Partitioning of Drug Analogs in Adsorbent Phases

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Polydimethylsiloxane (PDMS) is currently employed for sampling volatile and semivolatile compounds in the field, extracting compounds such as pesticides from the air and protecting them until laboratory analysis. PDMS coated glass fibers have recently been proposed to extract and concentrate analytes from breath. The ability to rapidly detect legal and illegal drugs by non-invasive methods is critical to law enforcement. Designer drugs, analogs of illegal drugs that are created to bypass legal restriction, present a moving target for drug quantitation by breath analysis. They are created by small modifications to the functional groups of an illegal drug, creating an unregulated product that may be more potent than the original drug. Here, we determine chemical-specific partitioning constants ($K_{PDMS/AIR}$) for drug analogs as a function of temperature, which are required for breath sampling applications. Our long-term goal is to accurately predict $K_{PDMS/AIR}$ for new drug analogs without any experimental input. To isolate the effect of functional groups, we determine $K_{PDMS/AIR}$ from isothermal gas chromatography retention time measurements for a variety of alkylbenzenes and phenethylamine derivatives. We present experimental values for these chemicals, which are structurally related to the Class II drugs amphetamine and methamphetamine, and a preliminary group contribution model that predicts $K_{PDMS/AIR}$ from first-order chemical structure.