

Estimating the octanol-water partition coefficients of NPAHs and PAHs by solid-phase microextraction and gas chromatography-ion trap detector

The solid-phase microextraction technique (SPME) was used for the measurement of the partition coefficients of eight nitro polycyclic aromatic hydrocarbons (NPAHs) and ten polycyclic aromatic hydrocarbons (PAHs) between the polymeric coating of polydimethylsiloxane used in SPME and water (K-SW). The results demonstrate that the technique is simple, rapid, and reproducible, and thus provides a viable alternative to the conventional methods used for such measurements. There is a strong linear correlation between $\log K_{\text{SW}}$ and the commonly used $\log K_{\text{OW}}$ (octanol - water partition coefficient) for PAHs, NPAHs, PCBs, and simple aromatics. The $\log K_{\text{OW}}$ values for NPAHs range from 2.78 to 4.75, and exhibit a general increase in value with increasing molecular weight. NPAHs are thus noticeably less hydrophobic than their parent PAHs counterparts, for which the $\log K_{\text{OW}}$ values range from 3.35 to 5.20.