

Abstract

Perfluorinated compounds are organic compounds in which all hydrogen atoms in a carbon chain are substituted with fluorine atoms. These compounds are highly stable, persistent and bioaccumulative. They are purely anthropogenic compounds contained in biota and abiota. Partition coefficient between n-octanol and water is the essential toxicological parameter of a compound. This parameter helps us to assess behaviour of compound in the environment as well as in the living organisms.

The shake flask method and the RP-HPLC method were employed to measure the K_{ow} of nine perfluorinated acids. Using the shake flask method, the surface activity of compounds and the acid dissociation caused false results of the measurement. But behaviour of these compounds in the environment can be assess. Accurate and precise results were measured by the RP-HPLC method using an acetate buffer. Log K_{ow} of perfluoro-carboxylic acids, with the carbon chain length of 5-14, were found out, their final value ranging between 1.66 and 5.10. Log K_{ow} of acid with 12 carbons was estimated based on the linear regression of dependence of log K_{ow} on the number of carbons. There were significant differences in the results obtained by various software. Thus, the results cannot be considered relevant. These software are not suitable for the calculation of log K_{ow} of perfluorinated compounds.

Key words: Perfluorinated acids, n-octanol/water, partition coefficient, shake flask, RP-HPLC.