RELATIONS BETWEEN WATER SOLUBILITY, TEST COCENTRATION AND BIOCONCENTRATION FACTOR IN BIOCONCENTRATION STUDY

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Abstract
The relation between the water solubility of a test substance and the nominal test concentration in the bio-concentration study was investigated, and analysis on the bioconcentration factor (BCF) obtained from the study was conducted. As a result, BCF obtained from the test concentration more than the water solubility have a difference according to the test concentration level about some substances with which high BCF data was obtained by the test concentration below the water solubility.
On the other hand, BCF obtained from the test concentration below the water solubility did not have a difference according to the test concentration level, and showed a steady state. If it is the test concentration below the water solubility, regardless of test concentration, the BCF will be obtained at a steady state, and it is judged that the proper degree of bio-concentration study is carried out.

Introduction
As for the super hydrophobic substance, the bio-concentration study is performed using the dispersant for preparing the stock solution. In order to prove that the proper BCF are obtained irrespective of the test concentration if the nominal test concentration is below the water solubility, relationships between the water solubility, the test concentration in the bio-concentration study and BCF was investigated.

Materials and Methods
Relations between the water solubility, the test concentration and BCF were investigated for existing substances which have more than 10-time differences between BCFs according to the test concentration and have the highest BCF of more than 100.

_Hydrogenated triphenyl (CAS 27985-87-1, K-448)
_Cyclododecane (CAS 294-62-2, K-467)
_Anthracene (CAS 120-12-7, K-74)
_Tetrabromopentane (CAS 3229-00-3, K-450)
_2-(2-hydroxy-3,3-di-t-butylphenyl)-5-chlorobenzotriazole (CAS 3864-99-1, K-334)
_[2-hydroxy-4-(octyl)phenyl]phenylmethanone (CAS 1843-05-6, K-352)
_2,2'-methylenebis (4-methyl-6-tert-butylphenol) (CAS 119-47-1, K-825)

Results and Discussion
Measured values of the water solubility (column elution method) of the substances which showed the test concentration dependence of BCF, calculated values of water solubility (WSKOWWin, U.S. EPA) and BCF are shown in Table 1. Moreover, the relation between BCF and the test concentration was shown in Fig.1. According to the results of seven substances investigated, the difference of BCF according to the test concentration was observed at the test concentration more than the water solubility. However, this difference of BCF was not appeared at the test concentration about or lower than the water solubility. According to the mentioned above, it is concluded that the correct BCF can be obtained if the test concentration is below the water solubility even if the study is performed with a dispersant. In addition, when the concentration dependence of BCF is seen temporarily in the test concentration level, it is thought that a possibility that the study is done by the concentration more than the water solubility is high.
Since the Chemical Substances Control Law was established in Japan, the bio-concentration study has been performed with two different test concentrations where the lower test concentration is 10 times lower than the higher test concentration, and additional test with further low test concentration has been requested when BCF shows the dependence on the test concentration. Therefore, it is considered that the current system of bio-concentration study

offers a proper method for the evaluation of the bio-concentration potential.

Acknowledgements
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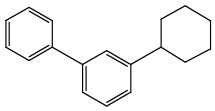
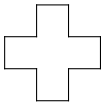
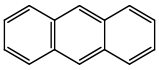
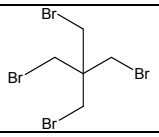
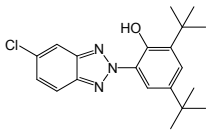
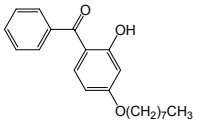
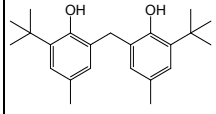
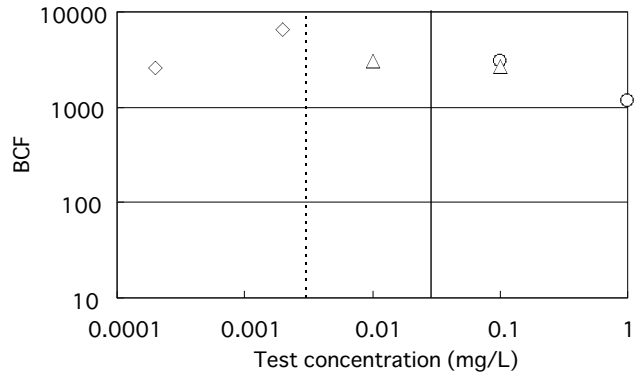
Table 1 Measured values of water solubility of test substances

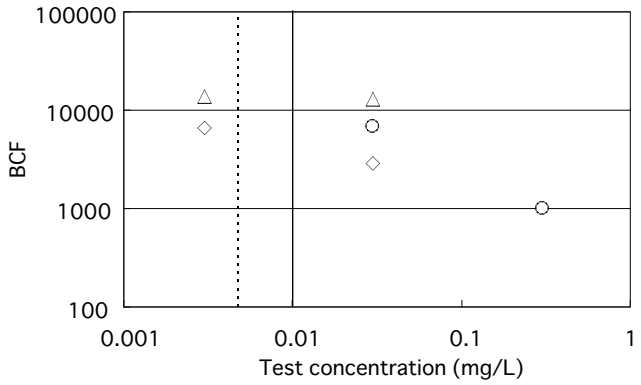
Substance (K-No)	Chemical structure	WS (purified water) (mg/L)	WS (test water) (mg/L)	WS (calculated*1) (mg/L)	Test concentration (mg/L)	BCF*2 1st –	BCF*2 2nd –	BCF*2 3rd –
Hydrogenated triphenyl (K-448)		0.0290	0.0349	0.00300	1	1165		
					0.1	3090	2708	
					0.01		3013	
					0.00199			6425*3
					0.000199			2550*3
Cyclododecane (K-467)		0.0102	0.0131	0.0047	0.3	1014		
					0.03	6813	12745	2853
					0.003		13938	6578
Anthracene (K-74)		0.0501	0.0499	0.0434	1.5	119	92	
					0.15	1225	1435	
					0.015		2448	2410
					0.0015			1618
Tetrabromopentane (K-450)		1.71	1.50	1.6	2	66		
					0.2	424		
					0.02	320		
2-(2-hydroxy-3,3-di-t-butylphenyl)-5-chlorobenzotriazole (K-334)		0.0000330		0.02628	0.4	1.0		
					0.04	6.0		
					0.001		910	
					0.0001		4875	7650
					0.00001			6625
[2-hydroxy-4-(octyl)phenyl]phenyl methanone (K-352)		0.00641		0.03693	0.5	26.5		
					0.05	39.8		
					0.002		180	
					0.0002		107	
2,2'-methylenebis (4-methyl-6-tert-butylphenol) (K-825)		0.0188		0.1235	1	25.0		
					0.1	113		
					0.002		700	
					0.0002		505	

*1 WSKOWWIN（U.S. Environmental Protection Agency, USA）
*2 Mean of last two values except not detection
*3 Weighted mean of 7 components

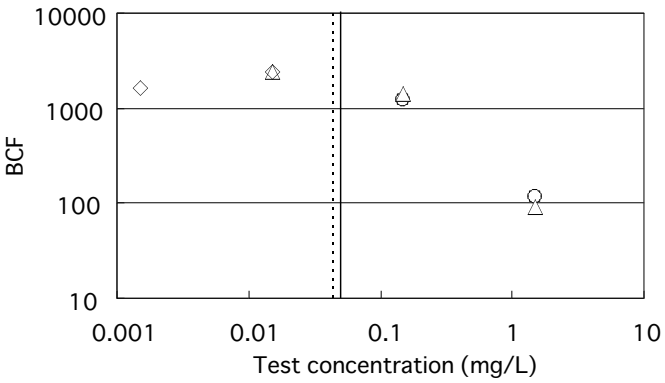
K-448



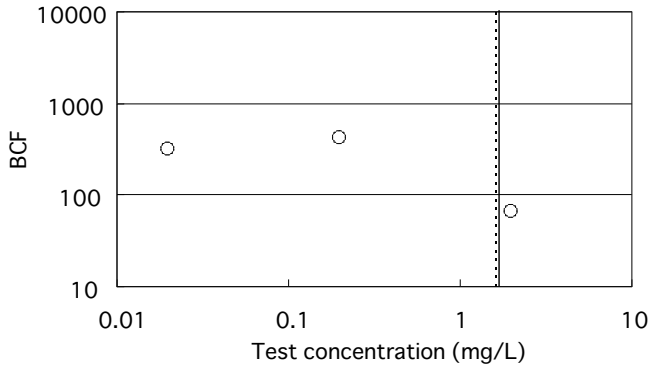
K-467



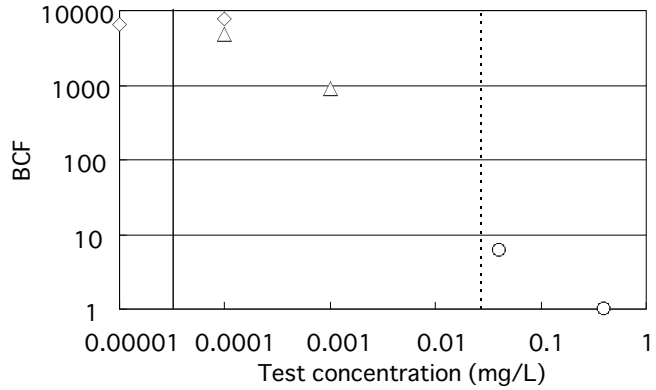
K-74



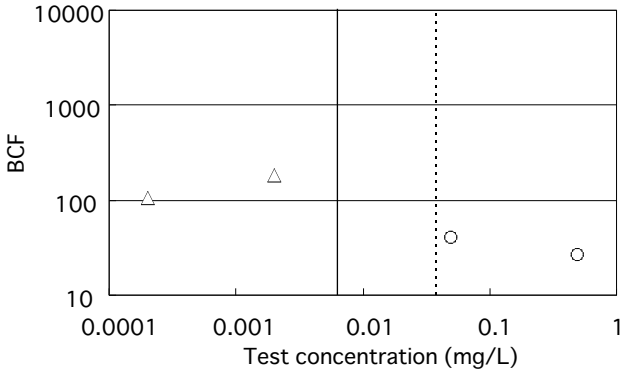
K-450



K-334



K-352



K-825

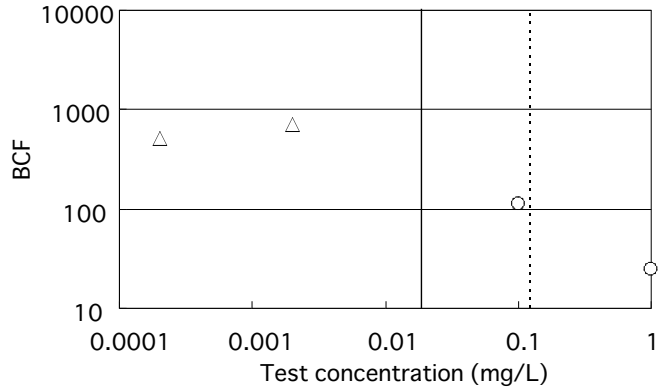


Fig. 1 Relationship between test concentration and BCF.
－：measured（purified water）、
---：calculated、
test number：_1st、_2nd、_3rd