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Evaluation of Bioconcentration Factors for Chemicals by using Category Approach.

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1. Introduction

Today, it is expected to utilize the evaluation method, for human and ecological hazards, such as QSAR, category approach and read-across, without making actual tests sacrificing animals and fishes in view of animal protection and cost saving.

The category approach is a risk evaluation method for untested chemicals by classifying the chemicals with known hazard properties by its chemical structure, physical-chemical properties and meaningful rules (categorization). This method has been developing internationally; especially OECD is developing intensively the OECD QSAR Application Toolbox (OECD Toolbox) [1]. The OECD Toolbox incorporates various database of hazard test data for chemicals provided by OECD countries and corporations. And it also provides the functions for supporting the category creation together with calculation of various descriptors such as logKow.

NITE has been developing the effective utilization of various evaluation methods for biodegradation and bioaccumulation. In the present research, we investigated the evaluation method for the bioaccumulation of chemicals in fish by using the category approach.

2. Method

In the development of categories, it is necessary to analyze the data of high reliability. For this purpose, we studied in detail the bioaccumulation test data for fish from the inventory of existing chemicals under the Chemical Substance Control Law (CSCL) and screened 511 chemicals that are low molecular weight organic compound [2]. And it is selected and analyzed the data of 397 chemicals of which the test concentration are lower than water solubility.

For the development of category, OECD Toolbox ver.1.0 was used. KOWWIN ver.1.62 was used for the calculation of logKow [3].

3. Results and Discussion

The correlation between logKow and logBCF was found very good for “Single Ring Benzenes” and “Nitro-Benzenes” categories. Fig.1 shows the plot of Single Ring Benzenes (26 chemicals) which were defined by the following conditions:

- I. Benzene ring in basic structure
- II. Number of ring: 1
- III. Consisting elements: just H, C, and halogen
- IV. No double or triple bond in side chain

The single ring benzene category showed good correlation ($R^2=0.9253$). This result can be explained that the chemicals in this category are taken into the living body by the simple passive diffusion, due to the lack of the functional groups of hydrogen bonding or dissociation ability [4].

On the other hand, "Phosphate esters" or "esters" did not show the good correlation between logKow and logBCF. Fig.2 shows the plot of phosphate esters (10 chemicals). In this case, all chemicals showed $\log BCF \leq 3$ and weak correlation between logKow and logBCF. Those 10 chemicals can be divided into chemicals with aromatic ring in side chain (2 chemicals) and aliphatic chain chemicals (8 chemicals), and aliphatic chain chemicals of $\log Kow \leq 4$ were analogue chemicals (7 chemicals). Those 7 analogues showed similar structure, similar physical-chemical properties and low BCF, and for those chemicals it could be applied the read-across effectively.

As described above, the application of Category Approach to the evaluation of bioaccumulation of chemicals in fish can show more precise and more comprehensive evaluation by using the analogue information and prediction basis for each untested chemicals.

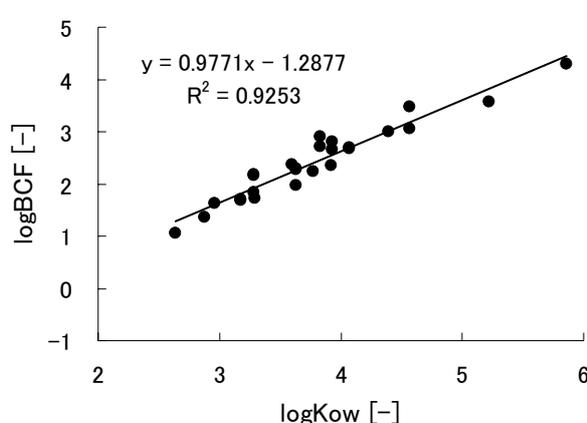


Fig.1 logKow vs. logBCF plot
(Single Ring Benzenes category)

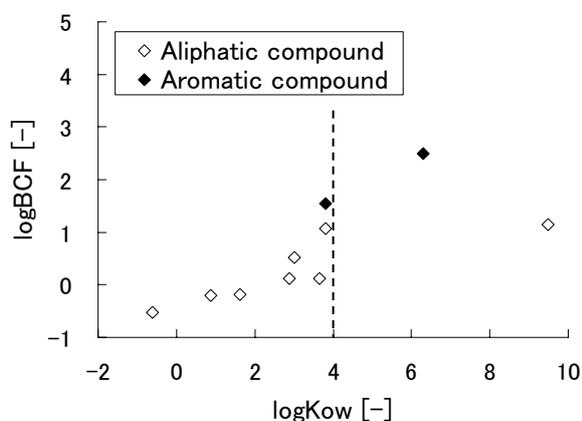


Fig.2 logKow vs. logBCF plot
(Phosphate esters category)

References

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4. Gennis RB., *Biomembranes: Molecular Structure and Function*, **1989**, 235-267.