**Table S5.** ICC values within different adsorbents including the 30 most common peaks for each adsorbent, and ICC values when data are adjusted for peaks in adjacent rel RT intervals.

| | | Adsorbent | | |
|---|---|---|---|---|
| Suggested names | Rel RT | C106 | CB | TTA |
| 2-Methyl-pentane | | -0,329 | 0,347 | |
| Pentane | 57,7 | 0,103 | | |
| Benzene | 73,2 | 0,663 | 0,468 | 0,631 |
| 3-Methyl-hexane | 75,7 | | 0,824 | |
| Heptane | 81,7 | 0,334 | 0,488 | 0,58 |
| Toluene | 100,2 | 0,618 | 0,29 | 0,658 |
| Hexanal | 107,7 | 0,054 | 0,136 | 0,612 |
| Tetrachloroethylene | 110,7 | 0,393 | 0,09 | 0,126 |
| Compound with very low qualifier | 112,2 | 0,089 | | |
| Ethylbenzene | 122,7 | | 0,341 | |
| Ethylbenzene | 123,2 | 0,182 | 0,331 | 0,194 |
| 1,3-Dimethyl-benzene | 124,7 | 0,398 | 0,463 | 0,137 |
| Styrene | 129,7 | 0,371 | 0,695 | 0,084 |
| 1,2-Dimethyl-benzene | 130,2 | 0,355 | 0,738 | 0,165 |
| Heptanal | 130,7 | 0,655 | 0,115 | 0,899 |
| alpha-Pinene | 139,2 | -0,021 | 0,759 | 0,482 |
| Camphene | 142,7 | | 0,293 | 0,693 |
| Benzaldehyde | 144,2 | | 0,363 | |
| Benzaldehyde | 144,7 | 0,414 | 0,571 | |
| Benzaldehyde | 145,2 | | 0,402 | |
| 1,3,5-Trimethyl-benzene | 145,7 | | 0,056 | |
| 6-Methyl-5-hepten-2-one | 148,2 | | 0,315 | |
| beta-Myrcene | 148,7 | | 0,915 | 0,732 |
| Decane | 149,7 | | | 0,141 |
| 1,2,3-Trimethyl-benzene | 150,7 | | 0,393 | 0,57 |
| Octanal | 151,2 | 0,229 | | |
| 2-Ethyl-1-hexanol | 155,7 | 0,195 | | |
| 1-Methyl-2-(1-Methylethyl)-Benzene | 156,2 | | 0,226 | |
| 1-Methyl-2-(1-Methylethyl)-Benzene | 156,7 | 0,22 | 0,829 | |
| D-Limonene | 157,2 | 0,965 | 0,798 | 0,943 |
| Eucalyptol | 158,2 | | | 0,701 |
| Acetophenone | 164,7 | -0,058 | | |
| Undecane | 167,7 | 0,905 | | 0,643 |
| 1-Methyl-4-(1-methylethenyl)-benzene | 168,7 | | | 0,895 |
| 1-Methyl-4-(1-methylethenyl)-benzene | 169,2 | 0,662 | -0,014 | 0,574 |
| 1,3-Diethenyl-benzene | 172,7 | -0,288 | | |
| 5-Methyl-2-(1-methylethyl)-cyclohexanone | 179,7 | | | 0,828 |
| (2-Methyl-1-butenyl)-benzene | 181,2 | -0,027 | | |
| Dodecane | 183,7 | | | 0,132 |
| Dodecane | 184,2 | -0,093 | | |
| Decanal | 185,7 | | -0,043 | |
| Naphthalene | 186,2 | 0,568 | | |
| Naphthalene | 186,7 | 0,45 | | |
| Nonanoic acid | 193,2 | | | 0,44 |

| | | | | |
|---|---|---|---|---|
| Phthalic anhydride | 205,7 | | 0,437 | |
| 1-[4-(1-Methylethenyl)phenyl]-ethanone | 211,7 | | | -0,127 |
| Tetradecane | 214,7 | | | 0,405 |
| Nonadecane | 226,2 | | | 0,172 |
| Butylated Hydroxyanisole | 226,7 | 0,214 | | -0,16 |
| 1-(6,6-Dimethylbicyclo[3.1.0]-hex-2-en-2-yl)-ethanone | 227,7 | | | 0,467 |
| Long aliphate 1 | 241,7 | 0,682 | | |
| 2,2,4-Trimethyl-pentanoic acid | 243,7 | | -0,073 | 0,552 |
| Long aliphate 2 | 278 | | | 0,447 |
| 1-Chloro-heptacosane | 284 | 0,889 | 0,267 | 0,971 |
| Long aliphate 3 | 312 | | 0,658 | |
| | | | | |
| Median | | 0,3445 | 0,363 | 0,552 |
| Min | | -0,329 | -0,073 | -0,16 |
| Max | | 0,965 | 0,915 | 0,971 |