 | | | | | | | | | | | t | 0.4 | t | 0.1 | t | t | | | t |
| Isopentyl isovalerate | 1080 | | | | | | | | | | | t | | t | t | t | t | t | t | t |
| α-Fenchol (*endo*-Fenchol) | 1085 | | | | | | | | | | | t | t | 0.2 | t | 0.2 | t | t | t | t |
| Camphor | 1102 | 0.7 | 0.7 | 0.4 | 0.5 | 0.6 | 0.5 | 0.5 | 0.4 | 0.2 | 0.5 | 0.3 | 0.5 | 0.5 | 0.5 | 0.5 | 0.3 | 0.4 | 0.2 | 0.5 |
| δ-Terpineol | 1134 | | | | | | | | | | | | t | t | t | t | | t | | |
| Terpinen-4-ol | 1148 | 0.1 | 0.1 | t | t | t | 0.1 | t | 0.1 | t | 0.1 | t | t | 0.1 | t | 0.1 | t | t | t | t |

| Components | RI | Accessions | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | **Fv20_P1 2020** | **Fv20_P2 2020** | **Fv20_B 2020** | **Fv20_VR1 2020** | **Fv20_VR2 2020** | **Fv20_VR3 2020** | **Fv20_VC1 2020** | **Fv20_VC2 2020** | **Fv20_VC3 2020** | **Fv20_CB 2020** | **Fv21_VR1 2021** | **Fv21_VR2 2021** | **Fv21_VR3 2021** | **Fv21_VR4 2021** | **Fv21_VR5 2021** | **Fv21_VC1 2021** | **Fv21_VC2 2021** | **Fv21_VC3 2021** | **Fv21_VC4 2021** |
| $\alpha$-Terpineol | 1159 | t | t | t | t | t | t | t | t | t | t | t | 0.1 | 0.1 | 0.1 | 0.2 | t | | t | t |
| Estragole (Methyl chavicol) | 1163 | **3.2** | **6.2** | **22.5** | **11.9** | **37.0** | **34.0** | **56.7** | **68.5** | **51.7** | **45.0** | **75.5** | **42.3** | **23.1** | **14.8** | **34.1** | **59.4** | **57.5** | **35.1** | **27.1** |
| *p*-Anisaldehyde | 1210 | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t |
| *cis*-Anethole | 1220 | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t | t |
| *trans*-Anethole | 1254 | **55.3** | **50.1** | **48.5** | **56.3** | **25.2** | **32.0** | **8.9** | **8.9** | **26.2** | **19.2** | **1.0** | **22.4** | **38.4** | **43.5** | **29.2** | **13.0** | **14.8** | **40.1** | **37.0** |
| Palmitic acid (Hexadecanoic acid) | 1908 | t | t | t | t | t | t | t | t | t | t | | | | | | | | | |
| **% Identification** | | 99.9 | 99.9 | 99.8 | 99.9 | 99.9 | 99.9 | 99.9 | 99.8 | 99.9 | 99.9 | 99.9 | 99.9 | 99.9 | 99.9 | 99.9 | 99.9 | 99.9 | 99.9 | 99.9 |
| **Grouped components** | | | | | | | | | | | | | | | | | | | | |
| Monoterpene hydrocarbons | | 7.5 | 8.3 | 6.6 | 7.9 | 6.4 | 9.1 | 7.0 | 3.5 | 4.1 | 7.9 | 6.7 | 6.2 | 13.2 | 9.9 | 9.4 | 9.3 | 6.9 | 9.6 | 6.9 |
| Oxygen-containing monoterpenes | | 33.9 | 35.3 | 22.2 | 23.8 | 31.3 | 24.8 | 27.3 | 18.9 | 17.9 | 27.8 | 16.7 | 29.0 | 25.2 | 31.7 | 27.2 | 18.2 | 20.7 | 15.1 | 28.9 |
| Phenylpropanoids | | 58.5 | 56.3 | 71.0 | 68.2 | 62.2 | 66.0 | 65.6 | 77.4 | 77.9 | 64.2 | 76.5 | 64.7 | 61.5 | 58.3 | 63.3 | 72.4 | 72.3 | 75.2 | 64.1 |
| Others | | t | t | t | t | t | t | t | t | t | t | | | | | | | | | |

RI: In-lab calculated retention index relative to $C_9$-$C_{20}$ *n*-alkanes on the DB-1 column. t: traces (t < 0.05%). Bold: dominant compounds relevant for each cluster.