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Structure-activity Relationships of Perfluoro Alkane Acids for Bioconcentraion

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1. Introduction

The tendency of chemicals to bioconcentrate in biota is generally expressed as a bioconcentration factor (BCF), defined as the ratio of the chemical concentration in biota to its steady state environment. Bioconcentration is thought to be the partitioning of compounds between the lipid phase of an organism and the water phase. A number of simple relationships have been reported between the octanol to water partition coefficient (Pow) and the BCF for fish [1]. These relationships take the general form:

$$\log BCF = a \log Pow + b \qquad (1)$$

where a is an empirical constant usually having a value approaching unity and b is an empirical constant with values ranging from -1 to -2. The BCF for chemicals with logPow values exceeding 6, was lower than that expected based on values extrapolated from the linear relationship [2].

For perfluoro alkane acids (PFAs) with a certain chain length, high BCF of fish greater than 10000 were reported [3]. However, it is known that equation (1) cannot be applied to PFAs. The reason for this is thought that PFAs cannot be assumed passive diffusion because PFAs can bind to some protein in blood and liver [4].

Recently, BCF for a series of PFAs have been measured under the activity of “Safety Inspections for Existing Chemical Substances under Japanese Chemical Substances Control Law (CSCL)” [5]. In this study we investigated the relationship between logBCF and calculated logPow of the PFAs by using this dataset.

2. Method

Measured bioconcentraion data for six PFAs (Perfluorooctanoic acid, Perfluoroundecanoic acid, Perfluorododecanoic acid, Perfluorotetradecanoic acid, Perfluorohexadecanoic acid, Perfluorooctadecanoic acid) are used in this study. The bioconcentration test for chemical substances in the CSCL is conducted as a part of the 305 method established by “The Organization for Economic Co-operation and Development (OECD) guidelines for the Testing of Chemicals” [5]. The test fish (carp) is exposed to two concentrations of the test chemical in water under flow-through conditions. The mean of the last three observed points of the BCF value under the lower concentration test condition was used as the average BCF value for each of the chemicals. The values for the logPow were calculated using the CLOGP and the KOWWIN program.

3. Results and Discussion

Figure 1 shows the relationship between logBCF and calculated logPow of the 6 PFAs. Parabolic relationships with high coefficient of correlations are obtained in both cases using the calculated logPow by CLOGP and KOWWIN whereas the logPow calculated by CLOGP and KOWWIN for same compounds are largely different.

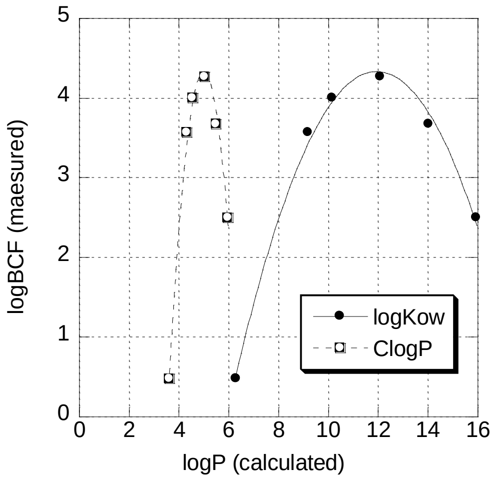

Fig1 relationship between logBCF and calculated logPow of the 6 PFAs

ClogP:	$y=-2.02(\log P)^2+20.1\log P-45.9$	r=0.997	(2)
KOWWIN	$y=-0.119(\log P)^2+2.85\log P-12.7$	r=0.997	(3)

Although the ranges of logPow are different these relationships (eq.2,3) are similar to that for general organic compound previously reported [2]. This result implies that the mechanism of bioconcentration of PFAs can be explained by passive diffusion.

References

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