**Table S7.** Compounds with high contribution to the PC1 and PC2 in Figure 3

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Code** | **Compound** | **Class** | **PC1** | **PC2** |
| 159 | elemene isomer | sesquiterpene | 0.87 | 0.03 |
| 27 | 2-hexenal | aldehyde | 0.86 | 0.02 |
| 8 | toluene | aromatic hydrocarbon | 0.82 | 0.06 |
| 17 | hexanal | aldehyde | 0.80 | 0.13 |
| 94 | *trans-β*-ocimene | monoterpene | 0.79 | 0.00 |
| 189 | *γ*-gurjunene | sesquiterpene | 0.77 | 0.15 |
| 64 | 1-octen-3-one | ketone | 0.76 | 0.13 |
| 170 | (-)-*β*-bourbonene | sesquiterpene | 0.76 | 0.15 |
| 150 | geranial | aldehyde | 0.76 | 0.17 |
| 185 | geranylaceton | ketone | 0.76 | 0.00 |
| 183 | aromandendrene | sesquiterpene | 0.75 | 0.05 |
| 68 | 6-methyl-5-hepten-2-one | ketone | 0.74 | 0.16 |
| 165 | *α*-ylangene | sesquiterpene | 0.74 | 0.19 |
| 66 | 3-octenol | alcohol | 0.73 | 0.25 |
| 197 | epizonarene | sesquiterpene | 0.73 | 0.18 |
| 180 | (*Z*)-caryophyllene | sesquiterpene | 0.53 | 0.42 |
| 54 | 4-methylhexanol | alcohol | 0.55 | 0.43 |
| 46 | heptanal | aldehyde | 0.48 | 0.44 |
| 6 | (*E*)-2-pentenal | aldehyde | 0.15 | 0.45 |
| 96 | 2-nonanone | ketone | 0.42 | 0.48 |
| 63 | heptanol | alcohol | 0.31 | 0.51 |
| 41 | 2-heptanone | ketone | 0.26 | 0.56 |
| 131 | (*E*)-2-nonenol | alcohol | 0.12 | 0.58 |
| 107 | octanol | alcohol | 0.37 | 0.59 |
| 43 | 2-butylfuran | furan | 0.19 | 0.71 |