

Determination of poly(dimethyl)siloxane-water partition coefficients for selected hydrophobic organic chemicals using ^{14}C -labeled analogs

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ABSTRACT

Aqueous solutions of ^{14}C -labeled analogs of seven hydrophobic organic chemicals (HOCs) were subject to solid-phase microextraction (SPME) under static conditions to assess their multi-compartment distribution and to compare poly(dimethyl)siloxane (PDMS)–water partition coefficients (K_{fs}) with previously reported values. To accomplish this, a protocol for quantitative desorption of radiolabelled HOCs from SPME fibers using hexane was developed. Time series extractions indicated that loading of SPME fibers had reached steady-state by Day 8 for PCB 52, 77 and 153, phenanthrene, benzo[a]pyrene, *p,p'*-DDT and *p,p'*-DDE. The recovery of spiked radioactivity among the (residual) aqueous phase, the PDMS coating, and all remaining wetted experimental surfaces ranged between 80 to 120%. K_f values based on ^{14}C -labeled analogs were in good agreement with previously published values that were determined at (or closely approaching) equilibrium conditions and without significant chemical depletion and/or uncorrected system losses. Because it allows for the direct determination of HOCs associated with the residual aqueous and experimental surface compartments, the use of radiolabelled HOC analogs is a powerful tool in discriminating among competing sorptive compartments encountered in most SPME fiber calibration methodologies employed to date.

Full Text

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