**Table S9.** Compounds with high contribution to the PC1 and PC2 in Figure 6

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Code** | **Compound** | **Class** | **PC1** | **PC2** |
| 233 | *β*-elemene | sesquiterpene | 0.97 | 0 |
| 266 | (*E*, *Z*)-2,6-dodecadienal | aldehyde | 0.96 | 0 |
| 210 | δ-eiemene | sesquiterpene | 0.96 | 0 |
| 277 | (*E*)-2-dodecenal | aldehyde | 0.96 | 0 |
| 296 | (-)-*cis-beta*-elemene | sesquiterpene | 0.96 | 0 |
| 197 | undecanal | aldehyde | 0.96 | 0 |
| 256 | *γ*-elemene | sesquiterpene | 0.96 | 0.01 |
| 260 | guaia-6,9-diene | sesquiterpene | 0.96 | 0 |
| 202 | (2*E*, 4*E*)-decadienal | aldehyde | 0.96 | 0.01 |
| 318 | germacrene B | sesquiterpene | 0.96 | 0 |
| 274 | RI1493 | sesquiterpene | 0.95 | 0 |
| 284 | *δ*-selinene | sesquiterpene | 0.95 | 0 |
| 320 | *trans*-nerolidol | alcohol | 0.94 | 0.02 |
| 265 | *cis*-muurola-3,5-diene | sesquiterpene | 0.93 | 0.03 |
| 315 | selina-3,7(11)-diene | sesquiterpene | 0.93 | 0.03 |
| 94 | (3*E*)-4,8-dimethylnona-1,3,7-triene | aromatic hydrocarbon | 0.57 | 0.38 |
| 154 | *trans*-8-*p*-menthen-2-one | ketone | 0.54 | 0.39 |
| 116 | 2,6-dimethylocta-1,5,7-trien-3-ol | alcohol | 0.33 | 0.55 |
| 128 | (*E*)-2-nonenal | aldehyde | 0.30 | 0.54 |
| 102 | *cis*-limonene oxide | epoxide | 0.26 | 0.45 |
| 26 | camphene | monoterpene | 0.19 | 0.47 |
| 107 | 2-methyl-6-methylideneocta-1,7-dien-3-one | ketone | 0.16 | 0.68 |
| 198 | nonyl acetate | ester | 0.15 | 0.37 |
| 352 | octadecane | aromatic hydrocarbon | 0.08 | 0.58 |
| 348 | heptadecane | aromatic hydrocarbon | 0.02 | 0.47 |