



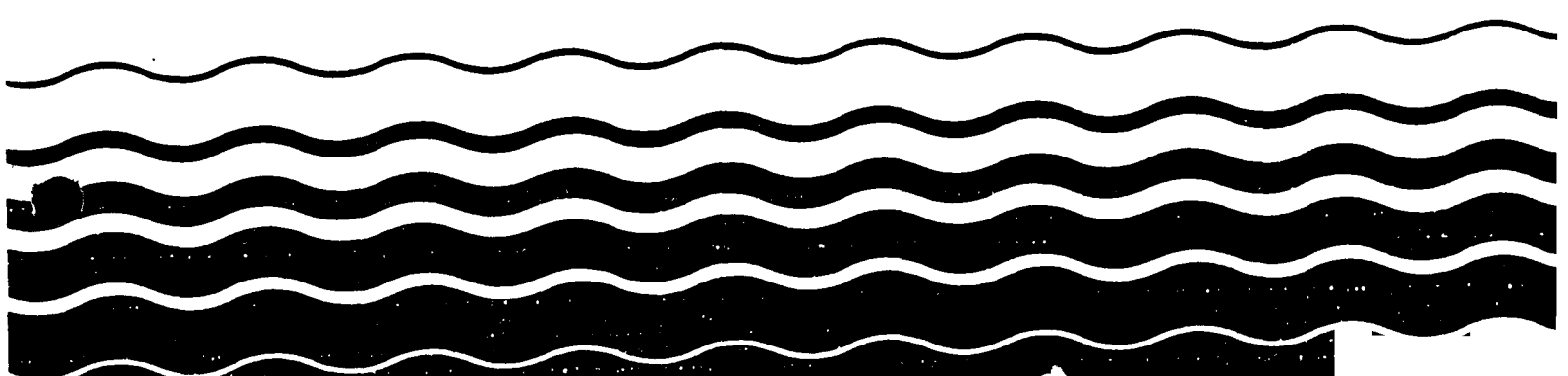
# Great Lakes Water Quality Initiative Technical Support Document for the Procedure to Determine Bioaccumulation Factors - July 1994

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**GREAT LAKES WATER QUALITY INITIATIVE  
TECHNICAL SUPPORT DOCUMENT FOR  
THE PROCEDURE TO DETERMINE BIOACCUMULATION FACTORS**

## **I. INTRODUCTION**

### **A. Purpose and Scope**

The purpose of this document is to provide the technical information and rational in support of the proposed procedures to determine bioaccumulation factors (BAFs). This document contains six sections: 1. Introduction; 2. BAFs based on the concentration of the freely dissolved chemical in water; 3. Prediction of bioconcentration factors (BCFs); 4. Food chain multipliers based on the 1993 Gobas model; 5. BAFs from biota-sediment accumulation factor (BSAF) measurements; 6. Bioaccumulation Equivalency Factors (BEFs); and 7. Derivation of BAFs for twenty-two chemicals.

Bioaccumulation factors are needed to determine both human health and wildlife Tier I water quality criteria and Tier II values. Also, they are used to define Bioaccumulative Chemicals of Concern among the Great Lakes Initiative universe of pollutants.

## **II. BAFs BASED ON THE CONCENTRATIONS OF THE FREELY DISSOLVED CHEMICALS IN WATER**

### **A. Relationship between BAFs reported on a total and freely dissolved basis**

The relationship between a BAF reported on the basis of the total concentration of the chemical in the water, i.e., freely dissolved plus that sorbed to particulate organic carbon (POC) and dissolved organic carbon (DOC), to a BAF reported on the basis of the freely dissolved concentration of the chemical in the water is as follows:

$$BAF_t^i = f_{fd} \bullet BAF_{fd}^i \quad (1)$$

where

$BAF_t^i$  = BAF (L/Kg of lipid) reported on the basis of the lipid-normalized concentration of chemical in the biota (Kg/Kg lipid) divided by the total concentration of the chemical in the water (Kg/L);

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$BAF_{fd}^{fd} = BAF$  (L/Kg of lipid) reported on the basis of the lipid-normalized concentration of chemical in the biota (Kg/Kg lipid) divided by the freely dissolved concentration of the chemical in the water (Kg/L);  
 $f_{fd}$  = fraction of the total chemical that is freely dissolved in the water.

#### **B. Determination of the fraction of the chemical that is freely dissolved in water**

The fraction of the chemical that is freely dissolved in the water,  $f_{fd}$ , can be determined using equation 2 with the  $K_{ow}$  for the chemical and the DOC and POC of the water.

$$f_{fd} = 1 / ( 1 + POC \bullet K_{ow} + DOC \bullet K_{ow} / 10 ) \quad (2)$$

where

POC = concentration of particulate organic carbon, Kg of organic carbon/L of water;  
DOC = concentration of dissolved organic carbon, Kg of organic carbon/L of water;  
 $K_{ow}$  = n-octanol/water partition coefficient.

#### **C. Derivation of the equation defining $f_{fd}$**

Experimental investigations have shown that hydrophobic organic chemicals exist in water in three phases, 1) the freely dissolved phase, 2) sorbed to suspended solids and 3) sorbed to dissolved organic matter (Hassett and Anderson (1979), Carter and Suffet (1982), Landrum et al. (1984), Gschwend and Wu (1985), McCarthy and Jimenez (1985), Eadie et al. (1990, 1992)). The total concentration of the chemical in water is the sum of the concentrations of the sorbed chemical and the freely dissolved chemical (Gschwend and Wu (1985) and Cook et al. (1993)):

$$C_w^t = C_w^{fd} + POC \bullet C_{poc} + DOC \bullet C_{doc} \quad (3)$$

where

$C_w^{fd}$  = concentration of freely dissolved chemical in the water, Kg of chemical/L of water;  
 $C_w^t$  = total concentration of the chemical in the water, Kg of chemical/L of water;  
 $C_{poc}$  = concentration of chemical sorbed to the particulate organic carbon in the water, Kg of chemical/Kg of organic carbon;

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- $C_{doc}$  = concentration of chemical sorbed to the dissolved organic carbon in the water, Kg of chemical/Kg of organic carbon;  
 $POC$  = concentration of particulate organic carbon, Kg of organic carbon/L of water;  
 $DOC$  = concentration of dissolved organic carbon, Kg of organic carbon/L of water.

The above equation can also be expressed using partitioning relationships as:

$$C_w^t = C_w^{fd} \bullet (1 + POC \bullet K_{poc} + DOC \bullet K_{doc}) \quad (4)$$

where

$$K_{poc} = C_{poc} / C_w^{fd} \quad \text{and} \quad K_{doc} = C_{doc} / C_w^{fd}$$

- $K_{poc}$  = equilibrium partition coefficient of the chemical between POC and the freely dissolved phase in the water,  
 $K_{doc}$  = equilibrium partition coefficient of the chemical between DOC and the freely dissolved phase in the water.

From equation 4, the fraction of the chemical which is freely dissolved in the water can be calculated using the following equations:

$$f_{fd} = C_w^{fd} / C_w^t \quad (5)$$

$$f_{fd} = 1 / (1 + POC \bullet K_{poc} + DOC \bullet K_{doc}) \quad (6)$$

Experimental investigations by Eadie et al. (1990, 1992), Landrum et al. (1984), Yin and Hassett (1986, 1989), Chin and Gschwend (1992), and Herbert et al. (1993) have shown that  $K_{doc}$  is directly proportional to the  $K_{ow}$  of the chemical and is less than the  $K_{ow}$ . The  $K_{doc}$  can be estimated using the following equation:

$$K_{doc} \approx K_{ow} / 10 \quad (7)$$

The above equation is based upon the results of Yin and Hassett (1986, 1989), Chin and Gschwend (1992), and Herbert et al. (1993). These investigations were done using unbiased methods, such as the dynamic headspace gas-partitioning (sparging) and the fluorescence methods, for determining the  $K_{doc}$ .

Experimental investigations by Eadie et al. (1990, 1992) and Dean et al. (1993) have shown that  $K_{poc}$  is approximately equal to the  $K_{ow}$  of the chemical. The  $K_{poc}$  can be estimated using the following equation:

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$$K_{poc} \approx K_{ow} \quad (8)$$

By substituting equations 7 and 8 into equation 6, the following equation is obtained:

$$f_{fd} \approx 1 / ( 1 + POC \bullet K_{ow} + DOC \bullet K_{ow} / 10 ) \quad (9)$$

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### III. PREDICTION OF BIOCONCENTRATION FACTORS (BCFs)

Numerous investigations have demonstrated a linear relationship between the logarithm of the bioconcentration factor (BCF) and the logarithm of the n-octanol/water partition coefficient ( $K_{ow}$ ) for lipophilic non-polar organic chemicals for fish and other aquatic organisms. Isnard and Lambert (1988) have listed various regression equations that illustrate this linear relationship. The underlying assumption for the linear relationship between the BCF and  $K_{ow}$  is that the bioconcentration process can be viewed as a partitioning of a chemical between the lipids of the aquatic organisms and water and that the  $K_{ow}$  is an useful surrogate for this partitioning process (Mackay (1982)).

The regression equations demonstrating the linear relationship between the logarithms of the BCF and  $K_{ow}$  have been developed using non-polar organic chemicals which are slowly, if at all, metabolized by fishes or other aquatic organisms. For metabolizable chemicals, the regression equations developed between BCF and  $K_{ow}$  for non-metabolizable chemicals in most cases predict BCFs which are larger than the measured BCFs. The losses of the chemicals due to metabolism are not accounted for in the simple partitioning model (Baron (1990), de Wolf et al. (1992)).

Mackay (1982) presented a thermodynamic basis for the partitioning process for bioconcentration and in essence, the BCF on a lipid-normalized basis (and freely dissolved concentration of the chemical in the water) should be similar if not equal to the  $K_{ow}$  for non-polar organic chemicals. Unfortunately, almost all of the reported regression equations have used BCFs reported on a wet weight basis instead of lipid-normalized. When regression equations are constructed using BCFs reported on a lipid-normalized basis, regression equations are obtained which have slopes and intercepts which are not significantly different from one and zero, respectively. For example, de Wolf et al. (1992) recalculated the linear relationship reported by Mackay (1982) assuming a 5% lipid content and obtained the following relationship:

$$\log \text{BCF} = 1.00 \log K_{ow} - 0.08 \quad (1)$$

For chemicals with large  $\log K_{ow}$ s, i.e. greater than 6.0, reported BCFs are often not equal to the  $K_{ow}$  for non-metabolizable chemicals. As discussed by Gobas et al. (1989), this non-equality between the BCF and  $K_{ow}$  is not caused by a breakdown of the BCF- $K_{ow}$  relationship but rather is caused by 1) not accounting for growth dilution which occurred during the BCF determination, 2) using the total concentration of the chemical in the water instead of the bioavailable (freely dissolved) concentration of the chemical in calculating the BCF, 3) not allowing

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sufficient time in the exposure to achieve steady-state conditions, and 4) not correcting for elimination of the chemical into the feces. BCFs for non-metabolizable chemicals are equal to the  $K_{ow}$  when the BCFs are reported on lipid-normalized basis, determined using the freely dissolved concentration of the chemical in the exposure water, corrected for growth dilution, determined from steady-state conditions or determined from accurate measurements of the chemical's uptake ( $k_1$ ) and elimination ( $k_2$ ) rate constants from and to the water, respectively, and determined using no solvent carriers in the exposure.

One option for the final GLWQI, is to estimate predicted BCFs using the following approximation:

$$BCF_i^{fd} \approx K_{ow} \quad (2)$$

where the  $BCF_i^{fd}$  is the BCF reported on lipid-normalized basis using the freely dissolved concentration of the chemical in the water. This relationship is applicable to lipophilic non-polar organic chemicals with  $\log K_{ow}$ s greater than 3 which are either slowly or not metabolized by aquatic organisms.

Equation 2 implicitly assumes that n-octanol is an appropriate surrogate for lipids in aquatic organisms. If n-octanol is not an appropriate surrogate for lipids, the slope and intercept of equation 2 will not be 1.0 and 0.0, respectively. The theoretical basis presented by Mackay (1982) and the experimental data suggest that n-octanol is a very reasonable surrogate for lipids.

Equation 2 is also supported and consistent with the food-chain model of Gobas (1993). For the Gobas model, the  $BCF_i^{fd}$  is equal to  $K_{ow}$  when the growth rate of the organisms and metabolism rate of the chemical by the organisms are set equal to zero. It should be noted that the model does not use the partitioning process described by Mackay (1982) for bioconcentration. Instead the food-chain model predicts the  $k_1$  and  $k_2$  rate constants for the fishes and the bioconcentration factor is determined by dividing the uptake rate constant from water ( $k_1$ ) by the elimination rate constant to water ( $k_2$ ).

The above equation is also supported and consistent with the equilibrium partitioning theory being developed by EPA for the derivation of sediment quality criteria (Di Toro et al. 1991). Both the sediment organic carbon-water equilibrium partition coefficient ( $\mu\text{g}$  of chemical/Kg of organic carbon in the sediment)/( $\mu\text{g}$  of freely dissolved chemical/L of sediment pore water) ( $K_{oc}$  or  $K_{oc}$ ) and the lipid/water equilibrium partition coefficient ( $\mu\text{g}$  of chemical/Kg of lipid)/( $\mu\text{g}$  of freely dissolved chemical/L of sediment pore water) ( $K_L$ ) have been demonstrated to be

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approximately equal to  $K_{ow}$  for non-polar organic chemicals in sediments and benthic organisms, respectively.

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#### IV. FOOD CHAIN MULTIPLIERS

Food chain multipliers (FCMs) for non-polar organic chemicals were determined using the model of Gobas (1993). This model includes both benthic and pelagic food chains thereby incorporating exposures of organisms to chemicals from both the sediment and the water column. This model does not predict FCMs but rather it predicts a) the chemical residues in the organisms and b) the freely dissolved concentration of the chemical in the water column. With this information, bioaccumulation factors (BAFs) for each species in the food chain can be predicted. FCMs can then be calculated from the predicted BAFs using the following equation:

$$FCM = BAF_i^{fd} / K_{ow} \quad (1)$$

where  $K_{ow}$  is the n-octanol/water partition coefficient for the chemical and  $BAF_i^{fd}$  is the BAF reported on a lipid-normalized basis using the freely dissolved concentration of the chemical in water.

##### A. Data for the Model

The data of Oliver and Niimi (1988) and Flint (1986) for Lake Ontario were used for the feeding preferences, weights, and lipid contents for each species in the food chain (Table 1). The mean water temperature of Lake Ontario was set to 8°C and the organic carbon content of sediment was set to 2.7% as reported by Oliver and Niimi (1988) (Table 1). Values for the densities of the lipid and organic carbon were taken directly from Gobas (1993) (Table 1). The metabolic transformation rate constant was set equal to zero. The organic carbon content of the water column was set to 0.0 kg/L (see B. Calculation of the FCMs).

With the values specified in Table 1, the remaining data needed for the model of Gobas (1993) are the concentrations of the chemical in the sediment and water column, and the  $K_{ow}$  of the chemical. The  $K_{ow}$  of the chemical is used as the independent variable in deriving the FCMs and thus only the two chemical concentrations need to be defined for the model.

To determine the relationship between the total concentration of the chemical in the sediment and the freely dissolved concentration of the chemical in the water

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column, the following sediment-water column chemical concentration quotient ( $\Pi_{\text{soc}}$ ) was calculated for each chemical reported by Oliver and Niimi (1988):

$$\Pi_{\text{soc}} = \frac{\text{ng of total chemical/Kg of organic carbon (in the sediment)}}{\text{ng of freely dissolved chemical/L of water (in the water column)}}$$

The freely dissolved concentrations of the chemicals in the water column were calculated from the data of Oliver and Niimi (1988) using the equations of Gschwend and Wu (1985) and Cook et al. (1993). These equations are:

$$\text{Freely dissolved fraction} = f_{\text{fd}} = 1/(1 + \text{DOC} \bullet K_{\text{doc}} + \text{POC} \bullet K_{\text{poc}})$$

$$\text{Freely dissolved concentration} = C_{\text{w}}^{\text{fd}} = C_{\text{w}}^{\text{t}} \bullet f_{\text{fd}}$$

where

- $f_{\text{fd}}$  = fraction of the chemical which is freely dissolved in the water,
- DOC = concentration of dissolved organic carbon,
- POC = concentration of particulate organic carbon,
- $K_{\text{doc}}$  = partition coefficient for the chemical between the DOC and the freely dissolved phase in the water,
- $K_{\text{poc}}$  = partition coefficient for the chemical between the POC phase and the freely dissolved phase in the water,
- $C_{\text{w}}^{\text{t}}$  = total concentration of the chemical in the water, and
- $C_{\text{w}}^{\text{fd}}$  = freely dissolved concentration of the chemical in the water.

The concentrations in the water reported by Oliver and Niimi (1988) were obtained by liquid-liquid extraction of aliquots of Lake Ontario water which had passed through a continuous-flow centrifuge to remove POC. Therefore, the concentrations in the water reported by Oliver and Niimi (1988) include both the freely dissolved chemical and the chemical associated with the DOC in the water sample. The above equations were used to derive the freely dissolved concentrations of the chemicals in the water by setting the  $\text{POC} = 0.0 \text{ mg/L}$ ,  $\text{DOC} = 2 \text{ mg/L}$ , and  $K_{\text{doc}} = K_{\text{ow}}/10$ .  $K_{\text{ow}}$ s used to derive the freely dissolved concentrations were obtained from Hawker and Connell (1988) for the PCBs, de Bruijn et al. (1989) for the chlorinated benzenes, *p,p*-DDT, *p,p*-DDE, *p,p*-DDD,  $\alpha$ -HCH, and  $\gamma$ -HCH, Pereira et al. (1988) and Chiou (1985) for hexachloro-1,3-butadiene, McKim et al. (1985) for mirex, and the CLogP program for 2,4,5-trichlorotoluene, 2,3,6-trichlorotoluene, 2,3,4,5,6-pentachlorotoluene, octachlorostyrene, and  $\gamma$ -chlordane (Leo 1988); for photomirex, its  $K_{\text{ow}}$  was set equal to the  $K_{\text{ow}}$  of mirex. The relationship for determining  $K_{\text{doc}}$  from  $K_{\text{ow}}$  was developed from the results reported by Yin and Hassett (1986, 1989), Eadie et al.

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(1990, 1992), Landrum et al. (1984), and Herbert et al. (1993) for partitioning to DOC.

In Figure 1, the ratios of  $\Pi_{\text{soc}}$  to  $K_{\text{ow}}$  are plotted against the  $\log K_{\text{ow}}$  for each chemical reported by Oliver and Niimi (1988). For the pesticides and PCB congeners, the ratios of the  $\Pi_{\text{soc}}$  to  $K_{\text{ow}}$  were nearly independent of the  $K_{\text{ow}}$  of the chemicals, i.e., Pearson correlation coefficients ( $r$ ) of -0.18 and -0.34 were obtained for the pesticides and PCBs, respectively. For the chlorinated benzenes, toluenes, and butadienes, the ratios of  $\Pi_{\text{soc}}$  to  $K_{\text{ow}}$  were slightly dependent upon the  $K_{\text{ow}}$  of the chemicals, i.e., Pearson correlation coefficient of -0.52. The average (standard deviation & number of values) ratios for the  $\Pi_{\text{soc}}$  to  $K_{\text{ow}}$  for pesticides, PCB congeners, pesticides and PCBs combined, and the group of chemicals consisting of the chlorinated benzenes, toluenes, and butadienes were 11.8 (8.4 & 9), 25.9 (26.8 & 46), 23.6 (25.3 & 55), and 294 (1188 & 12), respectively.

Based upon the independence of the ratios of  $\Pi_{\text{soc}}$  to  $K_{\text{ow}}$  on  $K_{\text{ow}}$  for the pesticides and PCBs and the average ratios above, a value of 25 was selected for this ratio. The resulting relationship between the concentration of the chemical in the sediment on an organic carbon basis ( $C_{\text{soc}}$ ) and the freely dissolved concentration of the chemical in the water column ( $C_w^{\text{fd}}$ ) is:

$$C_{\text{soc}} = 25 \bullet K_{\text{ow}} \bullet C_w^{\text{fd}} \quad (2)$$

and this relationship is applicable to chemicals with  $\log K_{\text{ow}}$ s from 2 to 10.

### B. Calculation of the FCMs

The model of Gobas (1993) (MS-DOS version) was run using the input data listed in Table 1 and the above relationship between the  $C_{\text{soc}}$  and  $C_w^{\text{fd}}$  for  $K_{\text{ow}}$ s of 3.5, 3.6, 3.7, 3.8, ..., and 9.0. The freely dissolved concentration of the chemical in the water was set to 1 ng/L and the concentration of the chemical in the sediment was calculated using the above sediment-water concentration relationship. To set the freely dissolved concentration of the chemical to 1 ng/L in the model of Gobas (1993), the DOC concentration was set equal to 0.0 mg/L.

It also should be noted that the model of Gobas (1993) does not include solubility controls or limitations, and thus, the concentration of the chemical in the water used with the model is arbitrary for determining the BAFs, i.e., the ratio of the concentration of the chemical in the tissue to the concentration of the chemical in the water column (BAF) obtained using a 1 ng/L concentration of the chemical will be equal to that obtained using a 150  $\mu\text{g/L}$  concentration of the chemical for a specified  $K_{\text{ow}}$ .

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It should be noted that the model of Gobas (1993) takes the inputted total concentration of the chemical in the water and before doing any predictions, calculates the freely dissolved concentration of the chemical in the water. The freely dissolved concentration of the chemical in the water is then used *in all subsequent calculations by the model*. By setting the concentration of the DOC to 0.0 mg/L, the total concentration of the chemical inputted to the model becomes equal to the freely dissolved concentration of the chemical in the water. This allowed the fixing of the chemical concentration relationship between sediment and water phases in the model. BAFs were determined by dividing the chemical residues predicted by the model of Gobas (1993) by the freely dissolved concentration of the chemical in the water and therefore, are not influenced by the concentration of DOC inputted to the model.

Listed in Table 2 are the FCMs calculated with equation 1 for the zooplankton, forage fish, and piscivorous fish.

### C. Evaluation of Food Chain Multipliers

BAFs were predicted for each chemical reported by Oliver and Niimi (1988). BAFs also were derived from the data of Oliver and Niimi (1988) by dividing the lipid-normalized concentration of the chemical in the fish by the freely dissolved concentration of the chemical in the water column. The freely dissolved concentration of the chemical in the water was determined as described above. These results are summarized in Tables 3 through 8 and Figures 2 through 7.

Measured chemical residues in fishes assigned to trophic level 3 can be higher than those in piscivorous fishes (trophic level 4) from the same food chain. Potential causes of the higher concentrations (on a lipid basis) in the trophic level 3 fish include a) growth rates which are much slower than the predator fishes, b) slower rates of metabolism than the predator fishes for the chemicals of interest, and c) the feeding preferences for the trophic level 3 fish that includes predation on other fish. In the development of FCMs, the feeding preferences for smelt (see Gobas 1993) consisted of a mixture of trophic level 2 and 3 organisms, i.e., mysids, *Diporeia* sp., and sculpin. This mixture of different trophic levels combined with bioenergetic factors for the smelt caused the predicted concentrations of the chemicals and subsequently, the derived FCMs, to be slightly larger than those for the piscivorous fishes (trophic level 4).

The average differences between the predicted and measured log BAFs were -0.59, 0.03, -0.15, -0.02, -0.08, and -0.11 for zooplankton, sculpin, alewives, small smelt, large smelt, and piscivorous fish, respectively.



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Table 1. Environmental parameters and species characteristics used with the model of Gobas (1993) for deriving the Food Chain Multipliers

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**Environmental parameters:**

Mean water temperature: 8°C  
 Organic carbon content of the sediment: 2.7%  
 Organic carbon content of the water column: 0.0 kg/L  
 Density of lipids: 0.9 kg/L  
 Density of organic carbon: 0.9 kg/L  
 Metabolic transformation rate constant: 0.0 day<sup>-1</sup>

**Species characteristics:**

**Phytoplankton**

Lipid content: 0.5%

**Zooplankton: Mysids (*Mysis relicta*)**

Lipid content: 5.0%

***Diporeia* sp.**

Lipid content: 3.0%

**Sculpin (*Cottus cognatus*)**

Lipid content: 8.0%

Weight: 5.4 g

Diet: 18% zooplankton, 82% *Diporeia* sp.

**Alewives (*Alosa pseudoharengus*)**

Lipid content: 7.0%

Weight: 32 g

Diet: 60% zooplankton, 40% *Diporeia* sp.

**Smelt (*Osmerus mordax*)**

Lipid content: 4.0%

Weight: 16 g

Diet: 54% zooplankton, 21% *Diporeia* sp., 25% sculpin

**Salmonids (*Salvelinus namaycush*, *Oncorhynchus mykiss*, *Oncorhynchus velinus namaycush*)**

Lipid content: 11.0%

Weight: 2410 g

Diet: 10% sculpin, 50% alewives, 40% smelt

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Table 2. Food Chain Multipliers for Zooplankton, Forage Fish and Piscivorous Fish

Log K <sub>ow</sub>	<u>Trophic Level 2</u>	<u>Trophic Level 3</u>			<u>Trophic Level 4</u>
	Zooplankton	Sculpin	Alewives	Smelt*	Piscivorous Fish
2.0	1.0	1.0	1.0	1.0	1.0
2.5	1.0	1.0	1.0	1.0	1.0
3.0	1.0	1.0	1.0	1.0	1.0
3.1	1.0	1.0	1.0	1.0	1.0
3.2	1.0	1.0	1.0	1.0	1.0
3.3	1.0	1.1	1.0	1.0	1.0
3.4	1.0	1.1	1.1	1.0	1.0
3.5	1.0	1.1	1.1	1.0	1.0
3.6	1.0	1.1	1.1	1.0	1.0
3.7	1.0	1.1	1.1	1.1	1.0
3.8	1.0	1.2	1.1	1.1	1.0
3.9	1.0	1.2	1.2	1.1	1.1
4.0	1.0	1.3	1.2	1.1	1.1
4.1	1.0	1.4	1.3	1.2	1.1
4.2	1.0	1.4	1.3	1.2	1.1
4.3	1.0	1.5	1.4	1.2	1.2
4.4	1.0	1.7	1.5	1.3	1.2
4.5	1.0	1.9	1.7	1.4	1.3
4.6	1.0	2.1	1.8	1.5	1.5
4.7	1.0	2.3	2.0	1.6	1.6
4.8	1.0	2.6	2.3	1.8	1.9
4.9	1.0	3.0	2.6	2.1	2.2
5.0	1.0	3.5	2.9	2.4	2.6
5.1	1.0	4.0	3.3	2.8	3.2
5.2	1.0	4.7	3.8	3.3	3.9
5.3	1.0	5.4	4.3	3.9	4.7
5.4	1.0	6.2	4.9	4.7	5.8
5.5	1.0	7.1	5.5	5.8	7.1
5.6	1.0	8.2	6.2	7.0	8.6
5.7	1.0	9.2	6.9	8.6	10.2
5.8	1.0	10.4	7.6	10.4	12.1
5.9	1.0	11.5	8.2	12.4	14.0
6.0	1.0	12.6	8.9	14.6	16.0
6.1	1.0	13.6	9.4	17.0	17.8
6.2	1.0	14.6	10.0	19.4	19.9
6.3	1.0	15.5	10.4	21.7	21.7
6.4	1.0	16.2	10.8	24.0	23.3
6.5	1.0	16.8	11.1	25.9	24.6
6.6	1.0	17.3	11.3	27.6	25.6

Table 2. Continued.

Log K <sub>ow</sub>	<u>Trophic Level 2</u>	<u>Trophic Level 3</u>			<u>Trophic Level 4</u>
	Zooplankton	Sculpin	Alewives	Smelt <sup>a</sup>	Piscivorous Fish
6.7	1.0	17.6	11.5	29.0	26.4
6.8	1.0	17.8	11.6	29.9	26.7
6.9	1.0	17.9	11.6	30.4	26.7
7.0	1.0	17.8	11.5	30.5	26.2
7.1	1.0	17.7	11.3	30.2	25.5
7.2	1.0	17.3	11.1	29.4	24.3
7.3	1.0	16.8	10.8	28.3	22.9
7.4	1.0	16.2	10.4	26.8	21.0
7.5	1.0	15.8	9.9	24.9	19.0
7.6	1.0	14.6	9.4	22.8	16.7
7.7	1.0	13.6	8.7	20.4	14.4
7.8	1.0	12.6	8.1	18.0	12.1
7.9	1.0	11.4	7.4	15.5	9.8
8.0	1.0	10.2	6.6	13.2	7.8
8.1	1.0	9.0	5.9	11.0	6.0
8.2	1.0	7.9	5.1	9.0	4.5
8.3	1.0	6.8	4.4	7.3	3.3
8.4	1.0	5.8	3.8	5.8	2.4
8.5	1.0	4.9	3.2	4.6	1.7
8.6	1.0	4.1	2.7	3.6	1.1
8.7	1.0	3.4	2.2	2.9	0.8
8.8	1.0	2.8	1.8	2.2	0.5
8.9	1.0	2.3	1.5	1.8	0.3
9.0	1.0	1.8	1.2	1.4	0.2

- <sup>a</sup> 25% of the smelt diet includes sculpin. Therefore, this species is at a trophic level slightly higher than 3.

Table 3. Measured and Predicted BAFs for Zooplankton. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water, i.e., ( $\mu\text{g}$  of chemical/Kg of lipid)/( $\mu\text{g}$  of freely dissolved chemical/L of water).

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
1	ppDDT	6.91	6.91	7.17
2	ppDDE	6.96	6.96	7.78
3	ppDDD	6.22	6.22	6.38
4	mirex	7.50	7.50	7.58
5	photomirex	7.50	7.50	7.80
6	g-chlordane	5.54	5.54	5.88
7	alpha-BHC	3.78	3.78	4.90
8	gamma-BHC	3.69	3.69	5.08
9	HCBD	4.84	4.84	5.05
10	OCS	7.94	7.94	7.85
11	HCB	5.73	5.73	5.77
12	QCB	5.18	5.18	6.38
13	1,2,3,5-TeCB	4.66	4.66	5.35
14	1,2,4,5-TeCB	4.60	4.60	5.14
15	1,2,3,4-TeCB	4.64	4.64	5.33
16	1,3,5-TCB	4.19	4.19	4.71
17	1,2,4-TCB	4.05	4.05	4.90
18	1,2,3-TCB	4.14	4.14	4.07
19	2,4,5-TCT	4.93	4.93	
20	2,3,6-TCT	4.93	4.93	5.71
21	PCT	6.36	6.36	
31	8	5.07	5.07	
32	6	5.06	5.06	
33	5	4.97	4.97	
34	12	5.22	5.22	
35	13	5.29	5.29	
36	28 + 31	5.67	5.67	6.48
37	18	5.24	5.24	5.69
38	22	5.58	5.58	6.21
39	26	5.66	5.66	
40	16	5.16	5.16	
41	33	5.60	5.60	5.79
42	17	5.25	5.25	5.69
43	25	5.67	5.67	
44	24 + 27	5.40	5.40	
45	32	5.44	5.44	
46	66	6.20	6.20	7.11
47	70 + 76	6.17	6.17	7.06
48	56 + 60 + 81	6.19	6.19	7.47

Table 3. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
49	52	5.84	5.84	6.10
50	47 + 48	5.82	5.82	5.97
51	44	5.75	5.75	6.27
52	74	6.20	6.20	7.02
53	49	5.85	5.85	6.34
54	64	5.95	5.95	6.96
55	42	5.76	5.76	7.01
56	53	5.62	5.62	
57	40	5.66	5.66	
58	41 + 71	5.84	5.84	
59	46	5.53	5.53	
60	45	5.53	5.53	
61	101	6.38	6.38	6.61
62	84	6.04	6.04	7.53
63	118	6.74	6.74	7.37
64	110	6.48	6.48	7.11
65	87 + 97	6.29	6.29	7.38
66	105	6.65	6.65	7.36
67	95	6.13	6.13	6.14
68	85	6.30	6.30	7.12
69	92	6.35	6.35	
70	82	6.20	6.20	7.50
71	91	6.13	6.13	6.33
72	99	6.39	6.39	6.51
73	153	6.92	6.92	7.50
74	138	6.83	6.83	7.43
75	149	6.67	6.67	7.31
76	146	6.89	6.89	7.93
77	141	6.82	6.82	7.46
78	128	6.74	6.74	
79	151	6.64	6.64	6.62
80	132	6.58	6.58	7.08
81	156	7.18	7.18	
82	136	6.22	6.22	6.34
83	129	6.73	6.73	
84	180	7.36	7.36	7.66
85	187 + 182	7.19	7.19	7.60
86	170 + 190	7.37	7.37	8.20
87	183	7.20	7.20	8.16
88	177	7.08	7.08	8.07
89	174	7.11	7.11	7.88

Table 3. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
90	178	7.14	7.14	
91	171	7.11	7.11	
92	185	7.11	7.11	
93	173	7.02	7.02	
94	203 + 196	7.65	7.65	8.26
95	201	7.62	7.62	
96	194	7.80	7.80	7.69
97	195	7.56	7.56	
98	198	7.62	7.62	
99	205	8.00	8.00	
100	206	8.09	8.09	
101	207	7.74	7.74	
102	209	8.18	8.18	
	Average difference			-0.59
	Standard deviation			0.40
	Number of values			61

<sup>a</sup> Chemical abbreviations taken from Oliver and Niimi (1988).

<sup>b</sup> Predicted BAFs were obtained by taking the product of the FCM and K<sub>ow</sub> for each chemical. Because the FCM is set to 1.0 for zooplankton, the predicted log BAF equals log K<sub>ow</sub>.

<sup>c</sup> Measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms ( $\mu\text{g}$  of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water ( $\mu\text{g}$  of freely dissolved chemical/L of water).



Table 4. Measured and Predicted BAFs for Sculpin. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water, i.e., ( $\mu\text{g}$  of chemical/Kg of lipid)/( $\mu\text{g}$  of freely dissolved chemical/L of water).

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
1	ppDDT	6.91	8.16	7.70
2	ppDDE	6.96	8.21	7.95
3	ppDDD	6.22	7.38	6.93
4	mirex	7.50	8.70	8.23
5	photomirex	7.50	8.70	8.15
6	g-chlordane	5.54	6.39	7.07
7	alpha-BHC	3.78	3.86	4.69
8	gamma-BHC	3.69	3.73	5.05
9	HCBD	4.84	5.25	5.55
10	OCS	7.94	9.00	8.89
11	HCB	5.73	6.69	6.54
12	QCB	5.18	5.85	5.67
13	1,2,3,5-TeCB	4.66	5.02	
14	1,2,4,5-TeCB	4.60	4.92	
15	1,2,3,4-TeCB	4.64	4.96	4.91
16	1,3,5-TCB	4.19	4.34	
17	1,2,4-TCB	4.05	4.20	4.57
18	1,2,3-TCB	4.14	4.29	
19	2,4,5-TCT	4.93	5.41	
20	2,3,6-TCT	4.93	5.41	
21	PCT	6.36	7.57	6.41
31	8	5.07	5.67	
32	6	5.06	5.66	
33	5	4.97	5.51	
34	12	5.22	5.89	
35	13	5.29	6.02	
36	28 + 31	5.67	6.63	6.37
37	18	5.24	5.91	5.97
38	22	5.58	6.49	
39	26	5.66	6.62	
40	16	5.16	5.83	
41	33	5.60	6.51	
42	17	5.25	5.98	
43	25	5.67	6.63	
44	24 + 27	5.40	6.19	
45	32	5.44	6.23	
46	66	6.20	7.36	7.45
47	70 + 76	6.17	7.33	7.06
48	56 + 60 + 81	6.19	7.35	7.48

Table 4. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
49	52	5.84	6.86	6.80
50	47 + 48	5.82	6.84	6.15
51	44	5.75	6.77	6.65
52	74	6.20	7.36	7.30
53	49	5.85	6.91	6.77
54	64	5.95	7.05	7.16
55	42	5.76	6.78	7.07
56	53	5.62	6.53	
57	40	5.66	6.62	
58	41 + 71	5.84	6.86	
59	46	5.53	6.38	
60	45	5.53	6.38	
61	101	6.38	7.59	7.30
62	84	6.04	7.14	8.05
63	118	6.74	7.99	7.86
64	110	6.48	7.71	7.44
65	87 + 97	6.29	7.48	7.54
66	105	6.65	7.90	7.82
67	95	6.13	7.26	6.98
68	85	6.30	7.49	7.50
69	92	6.35	7.56	7.70
70	82	6.20	7.36	7.60
71	91	6.13	7.26	6.44
72	99	6.39	7.60	
73	153	6.92	8.17	8.05
74	138	6.83	8.08	8.06
75	149	6.67	7.92	7.28
76	146	6.89	8.14	8.49
77	141	6.82	8.07	8.11
78	128	6.74	7.99	
79	151	6.64	7.88	8.34
80	132	6.58	7.82	7.41
81	156	7.18	8.42	
82	136	6.22	7.38	7.13
83	129	6.73	7.98	
84	180	7.36	8.57	8.45
85	187 + 182	7.19	8.43	8.07
86	170 + 190	7.37	8.58	9.15
87	183	7.20	8.44	8.81
88	177	7.08	8.33	8.63
89	174	7.11	8.36	8.24

Table 4. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
90	178	7.14	8.39	
91	171	7.11	8.36	
92	185	7.11	8.36	
93	173	7.02	8.27	
94	203 + 196	7.65	8.78	9.14
95	201	7.62	8.78	
96	194	7.80	8.90	8.52
97	195	7.56	8.72	
98	198	7.62	8.78	
99	205	8.00	9.01	
100	206	8.09	9.04	
101	207	7.74	8.87	
102	209	8.18	9.08	
	Average difference			0.03
	Standard deviation			0.43
	Number of values			54

<sup>a</sup> Chemical abbreviations taken from Oliver and Niimi (1988).

<sup>b</sup> Predicted BAFs were obtained by taking the product of the FCM and K<sub>ow</sub> for each chemical.

<sup>c</sup> Measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms ( $\mu\text{g}$  of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water ( $\mu\text{g}$  of freely dissolved chemical/L of water).

Table 5. Measured and Predicted BAFs for Alewives. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water, i.e., ( $\mu\text{g}$  of chemical/ $\text{Kg}$  of lipid)/( $\mu\text{g}$  of freely dissolved chemical/ $\text{L}$  of water).

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
1	ppDDT	6.91	7.97	7.84
2	ppDDE	6.96	8.02	7.98
3	ppDDD	6.22	7.22	6.82
4	mirex	7.50	8.50	8.18
5	photomirex	7.50	8.50	8.09
6	g-chlordane	5.54	6.28	6.63
7	alpha-BHC	3.78	3.82	4.82
8	gamma-BHC	3.69	3.73	5.00
9	HCBD	4.84	5.20	
10	OCS	7.94	8.81	8.89
11	HCB	5.73	6.57	6.32
12	QCB	5.18	5.76	
13	1,2,3,5-TeCB	4.66	4.96	
14	1,2,4,5-TeCB	4.60	4.86	
15	1,2,3,4-TeCB	4.64	4.90	
16	1,3,5-TCB	4.19	4.30	
17	1,2,4-TCB	4.05	4.16	
18	1,2,3-TCB	4.14	4.25	
19	2,4,5-TCT	4.93	5.34	
20	2,3,6-TCT	4.93	5.34	
21	PCT	6.36	7.39	6.53
31	8	5.07	5.59	
32	6	5.06	5.58	
33	5	4.97	5.43	
34	12	5.22	5.80	
35	13	5.29	5.92	
36	28 + 31	5.67	6.51	6.68
37	18	5.24	5.82	6.39
38	22	5.58	6.37	
39	26	5.66	6.50	
40	16	5.16	5.74	
41	33	5.60	6.39	
42	17	5.25	5.88	
43	25	5.67	6.51	
44	24 + 27	5.40	6.09	
45	32	5.44	6.13	
46	66	6.20	7.20	7.57
47	70 + 76	6.17	7.17	7.31
48	56 + 60 + 81	6.19	7.19	7.79

Table 5. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
49	52	5.84	6.72	6.84
50	47 + 48	5.82	6.70	6.85
51	44	5.75	6.63	6.86
52	74	6.20	7.20	7.35
53	49	5.85	6.76	6.98
54	64	5.95	6.90	7.30
55	42	5.76	6.64	7.38
56	53	5.62	6.41	
57	40	5.66	6.50	
58	41 + 71	5.84	6.72	
59	46	5.53	6.27	
60	45	5.53	6.27	
61	101	6.38	7.41	7.25
62	84	6.04	6.99	7.90
63	118	6.74	7.80	7.71
64	110	6.48	7.53	7.51
65	87 + 97	6.29	7.31	7.89
66	105	6.65	7.71	7.72
67	95	6.13	7.10	7.14
68	85	6.30	7.32	7.67
69	92	6.35	7.38	7.93
70	82	6.20	7.20	7.86
71	91	6.13	7.10	6.74
72	99	6.39	7.42	7.37
73	153	6.92	7.98	7.82
74	138	6.83	7.89	7.89
75	149	6.67	7.73	7.75
76	146	6.89	7.95	8.30
77	141	6.82	7.88	7.96
78	128	6.74	7.80	
79	151	6.64	7.69	8.17
80	132	6.58	7.63	7.45
81	156	7.18	8.23	
82	136	6.22	7.22	7.25
83	129	6.73	7.79	
84	180	7.36	8.38	8.15
85	187 + 182	7.19	8.24	7.99
86	170 + 190	7.37	8.39	8.84
87	183	7.20	8.25	8.46
88	177	7.08	8.13	8.54
89	174	7.11	8.16	8.51

Table 5. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
90	178	7.14	8.19	
91	171	7.11	8.16	
92	185	7.11	8.16	
93	173	7.02	8.08	
94	203 + 196	7.65	8.59	8.82
95	201	7.62	8.59	
96	194	7.80	8.71	8.22
97	195	7.56	8.53	
98	198	7.62	8.59	
99	205	8.00	8.82	
100	206	8.09	8.86	
101	207	7.74	8.68	
102	209	8.18	8.89	
	Average difference			-0.15
	Standard deviation			0.40
	Number of values			51

<sup>a</sup> Chemical abbreviations taken from Oliver and Niimi (1988).

<sup>b</sup> Predicted BAFs were obtained by taking the product of the FCM and K<sub>ow</sub> for each chemical.

<sup>c</sup> Measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms ( $\mu\text{g}$  of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water ( $\mu\text{g}$  of freely dissolved chemical/L of water).

Table 6. Measured and Predicted BAFs for Small Smelt. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water, i.e., ( $\mu\text{g}$  of chemical/Kg of lipid)/( $\mu\text{g}$  of freely dissolved chemical/L of water).

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
1	ppDDT	6.91	7.97	7.65
2	ppDDE	6.96	8.02	8.22
3	ppDDD	6.22	7.22	6.83
4	mirex	7.50	8.50	8.19
5	photomirex	7.50	8.50	8.21
6	g-chlordane	5.54	6.28	6.39
7	alpha-BHC	3.78	3.82	4.56
8	gamma-BHC	3.69	3.73	4.77
9	HCBD	4.84	5.20	
10	OCS	7.94	8.81	8.73
11	HCB	5.73	6.57	6.15
12	QCB	5.18	5.76	
13	1,2,3,5-TeCB	4.66	4.96	
14	1,2,4,5-TeCB	4.60	4.86	
15	1,2,3,4-TeCB	4.64	4.90	
16	1,3,5-TCB	4.19	4.30	
17	1,2,4-TCB	4.05	4.16	
18	1,2,3-TCB	4.14	4.25	
19	2,4,5-TCT	4.93	5.34	
20	2,3,6-TCT	4.93	5.34	
21	PCT	6.36	7.39	
31	8	5.07	5.59	
32	6	5.06	5.58	
33	5	4.97	5.43	
34	12	5.22	5.80	
35	13	5.29	5.92	
36	28 + 31	5.67	6.51	6.57
37	18	5.24	5.82	
38	22	5.58	6.37	
39	26	5.66	6.50	
40	16	5.16	5.74	
41	33	5.60	6.39	
42	17	5.25	5.88	
43	25	5.67	6.51	
44	24 + 27	5.40	6.09	
45	32	5.44	6.13	
46	66	6.20	7.20	7.46
47	70 + 76	6.17	7.17	7.32
48	56 + 60 + 81	6.19	7.19	7.73

Table 6. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
49	52	5.84	6.72	6.54
50	47 + 48	5.82	6.70	6.73
51	44	5.75	6.63	6.40
52	74	6.20	7.20	7.31
53	49	5.85	6.76	6.46
54	64	5.95	6.90	7.14
55	42	5.76	6.64	7.18
56	53	5.62	6.41	
57	40	5.66	6.50	
58	41 + 71	5.84	6.72	
59	46	5.53	6.27	
60	45	5.53	6.27	
61	101	6.38	7.41	7.05
62	84	6.04	6.99	7.90
63	118	6.74	7.80	7.76
64	110	6.48	7.53	7.41
65	87 + 97	6.29	7.31	7.79
66	105	6.65	7.71	7.71
67	95	6.13	7.10	6.83
68	85	6.30	7.32	7.41
69	92	6.35	7.38	7.17
70	82	6.20	7.20	7.77
71	91	6.13	7.10	6.40
72	99	6.39	7.42	6.43
73	153	6.92	7.98	7.93
74	138	6.83	7.89	7.87
75	149	6.67	7.73	7.63
76	146	6.89	7.95	8.30
77	141	6.82	7.88	7.84
78	128	6.74	7.80	
79	151	6.64	7.69	7.74
80	132	6.58	7.63	7.06
81	156	7.18	8.23	
82	136	6.22	7.22	
83	129	6.73	7.79	
84	180	7.36	8.38	8.18
85	187 + 182	7.19	8.24	8.01
86	170 + 190	7.37	8.39	8.86
87	183	7.20	8.25	8.59
88	177	7.08	8.13	8.54
89	174	7.11	8.16	8.31



Table 6. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
90	178	7.14	8.19	
91	171	7.11	8.16	
92	185	7.11	8.16	
93	173	7.02	8.08	
94	203 + 196	7.65	8.59	8.79
95	201	7.62	8.59	
96	194	7.80	8.71	8.24
97	195	7.56	8.53	
98	198	7.62	8.59	
99	205	8.00	8.82	
100	206	8.09	8.86	
101	207	7.74	8.68	
102	209	8.18	8.89	
	Average difference			-0.02
	Standard deviation			0.40
	Number of values			48

<sup>a</sup> Chemical abbreviations taken from Oliver and Niimi (1988).

<sup>b</sup> FCMs for alewives were used for the small smelt. Predicted BAFs were obtained by taking the product of the FCM and K<sub>ow</sub> for each chemical.

<sup>c</sup> Measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms ( $\mu\text{g}$  of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water ( $\mu\text{g}$  of freely dissolved chemical/L of water).

Table 7. Measured and Predicted BAFs for Large Smelt. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water, i.e., ( $\mu\text{g}$  of chemical/ $\text{Kg}$  of lipid)/( $\mu\text{g}$  of freely dissolved chemical/ $\text{L}$  of water).

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
1	ppDDT	6.91	8.39	8.15
2	ppDDE	6.96	8.44	8.38
3	ppDDD	6.22	7.51	6.88
4	mirex	7.50	8.90	8.50
5	photomirex	7.50	8.90	8.43
6	g-chlordane	5.54	6.30	6.45
7	alpha-BHC	3.78	3.82	4.71
8	gamma-BHC	3.69	3.73	4.82
9	HCBD	4.84	5.10	
10	OCS	7.94	9.13	8.97
11	HCB	5.73	6.66	6.41
12	OCB	5.18	5.70	5.88
13	1,2,3,5-TeCB	4.66	4.86	
14	1,2,4,5-TeCB	4.60	4.78	
15	1,2,3,4-TeCB	4.64	4.82	
16	1,3,5-TCB	4.19	4.27	
17	1,2,4-TCB	4.05	4.13	
18	1,2,3-TCB	4.14	4.22	
19	2,4,5-TCT	4.93	5.25	
20	2,3,6-TCT	4.93	5.25	
21	PCT	6.36	7.74	
31	8	5.07	5.52	
32	6	5.06	5.51	
33	5	4.97	5.35	
34	12	5.22	5.74	
35	13	5.29	5.88	
36	28 + 31	5.67	6.60	6.92
37	18	5.24	5.76	
38	22	5.58	6.43	
39	26	5.66	6.59	
40	16	5.16	5.68	
41	33	5.60	6.45	
42	17	5.25	5.84	
43	25	5.67	6.60	
44	24 + 27	5.40	6.07	
45	32	5.44	6.11	
46	66	6.20	7.49	7.88
47	70 + 76	6.17	7.46	7.71
48	56 + 60 + 81	6.19	7.48	8.12

Table 7. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
49	52	5.84	6.86	6.91
50	47 + 48	5.82	6.84	7.22
51	44	5.75	6.77	6.92
52	74	6.20	7.49	7.66
53	49	5.85	6.94	7.03
54	64	5.95	7.11	7.54
55	42	5.76	6.78	7.63
56	53	5.62	6.47	
57	40	5.66	6.59	
58	41 + 71	5.84	6.86	
59	46	5.53	6.29	
60	45	5.53	6.29	
61	101	6.38	7.76	7.35
62	84	6.04	7.20	8.29
63	118	6.74	8.20	8.13
64	110	6.48	7.89	7.81
65	87 + 97	6.29	7.63	8.06
66	105	6.65	8.11	8.11
67	95	6.13	7.36	7.17
68	85	6.30	7.64	7.85
69	92	6.35	7.73	7.80
70	82	6.20	7.49	8.14
71	91	6.13	7.36	6.90
72	99	6.39	7.77	7.40
73	153	6.92	8.40	8.24
74	138	6.83	8.31	8.22
75	149	6.67	8.13	7.99
76	146	6.89	8.37	8.66
77	141	6.82	8.30	8.17
78	128	6.74	8.20	
79	151	6.64	8.08	8.28
80	132	6.58	8.02	7.67
81	156	7.18	8.65	
82	136	6.22	7.51	
83	129	6.73	8.19	
84	180	7.36	8.79	8.45
85	187 + 182	7.19	8.66	8.34
86	170 + 190	7.37	8.80	9.02
87	183	7.20	8.67	8.85
88	177	7.08	8.56	8.78
89	174	7.11	8.59	8.71

Table 7. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
90	178	7.14	8.62	
91	171	7.11	8.59	
92	185	7.11	8.59	
93	173	7.02	8.50	
94	203 + 196	7.65	8.96	9.13
95	201	7.62	8.98	
96	194	7.80	9.06	8.50
97	195	7.56	8.92	
98	198	7.62	8.98	
99	205	8.00	9.12	
100	206	8.09	9.13	
101	207	7.74	9.05	
102	209	8.18	9.13	
	Average difference			-0.08
	Standard deviation			0.40
	Number of values			49

<sup>a</sup> Chemical abbreviations taken from Oliver and Niimi (1988).

<sup>b</sup> Predicted BAFs were obtained by taking the product of the FCM and K<sub>ow</sub> for each chemical.

<sup>c</sup> Measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms ( $\mu\text{g}$  of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water ( $\mu\text{g}$  of freely dissolved chemical/L of water).

Table 8. Measured and Predicted BAFs for Piscivorous Fish. BAFs are reported on a lipid weight basis using the freely dissolved concentration of the chemical in water, i.e., ( $\mu\text{g}$  of chemical/Kg of lipid)/( $\mu\text{g}$  of freely dissolved chemical/L of water).

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
1	ppDDT	6.91	8.34	8.00
2	ppDDE	6.96	8.38	8.46
3	ppDDD	6.22	7.52	7.03
4	mirex	7.50	8.78	8.59
5	photomirex	7.50	8.78	8.53
6	g-chlordane	5.54	6.39	6.74
7	alpha-BHC	3.78	3.78	4.69
8	gamma-BHC	3.69	3.69	4.93
9	HCBD	4.84	5.12	
10	OCS	7.94	8.93	9.20
11	HCB	5.73	6.74	6.41
12	QCB	5.18	5.77	5.81
13	1,2,3,5-TeCB	4.66	4.86	
14	1,2,4,5-TeCB	4.60	4.78	
15	1,2,3,4-TeCB	4.64	4.82	5.07
16	1,3,5-TCB	4.19	4.23	
17	1,2,4-TCB	4.05	4.09	
18	1,2,3-TCB	4.14	4.18	
19	2,4,5-TCT	4.93	5.27	
20	2,3,6-TCT	4.93	5.27	
21	PCT	6.36	7.73	
31	8	5.07	5.58	
32	6	5.06	5.57	
33	5	4.97	5.38	
34	12	5.22	5.81	
35	13	5.29	5.96	
36	28 + 31	5.67	6.68	6.89
37	18	5.24	5.83	5.75
38	22	5.58	6.51	6.39
39	26	5.66	6.67	
40	16	5.16	5.75	5.92
41	33	5.60	6.53	5.32
42	17	5.25	5.92	5.52
43	25	5.67	6.68	
44	24 + 27	5.40	6.16	
45	32	5.44	6.20	6.76
46	66	6.20	7.50	7.79
47	70 + 76	6.17	7.47	7.56
48	56 + 60 + 81	6.19	7.49	7.96

Table 8. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
49	52	5.84	6.92	7.01
50	47 + 48	5.82	6.90	7.18
51	44	5.75	6.83	6.96
52	74	6.20	7.50	7.66
53	49	5.85	7.00	7.13
54	64	5.95	7.15	7.51
55	42	5.76	6.84	7.49
56	53	5.62	6.55	6.51
57	40	5.66	6.67	6.55
58	41 + 71	5.84	6.92	
59	46	5.53	6.38	
60	45	5.53	6.38	
61	101	6.38	7.75	7.45
62	84	6.04	7.24	8.28
63	118	6.74	8.16	8.15
64	110	6.48	7.87	7.79
65	87 + 97	6.29	7.63	8.08
66	105	6.65	8.07	8.13
67	95	6.13	7.38	7.25
68	85	6.30	7.64	7.89
69	92	6.35	7.72	8.11
70	82	6.20	7.50	8.13
71	91	6.13	7.38	6.92
72	99	6.39	7.76	7.39
73	153	6.92	8.35	8.32
74	138	6.83	8.26	8.30
75	149	6.67	8.09	7.99
76	146	6.89	8.32	8.73
77	141	6.82	8.25	8.32
78	128	6.74	8.16	
79	151	6.64	8.05	8.51
80	132	6.58	7.99	7.56
81	156	7.18	8.57	
82	136	6.22	7.52	7.37
83	129	6.73	8.15	
84	180	7.36	8.68	8.58
85	187 + 182	7.19	8.58	8.43
86	170 + 190	7.37	8.69	9.20
87	183	7.20	8.59	9.03
88	177	7.08	8.49	9.01
89	174	7.11	8.52	8.74

Table 8. Continued.

	Chemical <sup>a</sup>	Log K <sub>ow</sub>	Predicted <sup>b</sup> Log BAF	Measured <sup>c</sup> Log BAF
90	178	7.14	8.55	
91	171	7.11	8.52	
92	185	7.11	8.52	
93	173	7.02	8.44	
94	203 + 196	7.65	8.81	9.26
95	201	7.62	8.84	
96	194	7.80	8.88	8.56
97	195	7.56	8.78	
98	198	7.62	8.84	
99	205	8.00	8.89	
100	206	8.09	8.87	
101	207	7.74	8.90	
102	209	8.18	8.83	
	Average difference			-0.11
	Standard deviation			0.40
	Number of values			59

<sup>a</sup> Chemical abbreviations taken from Oliver and Niimi (1988).

<sup>b</sup> Predicted BAFs were obtained by taking the product of the FCM and K<sub>ow</sub> for each chemical.

<sup>c</sup> Measured BAFs were determined by dividing the chemical residues on a lipid weight basis in the organisms ( $\mu\text{g}$  of chemical/Kg of lipid) by the freely dissolved concentration of the chemical in water ( $\mu\text{g}$  of freely dissolved chemical/L of water).

Figure 1. Sediment-water column chemical concentration quotient for Lake Ontario data of Oliver and Niimi (1988)

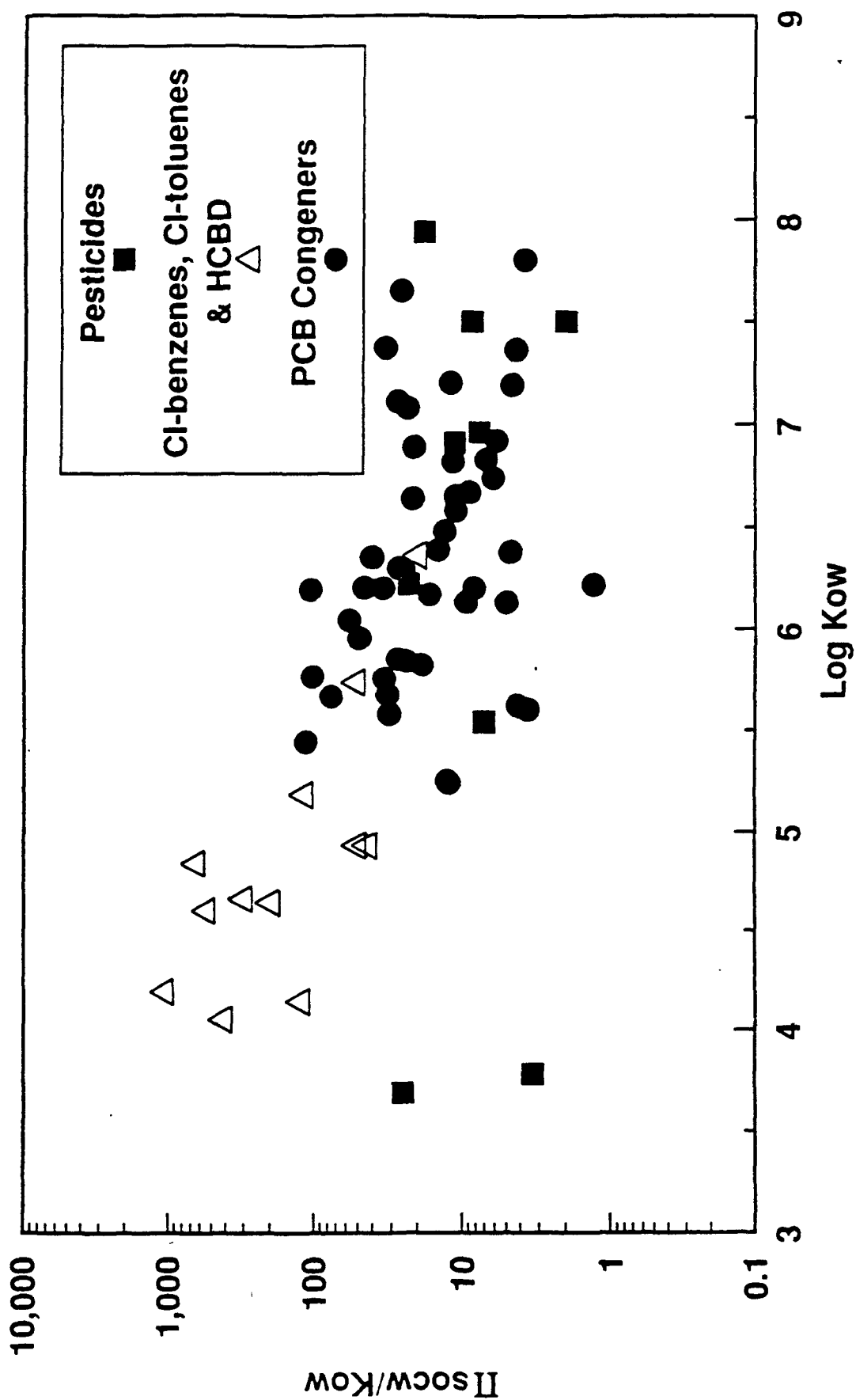
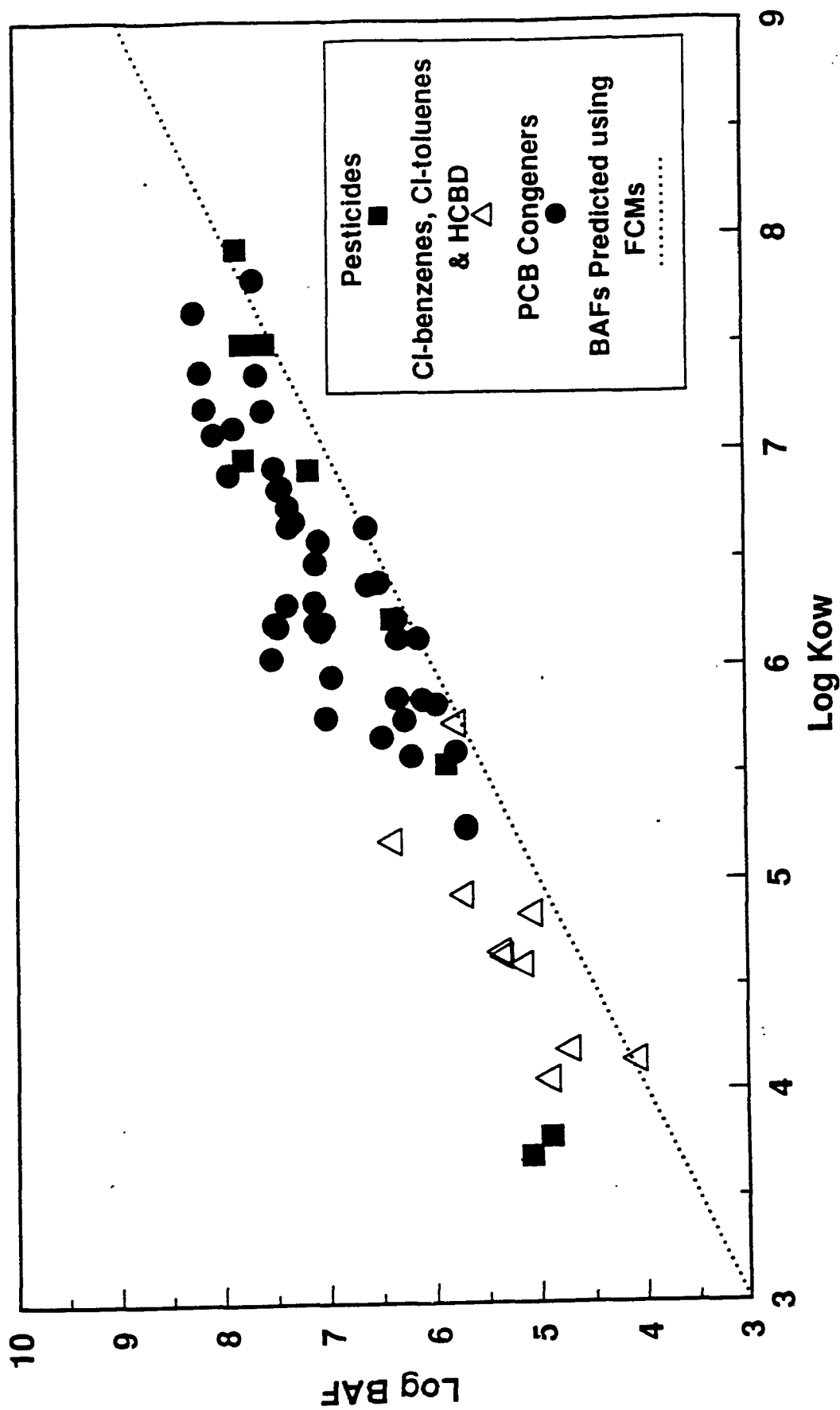


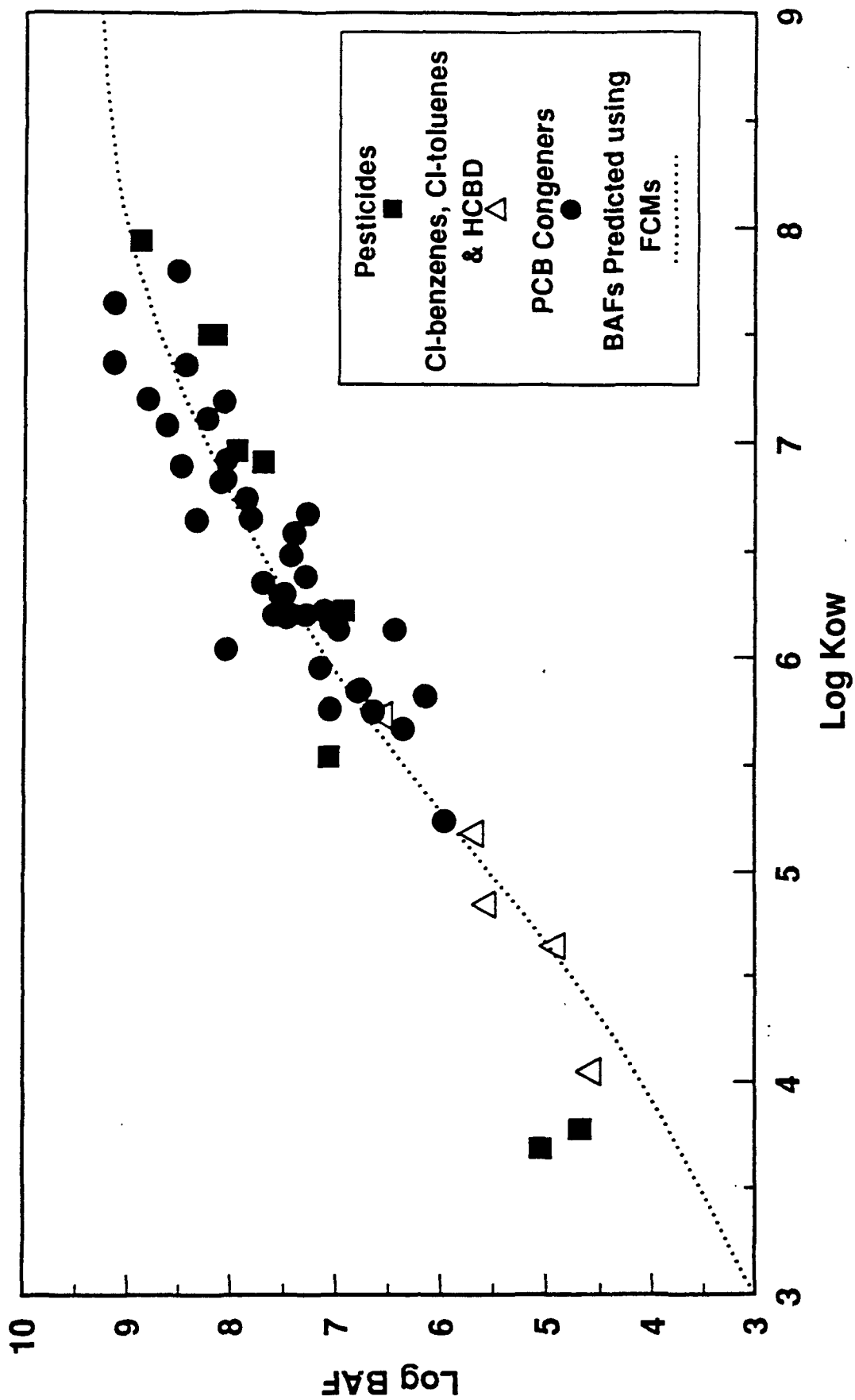


Figure 2. Measured and Predicted BAFs for  
Zooplankton  
Measured BAFs from Oliver and Niimi (1988)



DOC = 2 mg/L & Kdoc = Kow/10  
Sediment organic carbon content = 2.7%

Figure 3. Measured and Predicted BAFs for  
Sculpin  
Measured BAFs from Oliver and Niimi (1988)



**Figure 4. Measured and Predicted BAFs for  
Alewives  
Measured BAFs from Oliver and Niimi (1988)**

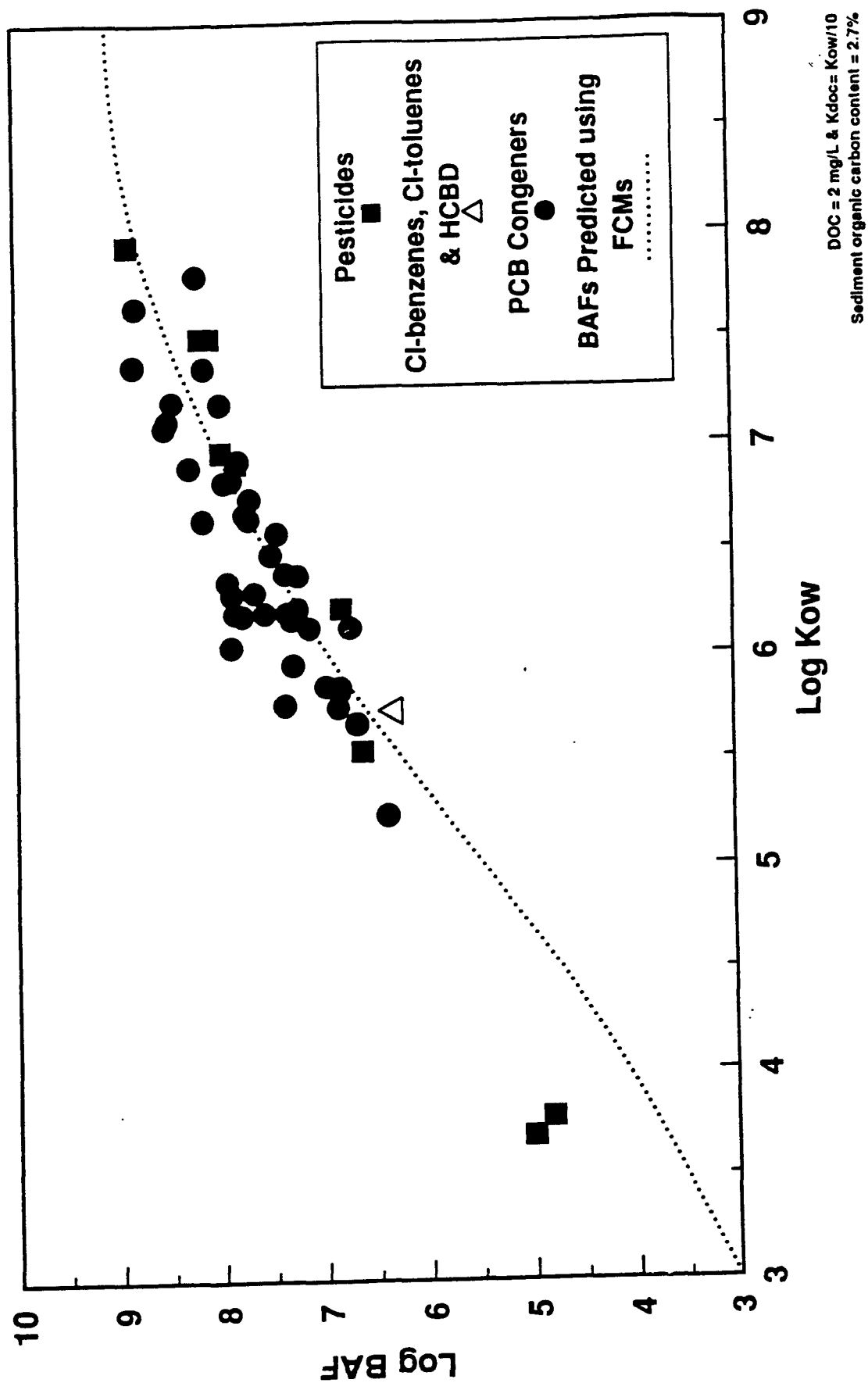


Figure 5. Measured and Predicted BAFs for  
Small Smelt  
Measured BAFs from Oliver and Niimi (1988)

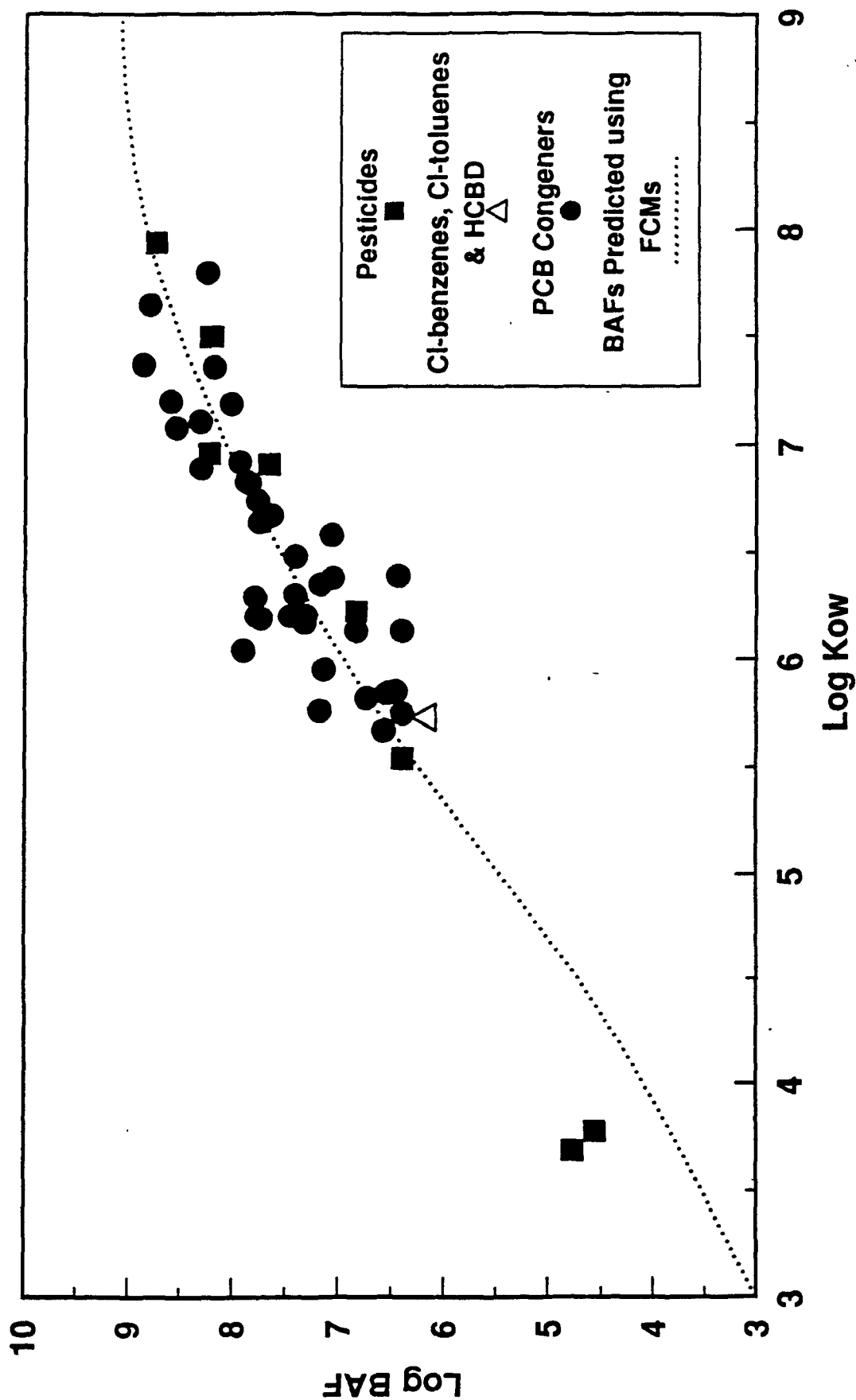
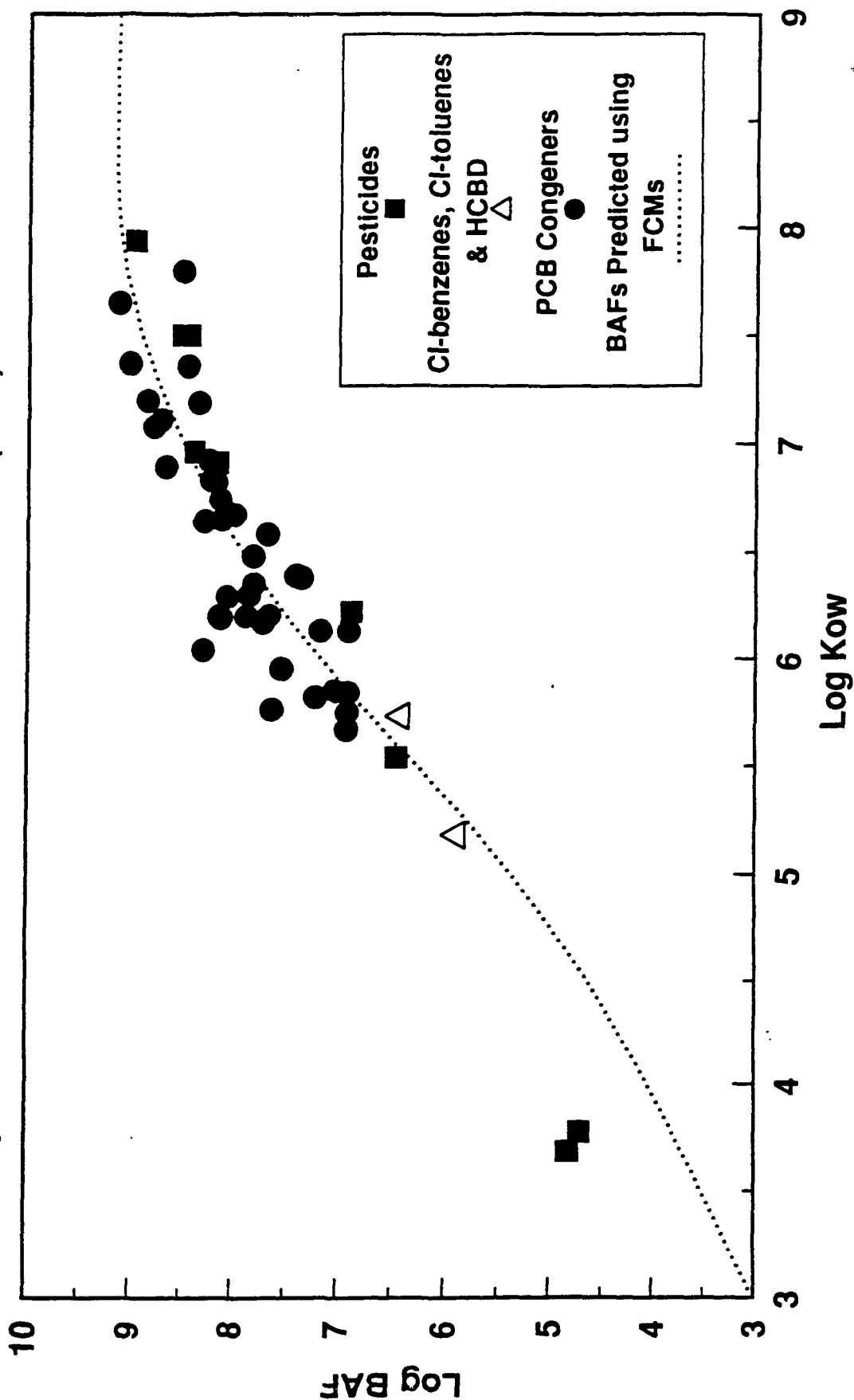
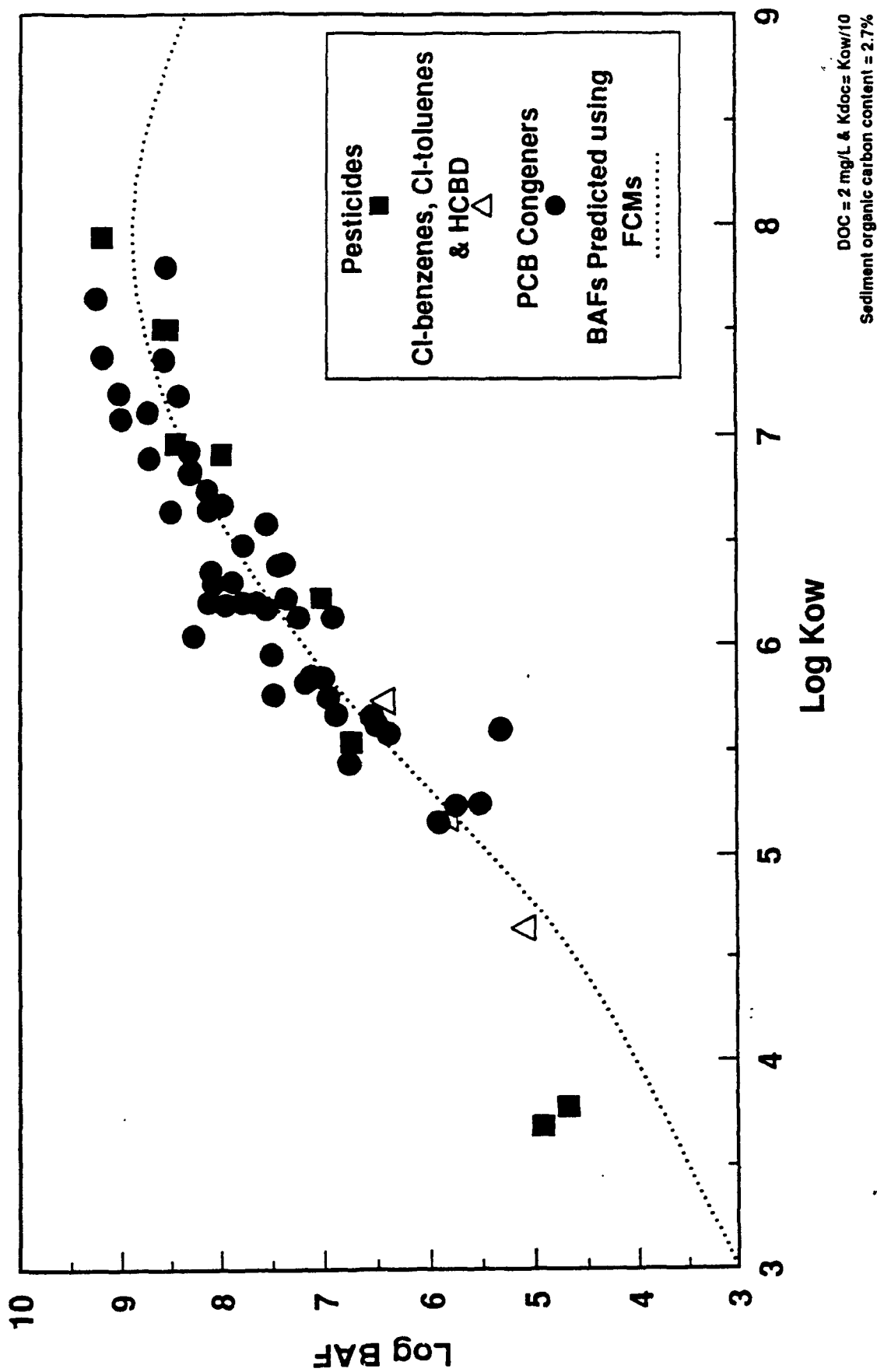


Figure 6. Measured and Predicted BAFs for  
Large Smelt  
Measured BAFs from Oliver and Niimi (1988)



DOC = 2 mg/L & Kdoc = Kow/10  
Sediment organic carbon content = 2.7%

Figure 7. Measured and Predicted BAFs for  
Piscivorous Fishes  
Measured BAFs from Oliver and Niimi (1988)



July 1994

## V. PREDICTION OF BIOACCUMULATION FACTORS (BAFs) FROM BIOTA-SEDIMENT ACCUMULATION FACTOR (BSAF) MEASUREMENTS

Biota-sediment accumulation factors may be used for measuring and predicting bioaccumulation directly from concentrations of chemicals in surface sediment. They may also be used to estimate  $BAF_i^{fd}$ s (Cook et al., 1993; 1994). Since BSAFs are based on field data and incorporate effects of metabolism, biomagnification, growth, etc.,  $BAF_i^{fd}$ s estimated from BSAFs will incorporate the net effect of all these factors. The BSAF approach is particularly beneficial for developing water quality criteria for chemicals such as polychlorinated dibenzo-p-dioxins, dibenzofurans and certain biphenyl congeners which are difficult to measure in water and have reduced bioaccumulation potential due to metabolism. The calculation of  $BAF_i^{fd}$ s from BSAFs also provides a method for validation of all measured or predicted  $BAF_i^{fd}$ s for nonpolar organic chemicals.

### A. Biota-sediment Accumulation Factors (BSAFs)

BSAFs are measured by relating lipid-normalized concentrations of chemicals in an organism to organic carbon-normalized concentrations of the chemicals in surface sediment samples associated with the average exposure environment of the organism. The BSAF equation is:

$$BSAF = \frac{C_i}{C_{soc}}$$

where

$C_i$  = lipid-normalized concentration of the chemical in tissues of the biota ( $\mu\text{g/g}$  lipid).

$C_{soc}$  = organic carbon-normalized concentration of the chemical in the surface sediment ( $\mu\text{g/g}$  sediment organic carbon).

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Since BSAFs are rarely measured for ecosystems which are at equilibrium, the BSAF inherently includes a measure of the disequilibrium of the ecosystem. This disequilibrium can be assessed for chemicals with  $\log K_{ow} > 3$  with the following relationship (equation 2):

$$BSAF \approx \frac{C_b^{fd} \cdot K_l}{C_s^{fd} \cdot K_{soc}} = D_{bs} \cdot \frac{K_l}{K_{soc}} \approx D_{bs} \cdot 2 \quad (2)$$

where

$C_b^{fd}$  = concentration of freely dissolved chemical (associated with water) in the tissues of biota ( $\mu\text{g/g}$  wet tissue).

$C_s^{fd}$  = concentration of freely dissolved chemical (associated with pore water) in the sediment ( $\mu\text{g/g}$  sediment organic carbon).

$K_l$  = lipid-water equilibrium partition coefficient =  $C_l/C_b^{fd}$ .

$K_{soc}$  = the sediment organic carbon-water equilibrium partition coefficient =  $C_{soc}/C_s^{fd}$ .

$D_{bs}$  = the disequilibrium (fugacity) ratio between biota and sediment ( $C_b^{fd}/C_s^{fd}$ ).

Measured BSAFs may range widely for different chemicals depending on  $K_l$ ,  $K_{soc}$ , and the actual ratio of  $C_b^{fd}$  to  $C_s^{fd}$ . At equilibrium, which rarely exists between sediment and pelagic organisms such as fish, the BSAF would be expected to equal the ratio of  $K_l/K_{soc}$  which is thought to range from 1-4. When chemical equilibrium between sediment and biota does not exist, the BSAF will equal the disequilibrium (fugacity) ratio between biota and sediment ( $D_{bs} = C_b^{fd}/C_s^{fd}$ ) times the ratio of the equilibrium partition coefficients (approximately 2).

The deviation of  $D_{bs}$  from the equilibrium value of 1.0 is determined by the net effect of all factors which contribute to the disequilibrium between sediment and aquatic organisms.  $D_{bs} > 1$  can occur due to biomagnification or when surface sediment has not reached steady-state with water.  $D_{bs} < 1$  can occur as a result of kinetic limitations for chemical transfer from sediment to water or water to food chain, and biological processes, such as growth or biotransformation of the chemical in the animal and its food chain. BSAFs are most useful when measured under steady-state conditions or pseudo-steady-state conditions in which chemical



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concentrations in water are linked to slowly changing concentrations in sediment. BSAFs measured for systems with new chemical loadings or rapid increases in loading may be unreliable due to underestimation of steady-state  $C_{soc}$ s.

### B. Relationship of BAFs to BSAFs

Differences between BSAFs for different organic chemicals are good measures of the relative bioaccumulation potentials of the chemicals. When calculated from a common organism/sediment sample set, chemical-specific differences in BSAFs reflect primarily the net effect of biomagnification, metabolism, and bioenergetic and bioavailability factors on each chemical's  $D_{bs}$ . Ratios of BSAFs of PCDDs and PCDFs to a BSAF for TCDD (bioaccumulation equivalency factors, BEFs) have been proposed in the GLWQI for evaluation of TCDD toxic equivalency associated with complex mixtures of these chemicals (see 58 FR 20802). The same approach is applicable to calculation of BAFs for other organic chemicals. The approach requires data for a steady-state or near steady-state condition between sediment and water for both a reference chemical (r) with a measured  $BAF_r^{fd}$  and other chemicals ( $n=i$ ) for which  $BAF_i^{fd}$ s are to be determined.  $BAF_i^{fd}$  for a chemical "i" is defined as:

$$(BAF_i^{fd})_i = \frac{(C_s)_i}{(C_w^{fd})_i} \quad (3)$$

where

$C_w^{fd}$  = concentration of freely dissolved chemical in water ( $\mu\text{g}/\mu\text{L}$  water).

Substitution of  $C_s$  from equation 1 into  $C_s$  of equation 3 for the chemical i gives:

$$(BAF_i^{fd})_i = (BSAF)_i \cdot \frac{(C_{soc})_i}{(C_w^{fd})_i} \quad (4)$$

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In order to avoid confusion with the equilibrium partition coefficients  $K_{soc}$ ,  $K_{poc}$  or  $K_{doc}$ , the chemical concentration quotient between sediment organic carbon and a freely dissolved state in overlying water is symbolized by  $\Pi_{soc}$ :

$$(\Pi_{soc})_i = \frac{(C_{soc})_i}{(C_w^{fd})_i} \quad (5)$$

Thus the ratio of  $BAF_i^{fd}$ s for chemical  $i$  and a reference chemical  $r$  is:

$$\frac{(BAF_i^{fd})_i}{(BAF_i^{fd})_r} = \frac{(BSAF)_i (\Pi_{soc})_i}{(BSAF)_r (\Pi_{soc})_r} \quad (6)$$

If both chemicals have similar fugacity ratios between water and sediment, as is the case for many chemicals in the open waters of the Great Lakes:

$$\frac{(\Pi_{soc})_i}{(\Pi_{soc})_r} = \frac{(K_{ow})_i}{(K_{ow})_r} \quad (7)$$

therefore:

$$(BAF_i^{fd})_i = (BAF_i^{fd})_r \cdot \frac{(BSAF)_i (K_{ow})_i}{(BSAF)_r (K_{ow})_r} \quad (8)$$

The assumption of equal or similar fugacity ratios between water and sediment for each chemical is equivalent to assuming that for all chemicals used in  $BAF_i^{fd}$  calculations: (1) the concentration ratios between sediment and suspended solids in the water and (2) the degree of equilibrium between suspended solids and  $C_w^{fd}$  are the same. Thus, errors could be introduced by inclusion of chemicals with non-steady-state external loading rates or chemicals with strongly reduced  $C_w^{fd}$  due to rapid volatilization from the water. Note that  $BAF_i^{fd}$ s calculated from BSAFs will incorporate any errors associated with measurement of the  $BAF_i^{fd}$  for the reference chemical and the  $K_{ow}$ s for both the reference and unknown chemicals. Such errors can be minimized by comparing results from several reference chemicals and assuring consistent use of  $C_w^{fd}$  values which are adjusted for dissolved organic

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carbon binding effects on the fraction of each chemical that is freely dissolved ( $f_{fd}$ ) in unfiltered, filtered or centrifuged water samples.  $BAF_i$ s based on total chemical concentration in water ( $BAF_i^t$ ) can be calculated on the basis of  $f_{fd}$  for the dissolved and particulate organic carbon concentrations in the water (POC and DOC):

$$BAF_i^t = BAF_i^{fd} \cdot f_{fd} \quad (9)$$

where:

$$f_{fd} = \frac{1}{1 + DOC \cdot K_{doc} + POC \cdot K_{poc}} \approx \frac{1}{1 + DOC \cdot K_{ow}/10 + POC \cdot K_{ow}} \quad (10)$$

Further information on calculation of concentrations of freely dissolved chemicals in water may be found in section II of this document titled "BAFs Based on Concentrations of the Freely Dissolved Chemical in Water".

### C. Calculation of $BAF_i^{fd}$ s from Lake Ontario Data

Two data sets are available to EPA for calculating  $BAF_i^{fd}$ s from BSAFs for fish in Lake Ontario. The Oliver and Niimi (1988) data set, which has been used extensively for construction of food chain models of bioaccumulation and calculation of food chain multipliers, biomagnification factors and  $BAF_i^{fd}$ s from chemical concentrations determined in organisms and water, also contains surface sediment data which allows calculation of lakewide average BSAFs. The second data set is provided by an extensive sampling of fish and sediments in 1987 for EPA's Lake Ontario TCDD Bioaccumulation Study (U.S. EPA, 1990) for the purpose of determining BSAFs. These samples were later analyzed for PCDD, PCDF, PCB congeners and some organochlorine pesticides at ERL-Duluth. Although these data should be submitted for publication within this year, they are needed here to provide a unique data set for checking  $BAF_i^{fd}$ s calculated from Oliver and Niimi data from samples collected between 1981-1984 and calculating  $BAF_i^{fd}$ s for organic chemicals not measured by Oliver and Niimi.

$BAF_i^{fd}$ s for salmonids were calculated for this demonstration of the BSAF ratio method using PCB congeners 52, 105 and 118 and DDT as reference chemicals. Several reference chemicals were used in order to examine the variability introduced by choice of reference chemical. The water analyses of Oliver and Niimi (1988) were adjusted for an estimated 2 mg/L residual dissolved organic carbon concentration in the centrifuged water (assumed no residual POC) and an estimated  $K_{doc} = K_{ow}/10$  in order to calculate  $C_w^{fd}$  from  $f_{fd}$  (equation 10). Log  $K_{ow}$ s for PCBs are those reported by Hawker and Connell (1988). Log  $K_{ow}$ s for PCDDs and PCDFs are those estimated by Burkhard and Kuehl (1986) except for the

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penta, hexa, and hepta chlorinated dibenzofurans which were estimated on the basis of assumed similarity to the trends reported for the PCDDs by Burkhard and Kuehl (1986). Log  $K_{ow}$ s for other chemicals are either as cited in the Appendix B of this document or noted in Table 1. Table 1 contains the measured and predicted log  $BAF_i^{fd}$ s from the two data sets.

#### D. Validity of $BAF_i^{fd}$ s Calculated from BSAFs

Figures 1, 2 and 3 show the relationship of log  $BAF_i^{fd}$ s to log  $K_{ow}$ s for (1) Oliver and Niimi (1988)  $BAF_i^{fd}$ s determined from measured concentrations of freely dissolved chemicals in Lake Ontario water in 1984; (2)  $BAF_i^{fd}$ s calculated from BSAFs derived from Oliver and Niimi data; and (3)  $BAF_i^{fd}$ s calculated from EPA BSAFs for lake trout in Lake Ontario in 1987 (Cook et al., 1994). The diagonal lines represent a 1:1 ratio of log BAF to log  $K_{ow}$ . The PCB congener  $BAF_i^{fd}$ s in all three sets of data appear quite similar. The EPA  $BAF_i^{fd}$ s predictions (figure 3) include a number of chemicals not in the Oliver and Niimi data set. These are the PCDDs, PCDFs, chlordanes, nonachlors and dieldrin. Only the dieldrin  $BAF_i^{fd}$  has been measured elsewhere. The  $BAF_i^{fd}$ s for five of six chlordanes and nonachlors are much greater than those for PCBs with the same estimated log  $K_{ow}$ . Therefore, the log  $K_{ow}$  values chosen here for the chlordanes and nonachlors may be significantly underestimated. The bioaccumulative PCDDs and PCDFs (2,3,7,8-chlorinated), as expected due to metabolism in fish, have  $BAF_i^{fd}$ s 10-1000 fold less than PCBs with similar  $K_{ow}$ s. Thus, the BSAF method for measuring  $BAF_i^{fd}$ s appears to work well for Lake Ontario.

Accuracy of the BSAF method can be best judged on the basis of comparison of the  $BAF_i^{fd}$ s calculated from BSAFs to measured  $BAF_i^{fd}$ s. Figure 4 illustrates the agreement between log  $BAF_i^{fd}$ s calculated from the Oliver and Niimi water data and those calculated from the sediment data. The  $BAF_i^{fd}$ s for chlorinated benzenes and toluenes may tend to be underestimated with BSAFs because the water-sediment fugacity gradient is altered in comparison to PCBs in response to rapid volatilization losses from water. Use of EPA BSAFs measured from a different set of fish and sediment samples collected several years after the Oliver and Niimi samples gives  $BAF_i^{fd}$ s that correlate equally well with the  $BAF_i^{fd}$ s calculated from Oliver and Niimi data (figure 5).

All of the above correlations were based on the BSAF method using the Oliver and Niimi measured Lake Ontario salmonid  $BAF_i^{fd}$  for PCB congener 52 as the reference. Very similar correlations result for comparisons of data in Table 1 for PCB congeners 105, 118 or DDT as reference chemicals. The BSAF method is strengthened through use of several reference chemicals with a range of  $K_{ow}$ s and greatest likelihood for accuracy in measurements of concentrations in water. The

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two data sets and four reference chemicals resulted in either four or eight determinations of  $BAF_i^{fd}$  for each chemical listed in Table 1. Mean log  $BAF_i^{fd}$ s (geometric means of  $BAF_i^{fd}$ s) for the 4-8 determinations from Lake Ontario data are reported in Table 2. The  $BAF_i^{fd}$  for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) at  $7.85 \times 10^6$  compares well to  $3.03 \times 10^6$  estimated by a different method for TCDD  $\log K_{ow} = 7$  by Cook et al. (1993). The small difference in the two estimates may be attributable to an underestimate of the sediment-disequilibrium between sediment and water by Cook et al. (1993) that resulted in an overestimate of  $C_w^{fd}$ .

The greatest test for robustness of the BSAF method for predicting  $BAF_i^{fd}$ s that are applicable throughout the Great Lakes would be a comparison of two totally independent data sets based on different ecosystems and conditions. Such a comparison can be made for bioaccumulation of PCBs in Lake Ontario fish and Green Bay fish. The EPA Green Bay/Fox River Mass Balance Study involved extensive sampling of water, sediment and fish in 1989. Green Bay is a shallower, smaller, and more eutrophic body of water than Lake Ontario. Measurement of bioaccumulation in Green Bay is complicated by the movement and interaction of biota through gradients of decreasing PCBs, nutrients and suspended organic carbon which extend from the Fox River to the outer bay and Lake Michigan. Table 1 contains brown trout  $BAF_i^{fd}$ s calculated from PCB BSAFs measured in the mid-bay region using PCB congeners 52 and 118 as reference chemicals. The reference chemical  $BAF_i^{fd}$ s were determined with water and brown trout data from the same region. Concentrations of freely dissolved PCBs were calculated, as for Lake Ontario, on the basis of dissolved organic carbon in the water samples and an assumed  $K_{doc} = K_{ow}/10$ . Despite the complex exposures of Green Bay fish, figures 6 and 7 illustrate  $\log BAF_i^{fd} - \log K_{ow}$  relationships found in Green Bay which are similar to those from the Oliver and Niimi and EPA Lake Ontario data sets. The correlations between the PCB  $BAF_i^{fd}$ s for Green Bay brown trout and  $BAF_i^{fd}$ s based on Oliver-Niimi salmonid and water measurements and EPA lake trout BSAFs are shown in figures 8-11 for reference chemicals PCB 52 and PCB 118, respectively. Good agreement exists between Green Bay brown trout predictions and Lake Ontario measured and BSAF-predicted  $BAF_i^{fd}$ s for both reference chemicals.

The means of log  $BAF_i^{fd}$ s calculated for each chemical from two sets of BSAFs and four reference chemicals for 124 chemicals measured in Lake Ontario trout (Table 2) are plotted against log  $K_{ow}$  in figure 12. Only 59 of these chemicals have measured  $BAF_i^{fd}$ s. Correlations between the mean Lake Ontario trout and Green Bay brown trout  $BAF_i^{fd}$ s (figures 13 and 14) indicate that the Green Bay brown trout estimates are slightly larger. This may be a sample set artifact associated with the complex Green Bay fish-water-sediment relationships in Green Bay rather than an actual site/species/food chain-specific difference in bioaccumulation. The Lake Ontario and Green Bay PCB congener 198  $BAF_i^{fd}$ s are noticeably different in

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figures 13 and 14 (greatest log  $BAF_i^{fd}$  based on Lake Ontario BSAFs) and cause most of the slight deviation of the slope of the linear regression lines from 1.0. The agreement of the Green Bay and Lake Ontario results demonstrates the general applicability of  $BAF_i^{fd}$ s calculated from BSAFs in predicting bioaccumulation in Great Lakes fish from estimated  $C_w^{fd}$ s.

#### **E. How to Apply the BSAF Method for Predicting $BAF_i^{fd}$ s**

If high quality data are not available for calculating  $BAF_i^{fd}$ s for organic chemicals that are expected to bioaccumulate, the mean  $BAF_i^{fd}$ s reported in Table 2 may be used. To apply the method for additional chemicals, site-specific determinations, or biota from different trophic levels than salmonids, the following steps and data requirements must be completed:

1. Reliable  $BAF_i^{fd}$ s which have been measured for several reference chemicals in biota in the ecosystem must be chosen. The water sample analyses should approximate the average exposure of the organism and its food chain over a time period that is most appropriate for the chemical, organism and ecosystem. Each  $C_w^{fd}$  used to calculate a  $BAF_i^{fd}$  should be based on a consistent adjustment of the concentration of total chemical in water for DOC and POC using equation 10. It is preferable to choose at least some reference chemicals on the basis of log  $K_{ow}$  and chemical class similarity with the test chemicals.
2. Measured (slow-stir method or equivalent preferred) or estimated Log  $K_{ow}$  values are chosen for each chemical.
3. Obtain chemical residue and % lipid data for representative samples of the tissues of the organisms. Migration patterns, food chain movement and hydrodynamic factors should be considered. For highly bioaccumulative chemicals variation of chemical residues in adult fish in the open waters of the Great Lakes within an annual cycle is usually slight.
4. Obtain chemical concentrations and % organic carbon data for surface sediment samples. Sediment sampling sites should be selected to allow prediction of ratios of freely dissolved chemical concentrations in the overlying water of the ecosystem region of interest. A 1 cm layer of surface sediment is ideal but 3 cm samples will work if sedimentation rates are large and periodic scouring events are not likely. Although desirable, sediment samples do not have to represent the average surface sediment condition in the area of the ecosystem affecting the exposure of the organisms for which bioaccumulation is to be measured. Since this is a ratio method, the concentrations of each chemical in sediment need only be predictive of the ratios of concentrations of the chemicals in the ecosystem water.

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5. With the data from steps 3 and 4, calculate BSAFs for chemicals of interest and reference chemicals (equation 1).

6. With BSAFs and  $K_{ow}$ s for each chemical, plus  $BAF_i^{fd}$ s for reference chemicals, calculate  $BAF_i^{fd}$ s using equation 8.

7. Use the  $BAF_i^{fd}$ s to predict chemical residues in fish and other biota or to establish unsafe concentrations of chemicals in water only on the basis of chemical concentration expressions for water and organisms that are consistent with the  $BAF_i^{fd}$  definition and measurement.

#### F. Summary

$BAF_i^{fd}$ s calculated from two different BSAF data sets for Lake Ontario salmonids are similar and agree well with measured  $BAF_i^{fd}$ s of Oliver and Niimi (1988). The BSAF method allows calculation of  $BAF_i^{fd}$ s for chemicals which have not been measured in Great Lakes water but are detectable in fish tissues and sediments.  $BAF_i^{fd}$ s can also be calculated for other fish species and biota at lower trophic levels in the food web.  $BAF_i^{fd}$ s calculated for PCBs in Green Bay brown trout agree well with the Lake Ontario salmonid/lake trout values despite differences in ecosystem, food chain and exposure conditions. Mean log  $BAF_i^{fd}$ s (geometric mean of  $BAF_i^{fd}$ s) from 4-8 determinations from Lake Ontario data are summarized in Table 2.

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Table 1. Great Lakes Trout BAF's Calculated from Measured BSAFs/BAFs - page 1a.

Chemical	log K <sub>ow</sub>	log BAF Oliver & Niimi <sup>a</sup> measured	BSAF Oliver & Niimi <sup>a</sup> measured	BSAF EPA <sup>b</sup> measured	log BAF Oliver & Niimi <sup>a</sup> ref PCB 52	log BAF EPA <sup>b</sup> ref PCB 52	log BAF Oliver & Niimi <sup>a</sup> ref PCB 105	log BAF EPA <sup>b</sup> ref PCB 105
dieldrin	5.40			6.65		7.77		7.05
ddt	6.91	8.00	1.09	1.67	8.33	8.68	8.00	7.96
dde	6.96	8.46	4.14	7.70	8.96	9.39	8.63	8.67
ddd	6.22	7.03	0.28		7.06		6.72	
mirex	7.50	8.59	1.43	1.31	9.04	9.16	8.70	8.45
photomirex	6.76	8.00	5.48		8.88		8.55	
g-chlordane	5.54	6.74	2.22		7.27		6.94	
t-chlordane	5.54			2.00		7.39		6.67
c-chlordane	5.54			4.77		7.77		7.05
t-nonachlor	5.66			10.50		8.23		7.51
c-nonachlor	5.66			0.51		6.91		6.20
alpha-hch	3.78	4.69	2.45		5.55		5.22	
gamma-hch	3.69	4.93	0.69		4.91		4.58	
hcbd	4.84							
ocs	7.94	9.20	0.98		9.32		8.98	
hch	5.73	6.41	0.09		6.08		5.75	
pcb	5.18	5.81	0.04		5.14		4.80	
1235tcb	4.66							
1245tcb	4.60							
1234tcb	4.64	5.07	0.01		4.16		3.83	
135tcb	4.19							
124tcb	4.05							
123tcb	4.14							
245tct	4.93							
236tct	4.93							
pct	6.36							

Table 1. Great Lakes Trout BAF's Calculated from Measured BSAFs/BAFs - page 2a.

Chemical	log K <sub>ow</sub>	log BAF Oliver & Niimi <sup>a</sup> measured	BSAF Oliver & Niimi <sup>a</sup> measured	BSAF EPA <sup>b</sup> measured	log BAF Oliver & Niimi <sup>a</sup> ref PCB 52	log BAF EPA <sup>b</sup> ref PCB 52	log BAF Oliver & Niimi <sup>a</sup> ref PCB 105	log BAF EPA <sup>b</sup> ref PCB 105
PCBs								
5	4.97							
6	5.06			0.36		6.16		5.44
8	5.07							
12	5.22			0.44		6.41		5.69
13	5.29							
16	5.16	5.92						
17	5.25	5.52	0.15	0.99	5.80	6.79	5.47	6.07
18	5.24	5.75	0.26	0.10	6.05	5.79	5.71	5.07
22	5.58	6.39	0.21	0.27	6.28	6.56	5.95	5.84
25	5.67		0.25	0.33	6.44	6.74	6.11	6.02
26	5.66		1.72	0.44	7.28	6.85	6.94	6.13
32	5.44	6.76	0.18		6.09		5.75	
33	5.60	5.32	0.15	0.49	6.15	6.84	5.82	6.12
40	5.66	6.55	0.10	0.18	6.06	6.46	5.72	5.74
42	5.76	7.49	0.52		6.86		6.53	
44	5.75	6.96	0.48	0.40	6.82	6.90	6.48	6.18
45	5.53			0.22		6.42		5.70
46	5.53		0.57	0.02	6.67	5.38	6.34	4.66
49	5.85	7.13	0.69		7.07		6.74	
52	5.84	7.01	0.61	0.42	7.01	7.01	6.67	6.29
53	5.62	6.51	1.84		7.27		6.93	
63	6.17			0.82		7.63		6.91
64	5.95	7.51	0.73		7.20		6.86	
66	6.20	7.79	0.85		7.52		7.18	
74	6.20	7.66	3.45	0.61	8.12	7.53	7.79	6.81
77	6.36			0.29		7.37		6.65
81	6.36			0.67		7.73		7.01
82	6.20	8.13	2.45	0.18	7.97	7.00	7.64	6.28
83	6.26			1.33		7.93		7.21
84	6.04	8.28	3.04		7.91		7.57	

Table 1. Great Lakes Trout BAF<sub>i</sub>s Calculated from Measured BSAFs/BAFs - page 3a.

Chemical	log K <sub>ow</sub>	log BAF Oliver & Niimi <sup>a</sup> measured	BSAF Oliver & Niimi <sup>a</sup> measured	BSAF EPA <sup>b</sup> measured	log BAF Oliver & Niimi <sup>a</sup> ref PCB 52	log BAF EPA <sup>b</sup> ref PCB 52	log BAF Oliver & Niimi <sup>a</sup> ref PCB 105	log BAF EPA <sup>b</sup> ref PCB 105
PCBs								
85	6.30	7.89	1.45	1.29	7.85	7.96	7.51	7.24
87	6.29			1.37		7.97		7.25
91	6.13	6.92	1.25	0.64	7.61	7.48	7.28	6.76
92	6.35	8.11	1.43		7.89		7.55	
95	6.13	7.25	1.40		7.66		7.33	
97	6.29			0.28		7.28		6.56
99	6.39	7.39	0.68	1.51	7.61	8.12	7.27	7.40
100	6.23			1.78		8.03		7.31
101	6.38	7.45	2.45	1.06	8.15	7.95	7.82	7.23
105	6.65	8.13	2.70	4.49	8.47	8.85	8.13	8.13
110	6.48	7.79	1.53	0.82	8.05	7.94	7.71	7.22
118	6.74	8.15	4.09	1.72	8.74	8.52	8.40	7.80
119	6.58			3.83		8.71		7.99
126	6.89			3.21		8.94		8.22
128	6.74		3.61	2.78	8.68	8.73	8.35	8.01
129	6.73		1.75	1.13	8.36	8.33	8.02	7.61
130	6.80			2.15		8.68		7.96
132	6.58	7.56	0.87		7.90		7.57	
136	6.22	7.37	10.87		8.64		8.30	
138	6.83	8.30	4.25		8.84		8.51	
141	6.82	8.32	2.75	1.74	8.64	8.61	8.31	7.89
146	6.89	8.73	3.22	1.25	8.78	8.53	8.45	7.81
149	6.67	7.99	2.33	0.93	8.42	8.19	8.09	7.47
151	6.64	8.51	3.38	1.65	8.55	8.40	8.22	7.69
153	6.92	8.32	4.22	1.91	8.93	8.75	8.59	8.03
156	7.18		3.97		9.16		8.83	
158	7.02			1.52		8.75		8.03
167	7.27			0.69		8.66		7.94
171	7.11		2.71		8.93		8.59	

Table 1. Great Lakes Trout BAF's Calculated from Measured BSAFs/BAFs - page 4a.

Chemical	log K <sub>ow</sub>	log BAF Oliver & Niimi <sup>a</sup> measured	BSAF Oliver & Niimi <sup>a</sup> measured	BSAF EPA <sup>b</sup> measured	log BAF Oliver & Niimi <sup>a</sup> ref PCB 52	log BAF EPA <sup>b</sup> ref PCB 52	log BAF Oliver & Niimi <sup>a</sup> ref PCB 105	log BAF EPA <sup>b</sup> ref PCB 105
PCBs								
172	7.33			1.36		9.01		8.29
174	7.11	8.74	1.54	1.25	8.68	8.75	8.35	8.03
177	7.08	9.01	3.53	1.91	9.01	8.91	8.68	8.19
178	7.14		4.48	2.76	9.18	9.13	8.84	8.41
180	7.36	8.58	3.78	3.26	9.32	9.42	8.99	8.70
183	7.20	9.03	5.62	2.68	9.33	9.17	9.00	8.46
185	7.11		1.55	2.24	8.68	9.01	8.35	8.29
189	7.71			0.71		9.11		8.39
194	7.80	8.56	1.53	2.47	9.37	9.74	9.03	9.02
195	7.56		1.90		9.22		8.89	
197	7.30			1.10		8.89		8.17
198	7.62			6.55		9.98		9.26
201	7.62		1.53	1.13	9.19	9.22	8.85	8.50
205	8.00		0.34	0.48	8.91	9.23	8.58	8.51
206	8.09		0.47	0.34	9.15	9.17	8.81	8.45
207	7.74		0.66	0.89	8.95	9.24	8.61	8.52
209	8.18		0.14	0.03	8.70	8.20	8.36	7.48
24 + 27	5.40		0.25	0.12	6.17	6.02	5.83	5.30
28 + 31	5.67	6.89	0.52	0.19	6.77	6.50	6.43	5.78
37 + 42	5.80			0.62		7.14		6.42
47 + 48	5.82	7.18	1.23	0.65	7.29	7.17	6.95	6.46
41 + 64 + 71	5.87			0.46		7.08		6.36
56 + 60	6.11			0.31		7.15		6.43
70 + 76	6.17	7.56	1.49	0.61	7.72	7.50	7.39	6.78
66 + 95	6.17			0.53		7.44		6.72
56 + 60 + 81	6.19	7.96	0.55		7.32		6.98	
84 + 92	6.20			1.22		7.83		7.11
87 + 97	6.29	8.08	2.45		8.06		7.73	
137 + 176	6.80			1.16		8.41		7.69

Table 1. Great Lakes Trout BAF<sub>g</sub>s Calculated from Measured BSAFs/BAFs - page 5a.

Chemical	log K <sub>ow</sub>	log BAF Oliver & Niimi <sup>a</sup> measured	BSAF Oliver & Niimi <sup>a</sup> measured	BSAF EPA <sup>b</sup> measured	log BAF Oliver & Niimi <sup>a</sup> ref PCB 52	log BAF EPA <sup>b</sup> ref PCB 52	log BAF Oliver & Niimi <sup>a</sup> ref PCB 105	log BAF EPA <sup>b</sup> ref PCB 105
PCBs								
138+163	6.91			2.23		8.81		8.09
156+171+202	7.18			1.25		8.82		8.10
182+187	7.19	8.43	3.80		9.15		8.81	
157+200	7.23			1.56		8.97		8.25
170+190	7.37	9.20	2.06	4.17	9.06	9.53	8.73	8.81
195+208	7.64			0.72		9.04		8.33
196+203	7.65	9.26	1.56	1.12	9.23	9.25	8.89	8.53
2378-TCDD	7.02			0.059		7.34		6.62
12378-PeCDD	7.50			0.054		7.78		7.06
123478-HxCDD	7.80			0.018		7.60		6.88
123678-HxCDD	7.80			0.0073		7.21		6.49
123789-HxCDD	7.80			0.0081		7.26		6.54
1234678-HpCDD	8.20			0.0031		7.24		6.52
OCDD	8.60			0.00074		7.02		6.30
2378-TCDF	5.80			0.047		6.02		5.30
12378-PeCDF	6.50			0.013		6.16		5.44
23478-PeCDF	7.00			0.095		7.52		6.81
123478-HxCDF	7.50			0.0045		6.70		5.98
123678-HxCDF	7.50			0.011		7.09		6.37
123789-HxCDF	7.50			0.037		7.61		6.90
234678-HxCDF	7.50			0.040		7.65		6.93
1234678-HpCDF	8.00			0.00065		6.36		5.64
1234789-HpCDF	8.00			0.023		7.91		7.19
OCDF	8.80			0.00099		7.34		6.62

<sup>a</sup> Oliver and Niimi, 1988

<sup>b</sup> Cook et al., 1994

Table 1. Great Lakes Trout BAF<sub>i</sub>'s Calculated from Measured BSAFs/BAFs - page 1b.

Chemical	log K <sub>ow</sub>	log BAF Oliv. & Niimi <sup>a</sup> measured	log BAF Oliv. & Niimi <sup>a</sup> DDT	log BAF EPA <sup>b</sup> DDT	log BAF Oliv. & Niimi <sup>a</sup> ref PCB 118	log BAF EPA <sup>b</sup> ref PCB 118	BT-BSAF EPA-G Bay	log BAF EPA-G Bay ref PCB 52	log BAF EPA-G Bay ref PCB118
dieldrin	5.40			7.09		7.40			
ddt	6.91	8.00	8.00	8.00	7.75	8.31			
dde	6.96	8.46	8.63	8.71	8.38	9.02			
ddd	6.22	7.03	6.72		6.47				
mirex	7.50	8.59	8.71	8.48	8.45	8.79			
photomirex	6.76	8.00	8.55		8.30				
p-chlordane	5.54	6.74	6.94		6.68				
t-chlordane	5.54			6.71		7.02			
c-chlordane	5.54			7.09		7.39			
t-nonachlor	5.66			7.55		7.86			
c-nonachlor	5.66			6.23		6.54			
alpha-hch	3.78	4.69	5.22		4.97				
gamma-hch	3.69	4.93	4.58		4.33				
hcbd	4.84								
ocs	7.94	9.20	8.98		8.73				
hcb	5.73	6.41	5.75		5.50				
pcb	5.18	5.81	4.80		4.55				
1235tcbl	4.66								
1245tcbl	4.60								
1234tcbl	4.64	5.07	3.83		3.58				
135tcbl	4.19								
124tcbl	4.05								
123tcbl	4.14								
245tcbl	4.93								
236tcbl	4.93								
pchl	6.36								

Table 1. Great Lakes Trout BAF<sub>i</sub>'s Calculated from Measured BSAFs/BAFs - page 2b.

Chemical	log K <sub>ow</sub>	log BAF Oliv. & Niimi <sup>a</sup> measured	log BAF Oliv. & Niimi <sup>a</sup> DDT	log BAF EPA <sup>b</sup> DDT	log BAF Oliv. & Niimi <sup>a</sup> ref PCB 118	log BAF EPA <sup>b</sup> ref PCB 118	BT-BSAF EPA-G Bay	log BAF EPA-G Bay ref PCB 52	log BAF EPA-G Bay ref PCB118
<b>PCBs</b>									
5	4.97						0.14	4.88	5.12
6	5.06			5.48		5.79	1.70	6.05	6.29
8	5.07						0.14	4.98	5.22
12	5.22			5.73		6.04			
13	5.29								
16	5.16	5.92							
17	5.25	5.52	5.47	6.11	5.22	6.42	0.75	5.89	6.13
18	5.24	5.75	5.71	5.11	5.46	5.41	0.64	5.81	6.05
22	5.58	6.39	5.95	5.88	5.70	6.19	0.39	5.94	6.18
25	5.67		6.11	6.06	5.86	6.36	0.73	6.30	6.54
26	5.66		6.95	6.17	6.69	6.48	0.95	6.40	6.64
32	5.44	6.76	5.76		5.50				
33	5.60	5.32	5.82	6.16	5.57	6.46	0.29	5.83	6.07
40	5.66	6.55	5.73	5.78	5.47	6.09	0.69	6.26	6.50
42	5.76	7.49	6.53		6.28				
44	5.75	6.96	6.48	6.22	6.23	6.53			
45	5.53			5.74		6.05	1.16	6.36	6.60
46	5.53		6.34	4.70	6.09	5.01	0.61	6.08	6.32
49	5.85	7.13	6.74		6.49		3.34	7.14	7.38
52	5.84	7.01	6.68	6.33	6.42	6.64	4.74	7.28	7.52
53	5.62	6.51	6.94		6.68		2.12	6.71	6.95
63	6.17			6.95		7.26	4.37	7.57	7.81
64	5.95	7.51	6.87		6.61				
66	6.20	7.79	7.18		6.93		3.10	7.46	7.70
74	6.20	7.66	7.79	6.85	7.54	7.16	2.46	7.36	7.60
77	6.36			6.69		7.00	4.12	7.74	7.98
81	6.36			7.05		7.36	11.60	8.19	8.43

Table 1. Great Lakes Trout BAF<sub>i</sub>s Calculated from Measured BSAFs/BAFs - page 3b.

Chemical	log K <sub>ow</sub>	log BAF Oliv. & Niimi <sup>a</sup> measured	log BAF Oliv. & Niimi <sup>a</sup> DDT	log BAF EPA <sup>b</sup> DDT	log BAF Oliv. & Niimi <sup>a</sup> ref PCB 118	log BAF EPA <sup>b</sup> ref PCB 118	BT-BSAF EPA-G Bay	log BAF EPA-G Bay ref PCB 52	log BAF EPA-G Bay ref PCB118
<b>PCBs</b>									
82	6.20	8.13	7.64	6.32	7.39	6.63	4.05	7.57	7.81
83	6.26			7.25		7.56	5.67	7.78	8.02
84	6.04	8.28	7.58		7.32		7.20	7.66	7.90
85	6.30	7.89	7.51	7.28	7.26	7.59	7.25	7.92	8.16
87	6.29			7.29		7.60	6.13	7.84	8.08
91	6.13	6.92	7.28	6.80	7.02	7.11	8.44	7.82	8.06
92	6.35	8.11	7.56		7.30				
95	6.13	7.25	7.33		7.08				
97	6.29			6.60		6.91	6.42	7.86	8.10
99	6.39	7.39	7.28	7.44	7.02	7.74	7.18	8.01	8.25
100	6.23			7.35		7.65	1.71	7.23	7.47
101	6.38	7.45	7.82	7.27	7.57	7.58	10.01	8.14	8.38
105	6.65	8.13	8.13	8.17	7.88	8.48	5.35	8.14	8.38
110	6.48	7.79	7.72	7.26	7.46	7.57	4.15	7.86	8.10
118	6.74	8.15	8.40	7.84	8.15	8.15	4.96	8.20	8.44
119	6.58			8.03		8.34	3.03	7.83	8.07
126	6.89			8.26		8.57			
128	6.74		8.35	8.05	8.10	8.36	10.21	8.51	8.75
129	6.73		8.03	7.65	7.77	7.96			
130	6.80			8.00		8.31	11.21	8.61	8.85
132	6.58	7.56	7.57		7.32				
136	6.22	7.37	8.31		8.05				
138	6.83	8.30	8.51		8.26				
141	6.82	8.32	8.31	7.93	8.06	8.24	9.30	8.55	8.79
146	6.89	8.73	8.45	7.85	8.20	8.16	10.02	8.66	8.90
149	6.67	7.99	8.09	7.51	7.84	7.81	8.70	8.37	8.61
151	6.64	8.51	8.22	7.72	7.97	8.03	9.70	8.39	8.63
153	6.92	8.32	8.60	8.07	8.34	8.38	5.35	8.41	8.65
156	7.18		8.83		8.58				
158	7.02			8.07		8.38			



Table 1. Great Lakes Trout BAF<sub>i</sub>'s Calculated from Measured BSAFs/BAFs - page 4b.

Chemical	log K <sub>ow</sub>	log BAF Oliv. & Niimi <sup>a</sup> measured	log BAF Oliv. & Niimi <sup>a</sup> DDT	log BAF EPA <sup>b</sup> DDT	log BAF Oliv. & Niimi <sup>a</sup> ref PCB 118	log BAF EPA <sup>b</sup> ref PCB 118	BT-BSAF EPA-G Bay	log BAF EPA-G Bay ref PCB 52	log BAF EPA-G Bay ref PCB118
<b>PCBs</b>									
167	7.27			7.98		8.28	16.02	9.24	9.48
171	7.11		8.60		8.34				
172	7.33			8.33		8.64			
174	7.11	8.74	8.35	8.07	8.10	8.38	4.46	8.52	8.76
177	7.08	9.01	8.68	8.23	8.43	8.54	8.04	8.75	8.99
178	7.14		8.84	8.45	8.59	8.76			
180	7.36	8.58	8.99	8.74	8.74	9.05	10.97	9.16	9.40
183	7.20	9.03	9.00	8.50	8.75	8.80	6.50	8.78	9.02
185	7.11		8.35	8.33	8.10	8.63	3.23	8.38	8.62
189	7.71			8.43		8.74	3.45	9.01	9.25
194	7.80	8.56	9.04	9.06	8.78	9.37	3.29	9.08	9.32
195	7.56		8.89		8.64				
197	7.30			8.21		8.52			
198	7.62			9.30		9.61	0.46	8.05	8.29
201	7.62		8.86	8.54	8.60	8.85	4.79	9.06	9.30
205	8.00		8.58	8.55	8.33	8.86	3.09	9.25	9.49
206	8.09		8.82	8.49	8.56	8.80	0.95	8.83	9.07
207	7.74		8.61	8.56	8.36	8.86	1.30	8.62	8.86
209	8.18		8.37	7.52	8.11	7.83	0.19	8.22	8.46
24 + 27	5.40		5.84	5.34	5.58	5.65	1.55	6.35	6.59
28 + 31	5.67	6.89	6.44	5.82	6.18	6.12	0.67	6.26	6.50
37 + 42	5.80			6.46		6.77	6.75	7.39	7.63
47 + 48	5.82	7.18	6.96	6.50	6.70	6.80	7.86	7.47	7.71
41 + 64 + 71	5.87			6.40		6.71	2.55	7.04	7.28
56 + 60	6.11			6.47		6.78	1.14	6.93	7.17
70 + 76	6.17	7.56	7.39	6.82	7.14	7.12	1.20	7.01	7.25
66 + 95	6.17			6.76		7.07	3.10	7.43	7.67
56 + 60 + 81	6.19	7.96	6.99		6.73		1.15	7.02	7.26
84 + 92	6.20			7.15		7.46	7.25	7.82	8.06

Table 1. Great Lakes Trout BAF<sub>i</sub>'s Calculated from Measured BSAFs/BAFs - page 5b.

Chemical	log K <sub>ow</sub>	log BAF Oliv. & Niimi <sup>a</sup> measured	log BAF Oliv. & Niimi <sup>a</sup> DDT	log BAF EPA <sup>b</sup> DDT	log BAF Oliv. & Niimi <sup>a</sup> ref PCB 118	log BAF EPA <sup>b</sup> ref PCB 118	BT-BSAF EPA-G Bay	log BAF EPA-G Bay ref PCB 52	log BAF EPA-G Bay ref PCB118
<b>PCBs</b>									
87 + 97	6.29	8.08	7.73		7.48		6.30	7.85	8.09
137 + 176	6.80			7.73		8.04	1.43	7.72	7.96
138 + 163	6.91			8.13		8.43	11.94	8.75	8.99
156 + 171 + 202	7.18			8.14		8.45	10.70	8.97	9.21
182 + 187	7.19	8.43	8.82		8.56		9.38	8.92	9.16
157 + 200	7.23			8.29		8.60	8.66	8.93	9.17
170 + 190	7.37	9.20	8.73	8.85	8.48	9.16	4.10	8.74	8.98
195 + 208	7.64			8.36		8.67	1.01	8.41	8.65
196 + 203	7.65	9.26	8.89	8.57	8.64	8.87	4.24	9.04	9.28
<b>OCDD</b>									
2378-TCDD	7.02			6.66		6.97			
12378-PeCDD	7.50			7.10		7.41			
123478-HxCDD	7.80			6.92		7.23			
123678-HxCDD	7.80			6.53		6.84			
123789-HxCDD	7.80			6.58		6.88			
1234678-HpCDD	8.20			6.56		6.87			
OCDD	8.60			6.34		6.64			
2378-TCDF	5.80			5.34		5.65			
12378-PeCDF	6.50			5.48		5.79			
23478-PeCDF	7.00			6.85		7.15			
123478-HxCDF	7.50			6.02		6.33			
123678-HxCDF	7.50			6.41		6.72			
123789-HxCDF	7.50			6.94		7.24			
234678-HxCDF	7.50			6.97		7.28			
1234678-HpCDF	8.00			5.68		5.99			
1234789-HpCDF	8.00			7.23		7.54			
OCDF	8.80			6.66		6.97			

Table 2. Mean BAF<sub>i</sub>s from Lake Ontario BSAFs for Salmonids - page 1

Chemical	log K <sub>ow</sub>	Number BAFs	Mean log BAF <sub>i</sub> <sup>d</sup>	Mean BAF <sub>i</sub> <sup>d</sup>
dieldrin	5.40	4	7.33	2.12e+07
ddt	6.91	8	8.13	1.34e+08
dde	6.96	8	8.80	6.30e+08
ddd	6.22	4	6.74	5.53e+06
mirex	7.50	8	8.72	5.29e+08
photomirex	6.76	4	8.57	3.71e+08
g-chlordane	5.54	4	6.96	9.07e+06
t-chlordane	5.54	4	6.95	8.81e+06
c-chlordane	5.54	4	7.32	2.10e+07
t-nonachlor	5.66	4	7.79	6.10e+07
c-nonachlor	5.66	4	6.47	2.96e+06
alpha-hch	3.78	4	5.24	1.74e+05
gamma-hch	3.69	4	4.60	3.96e+04
hcbd	4.84			
ocs	7.94	4	9.00	1.01e+09
hcb	5.73	4	5.77	5.90e+05
pcb	5.18	4	4.82	6.63e+04
1235tcb	4.66			
1245tcb	4.60			
1234tcb	4.64	4	3.85	7.10e+03
135tcb	4.19			
124tcb	4.05			
123tcb	4.14			
245tct	4.93			
236tct	4.93			
pct	6.36			
PCBs				
5	4.97			
6	5.06	4	5.72	5.25e+05
8	5.07			
12	5.22	4	5.97	9.28e+05
13	5.29			
16	5.16			
17	5.25	8	5.92	8.31e+05
18	5.24	8	5.54	3.45e+05
22	5.58	8	6.04	1.10e+06
25	5.67	8	6.21	1.63e+06
26	5.66	8	6.69	4.86e+06

Table 2. Mean BAF<sub>i</sub><sup>d</sup>s from Lake Ontario BSAFs for Salmonids - page 2

Chemical	log K <sub>ow</sub>	Number BAFs	Mean log BAF <sub>i</sub> <sup>d</sup>	Mean BAF <sub>i</sub> <sup>d</sup>
PCBs				
32	5.44	4	5.78	5.97e+05
33	5.60	8	6.12	1.31e+06
40	5.66	8	5.88	7.61e+05
42	5.76	4	6.55	3.54e+06
44	5.75	8	6.48	3.02e+06
45	5.53	4	5.98	9.47e+05
46	5.53	8	5.65	4.44e+05
49	5.85	4	6.76	5.77e+06
52	5.84	8	6.63	4.28e+06
53	5.62	4	6.96	9.04e+06
63	6.17	4	7.19	1.54e+07
64	5.95	4	6.89	7.67e+06
66	6.20	4	7.20	1.59e+07
74	6.20	8	7.45	2.81e+07
77	6.36	4	6.93	8.44e+06
81	6.36	4	7.29	1.95e+07
82	6.20	8	7.11	1.29e+07
83	6.26	4	7.49	3.08e+07
84	6.04	4	7.59	3.92e+07
85	6.30	8	7.52	3.34e+07
87	6.29	4	7.53	3.39e+07
91	6.13	8	7.17	1.48e+07
92	6.35	4	7.58	3.77e+07
95	6.13	4	7.35	2.23e+07
97	6.29	4	6.84	6.94e+06
99	6.39	8	7.48	3.05e+07
100	6.23	4	7.58	3.84e+07
101	6.38	8	7.68	4.73e+07
105	6.65	8	8.28	1.90e+08
110	6.48	8	7.62	4.13e+07
118	6.74	8	8.25	1.78e+08
119	6.58	4	8.27	1.85e+08
126	6.89	4	8.50	3.17e+08
128	6.74	8	8.33	2.13e+08
129	6.73	8	7.97	9.25e+07
130	6.80	4	8.24	1.72e+08
132	6.58	4	7.59	3.90e+07
136	6.22	4	8.33	2.12e+08
138	6.83	4	8.53	3.39e+08
141	6.82	8	8.25	1.77e+08

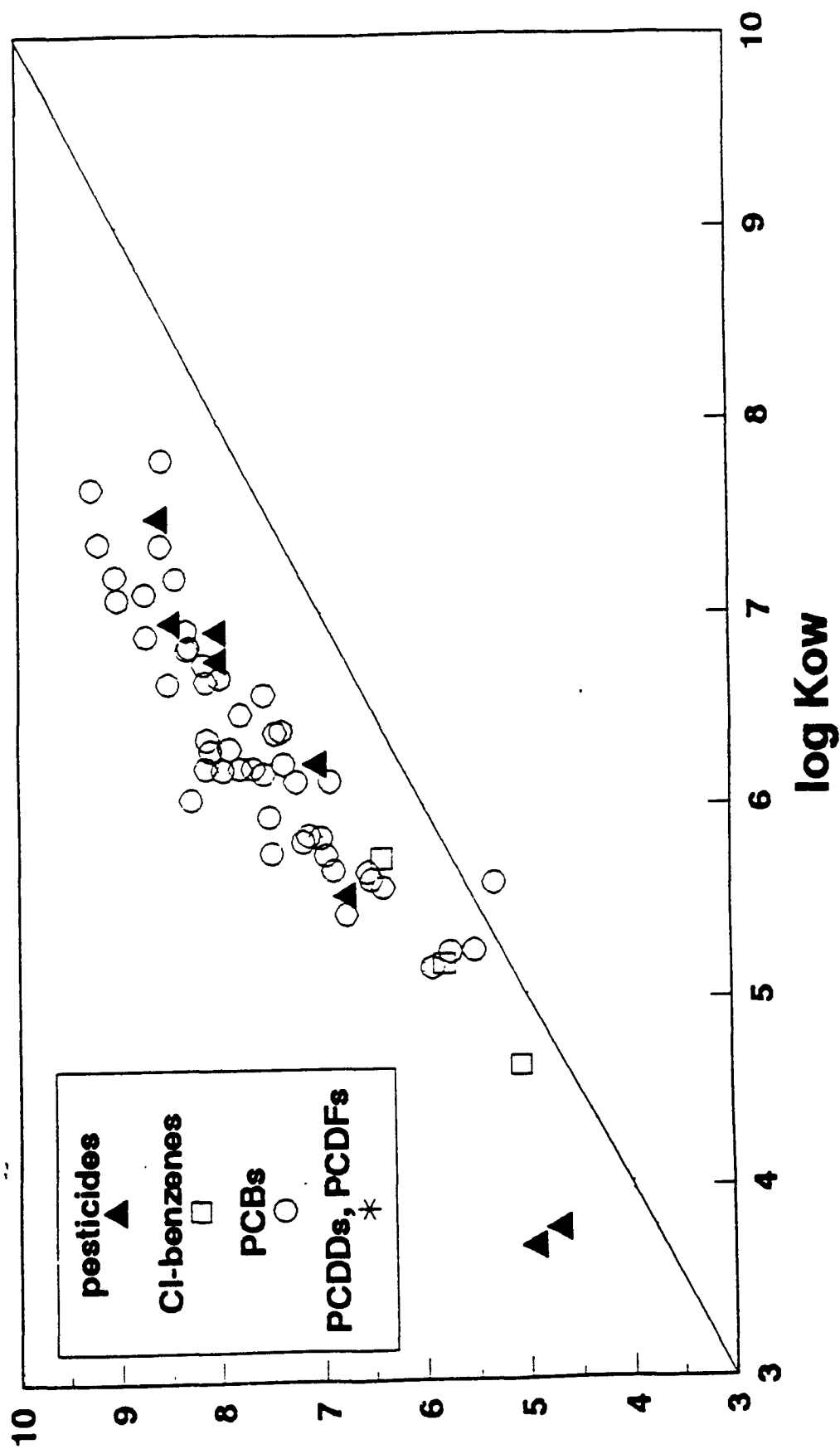
Table 2. Mean BAF<sub>i</sub><sup>d</sup>s from Lake Ontario BSAFs for Salmonids - page 3

Chemical	log K <sub>ow</sub>	Number BAFs	Mean log BAF <sub>i</sub> <sup>d</sup>	Mean BAF <sub>i</sub> <sup>d</sup>
PCBs				
146	6.89	8	8.28	1.91e+08
149	6.67	8	7.93	8.43e+07
151	6.64	8	8.10	1.26e+08
153	6.92	8	8.46	2.89e+08
156	7.18	4	8.85	7.08e+08
158	7.02	4	8.31	2.02e+08
167	7.27	4	8.21	1.63e+08
171	7.11	4	8.61	4.12e+08
172	7.33	4	8.57	3.69e+08
174	7.11	8	8.34	2.19e+08
177	7.08	8	8.58	3.82e+08
178	7.14	8	8.77	5.94e+08
180	7.36	8	8.99	9.83e+08
183	7.20	8	8.88	7.53e+08
185	7.11	8	8.47	2.93e+08
189	7.71	4	8.67	4.63e+08
194	7.80	8	9.18	1.50e+09
195	7.56	4	8.91	8.13e+08
197	7.30	4	8.45	2.79e+08
198	7.62	4	9.54	3.47e+09
201	7.62	8	8.83	6.71e+08
205	8.00	8	8.69	4.92e+08
206	8.09	8	8.78	6.02e+08
207	7.74	8	8.71	5.16e+08
209	8.18	8	8.07	1.18e+08
24+27	5.40	8	5.72	5.21e-07
28+31	5.67	8	6.25	1.80e+06
37+42	5.80	4	6.70	4.97e+06
47+48	5.82	8	6.85	7.14e+06
41+64+71	5.87	4	6.64	4.33e+06
56+60	6.11	4	6.71	5.07e+06
70+76	6.17	8	7.23	1.71e+07
66+95	6.17	4	7.00	9.96e+06
56+60+81	6.19	4	7.01	1.01e+07
84+92	6.20	4	7.39	2.46e+07
87+97	6.29	4	7.75	5.64e+07
137+176	6.80	4	7.97	9.30e+07
138+163	6.91	4	8.36	2.30e+08
156+171+202	7.18	4	8.38	2.40e+08
182+187	7.19	4	8.84	6.85e+08

Table 2. Mean BAF<sub>f</sub><sup>d</sup>s from Lake Ontario BSAFs for Salmonids - page 4

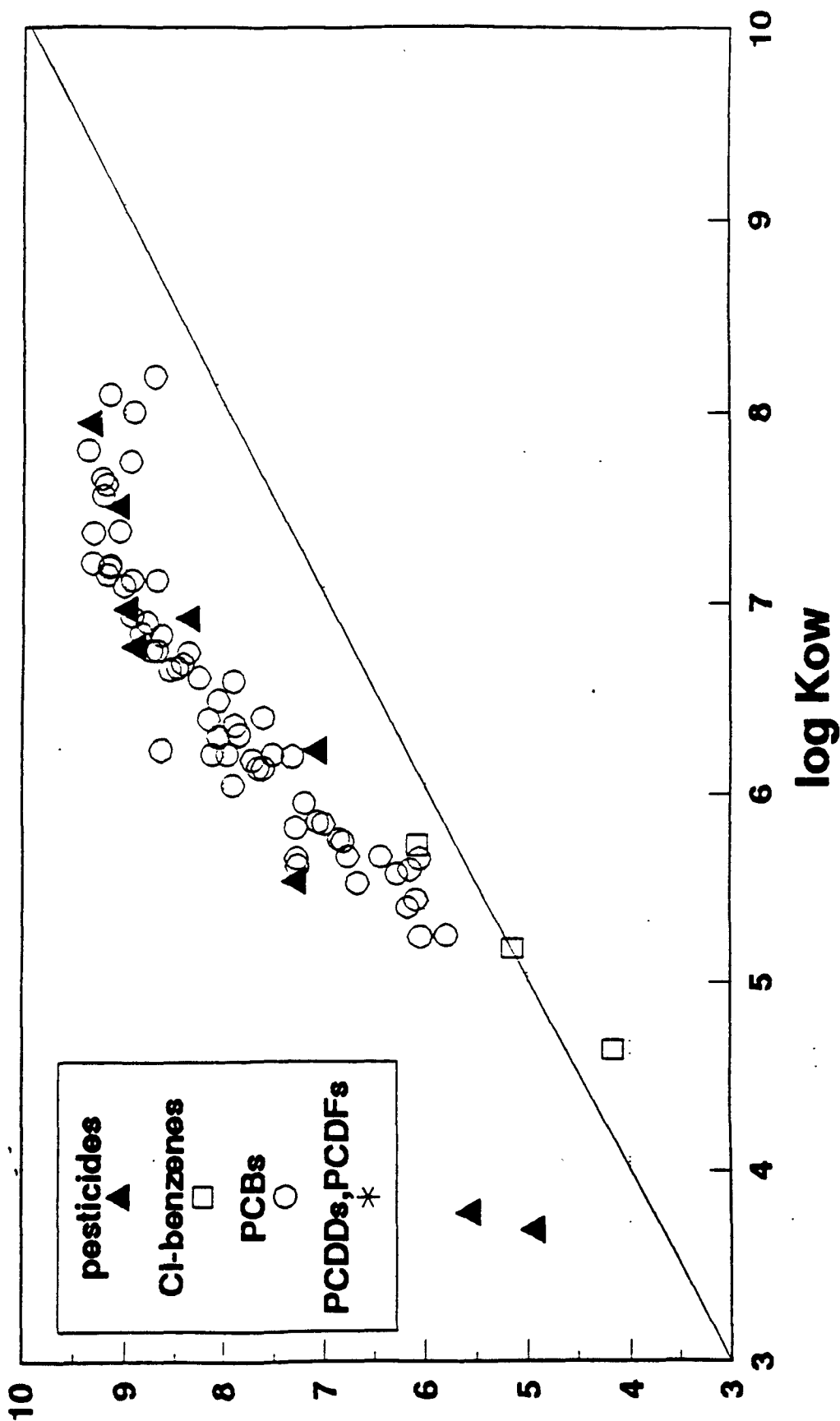
Chemical	log K <sub>ow</sub>	Number BAFs	Mean log BAF <sub>f</sub> <sup>d</sup>	Mean BAF <sub>f</sub> <sup>d</sup>
PCBs				
157+200	7.23	4	8.53	3.37e+08
170+190	7.37	8	8.92	8.31e+08
195+208	7.64	4	8.60	3.99e+08
196+203	7.65	8	8.86	7.22e+08
PCDDs				
2378-TCDD	7.02	4	6.89	7.85e+06
12378-PeCDD	7.50	4	7.34	2.17e+07
123478-HxCDD	7.80	4	7.16	1.44e+07
123678-HxCDD	7.80	4	6.77	5.85e+06
123789-HxCDD	7.80	4	6.81	6.49e+06
1234678-HpCDD	8.20	4	6.80	6.24e+06
OCDD	8.60	4	6.57	3.74e+06
PCDFs				
2378-TCDF	5.80	4	5.58	3.77e+05
12378-PeCDF	6.50	4	5.72	5.22e+05
23478-PeCDF	7.00	4	7.08	1.21e+07
123478-HxCDF	7.50	4	6.26	1.81e+06
123678-HxCDF	7.50	4	6.65	4.42e+06
123789-HxCDF	7.50	4	7.17	1.49e+07
234678-HxCDF	7.50	4	7.21	1.61e+07
1234678-HpCDF	8.00	4	5.92	8.26e+05
1234789-HpCDF	8.00	4	7.47	2.92e+07
OCDF	8.80	4	6.90	7.94e+06

**Figure 1. Measured Lake Ontario Salmonid BAFs**  
**log BAF from Oliver & Niimi (1988)**



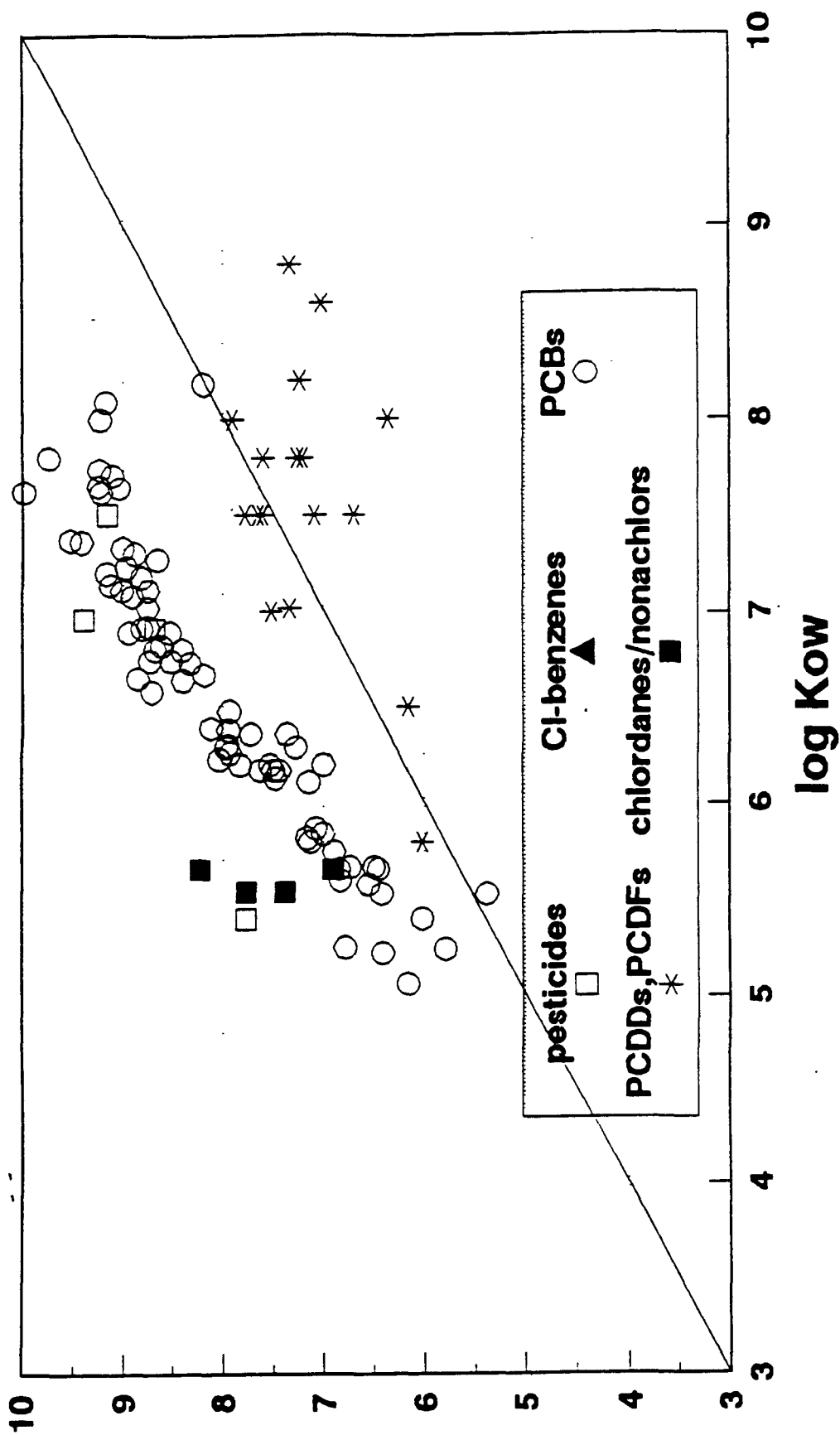
BAFs based on measured conc. in water  
 $Doc = 2mg/L$  &  $K_{doc} = K_{ow}/10$

**Figure 2. Predicted Lake Ontario Salmonid BAFs**  
**log BAF from Oliver & Niimi BSAFs**





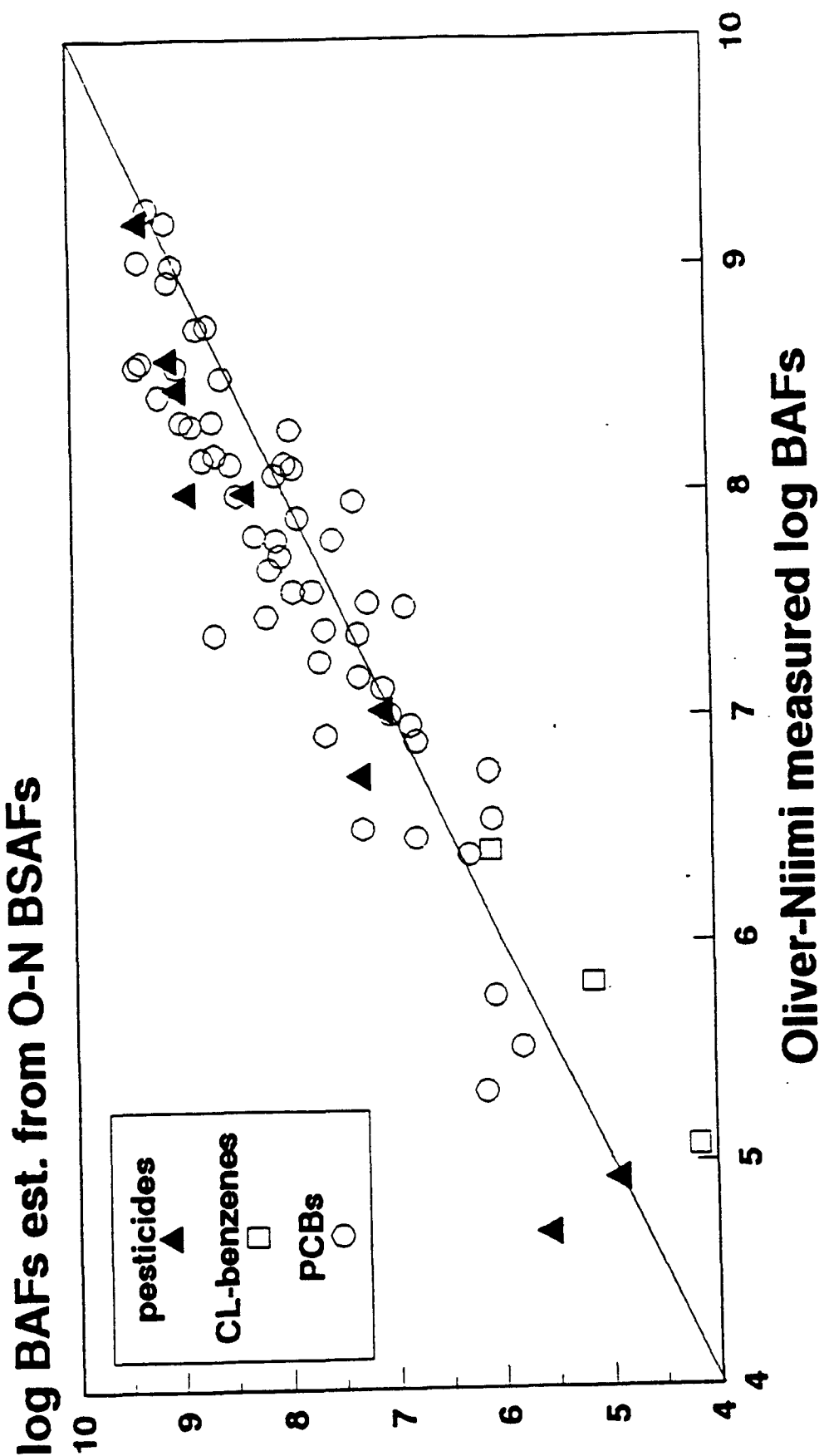
**Figure 3. Predicted Lake Ontario Lake Trout BAFs**  
**log BAF from EPA BSAFs (Cook et al., 1994)**



Referenced to O-N BAF for PCB 52  
 Doc=2mg/L & Kdoc=K<sub>ow</sub>/10

# Figure 4. Lake Ontario Salmonid BAFs

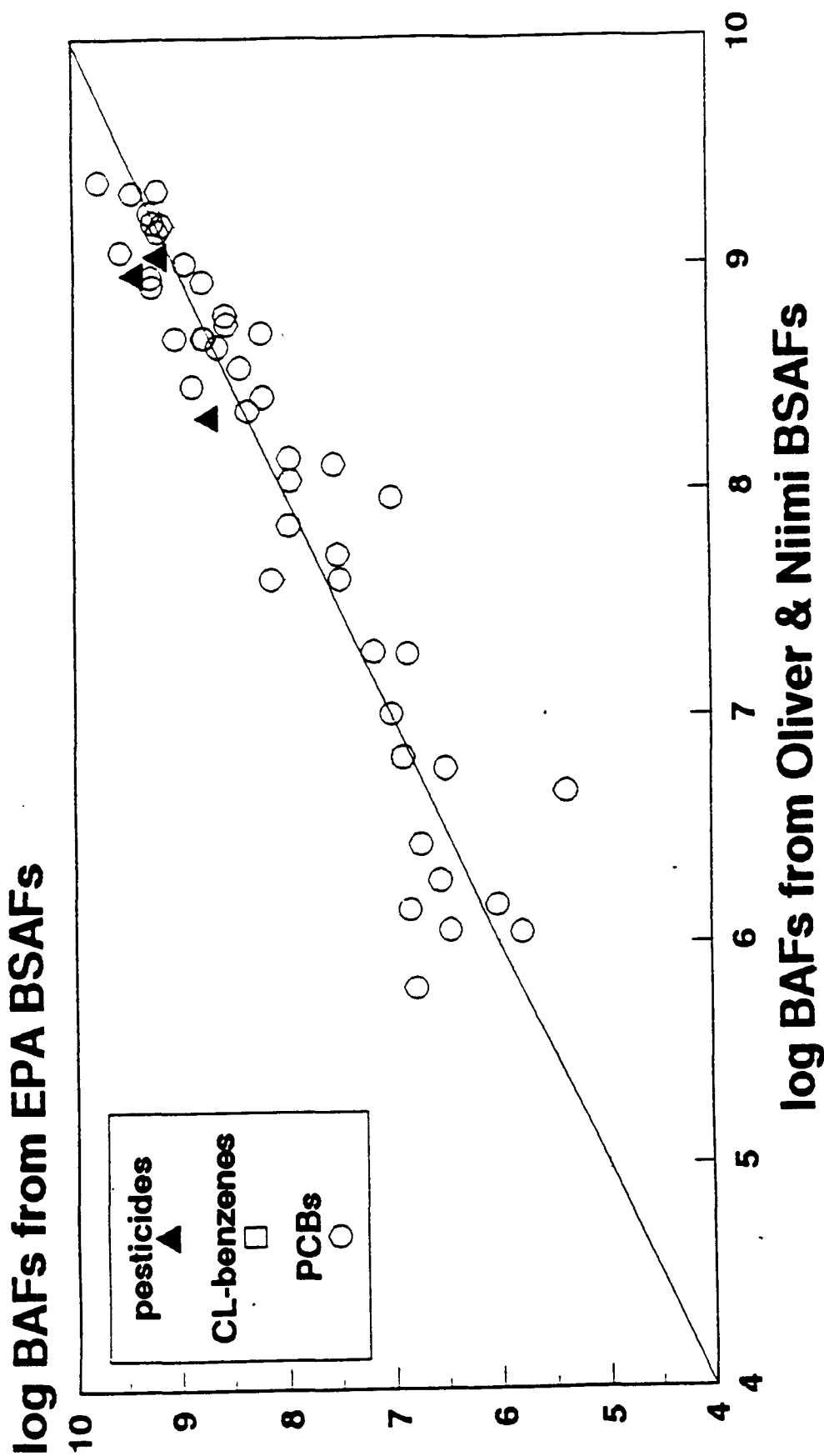
Correlation of Measured BAFs to BSAF Predicted



Oliver & Niimi - Referenced to BAF for PCB 52  
Doc=2mg/L & Kdoc=Kow/10

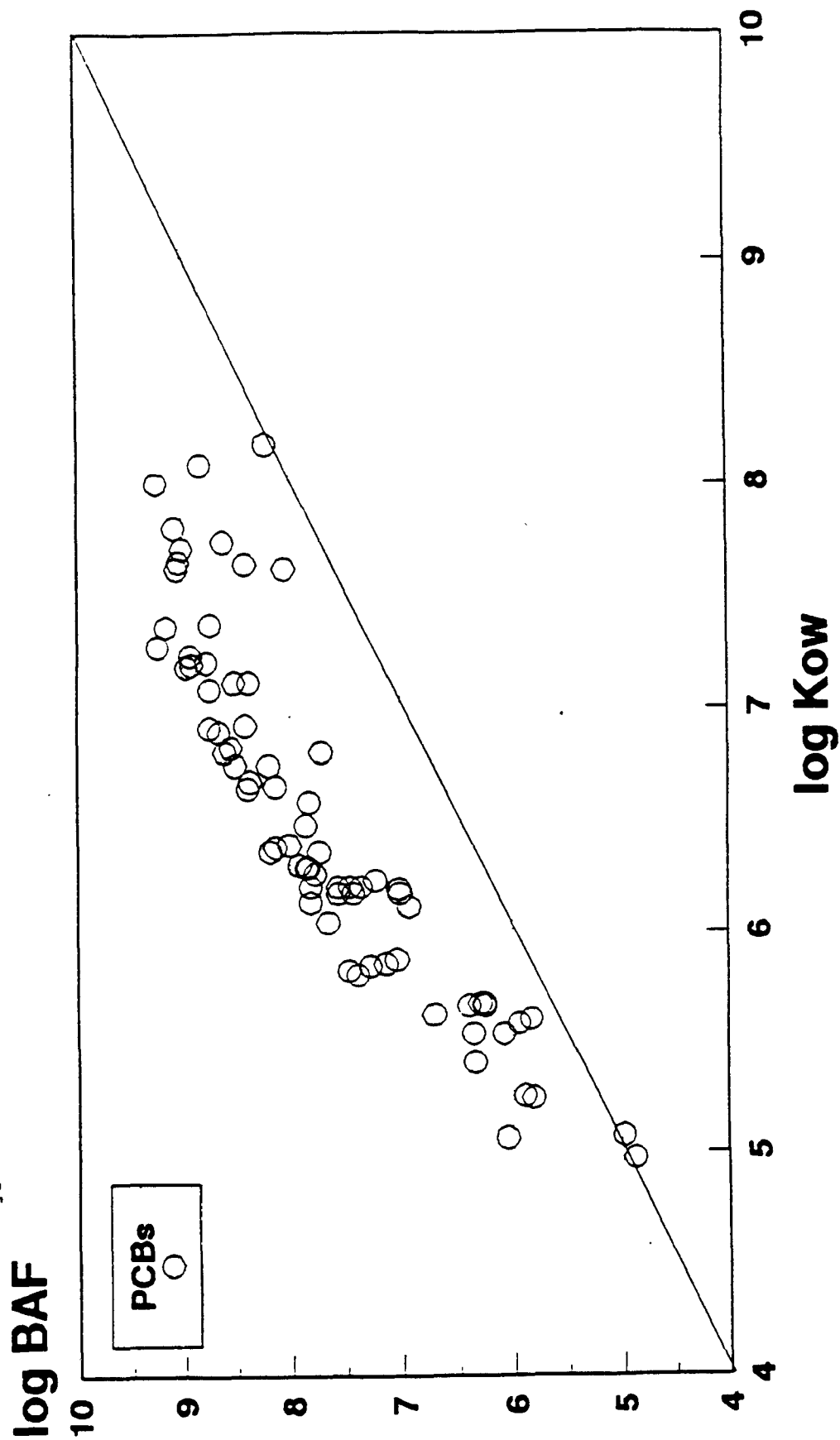
# Figure 5. Lake Ontario Salmonid BAFs

Correlation of EPA BSAF-pred. to O-N BSAF-pred.



# Figure 6. PCB BAFs for Brown Trout in Green Bay

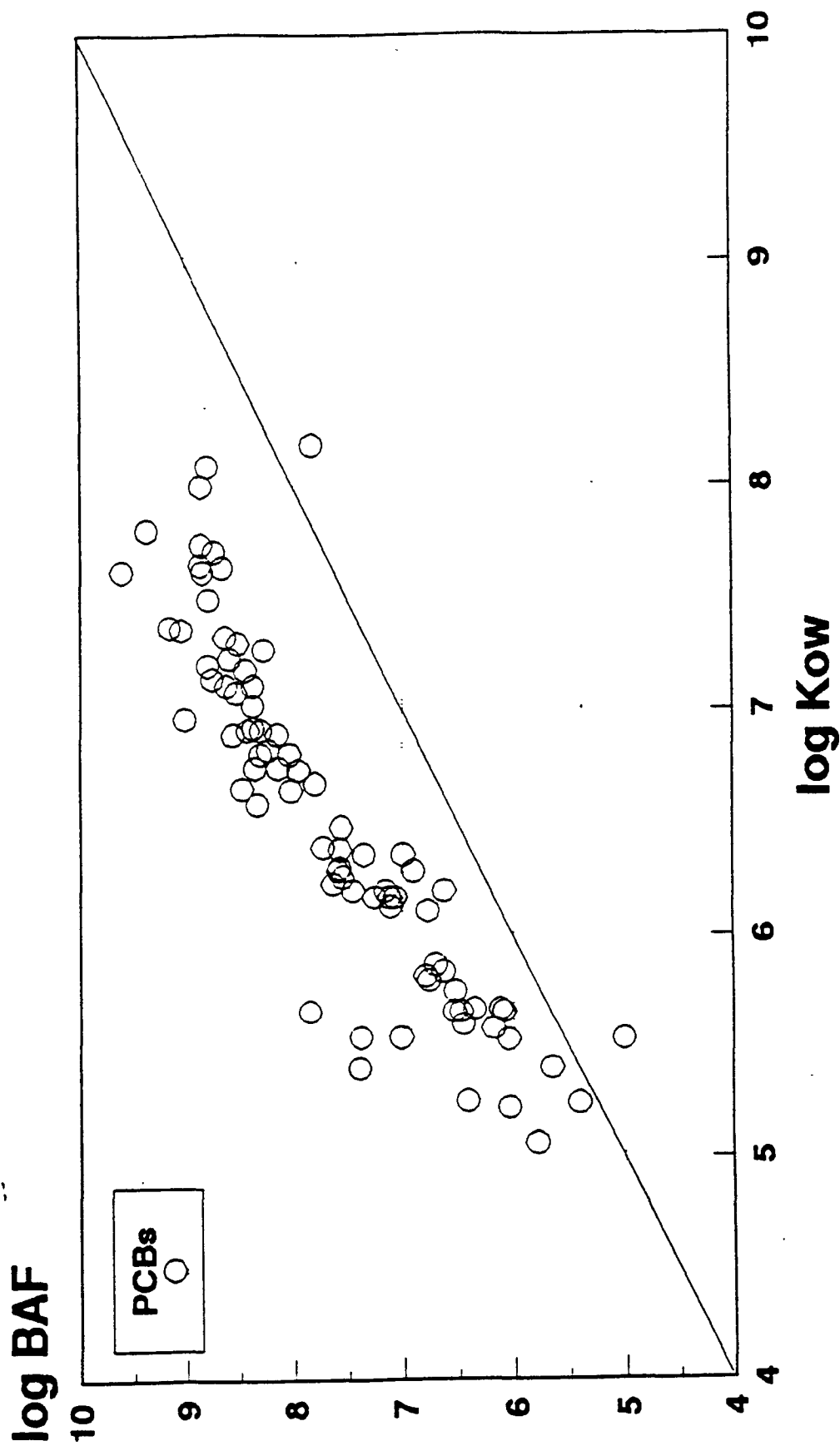
Calculated from BSAFs



EPA GB B. Trout-Region 3A/3B BAFs ref to PCB 52  
Doc=2-5mg/L & K<sub>oc</sub>=K<sub>ow</sub>/10

# Figure 7. PCB BAFs for Brown Trout in Green Bay

Calculated from BSAFs



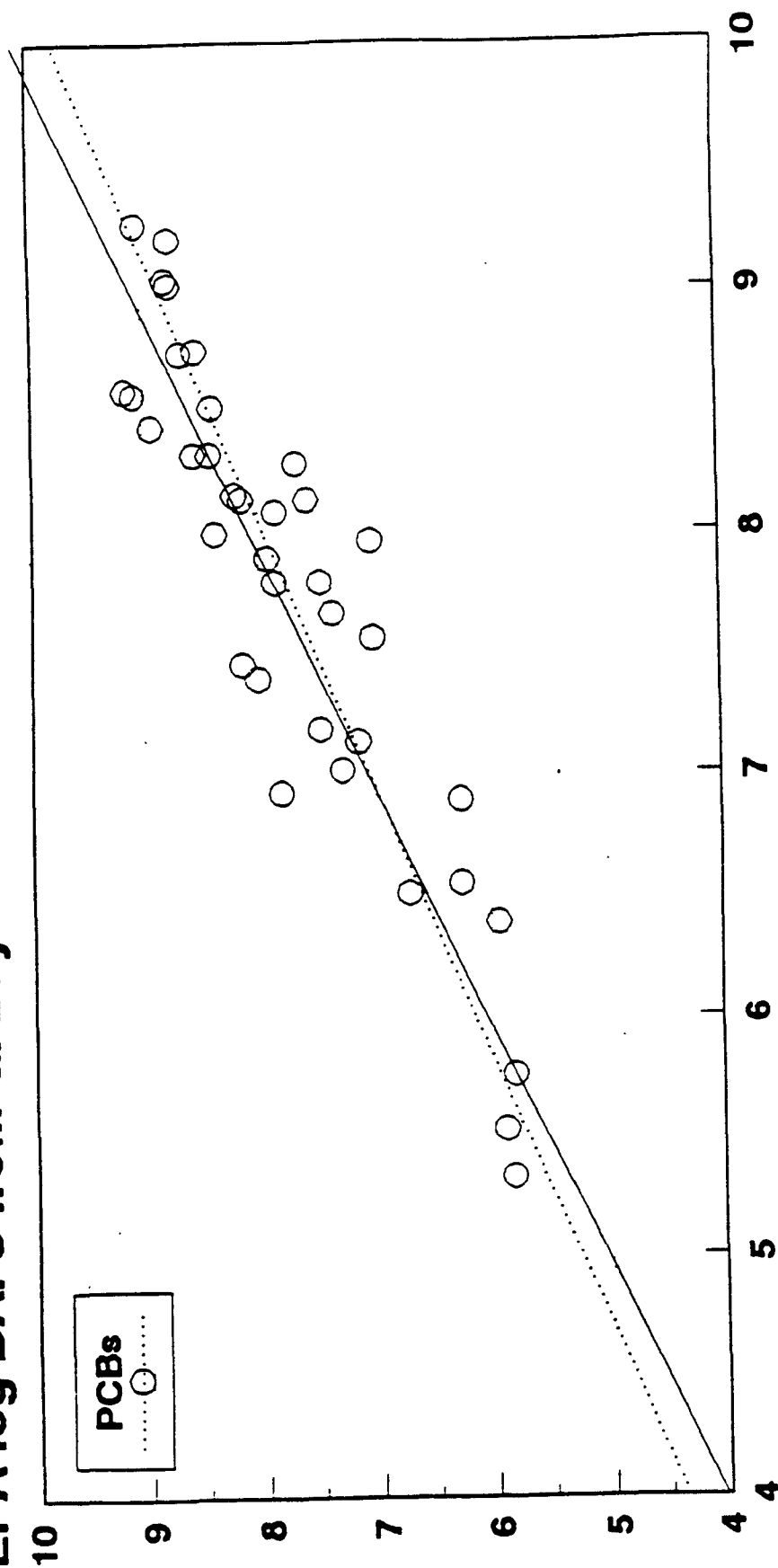
EPA GB B. Trout-Region 3A/3B BAFs ref to PCB 118

Doc=2.5mg/L & Koc=Kow/10

# Fig. 8. Correlation of L. Ont. & G. Bay BAFs

Lake Ont. Measured vs. G. Bay BT BSAF-predicted

EPA log BAFs from G. Bay BT BSAFs



Oliver & Niimi Meas. log BAFs

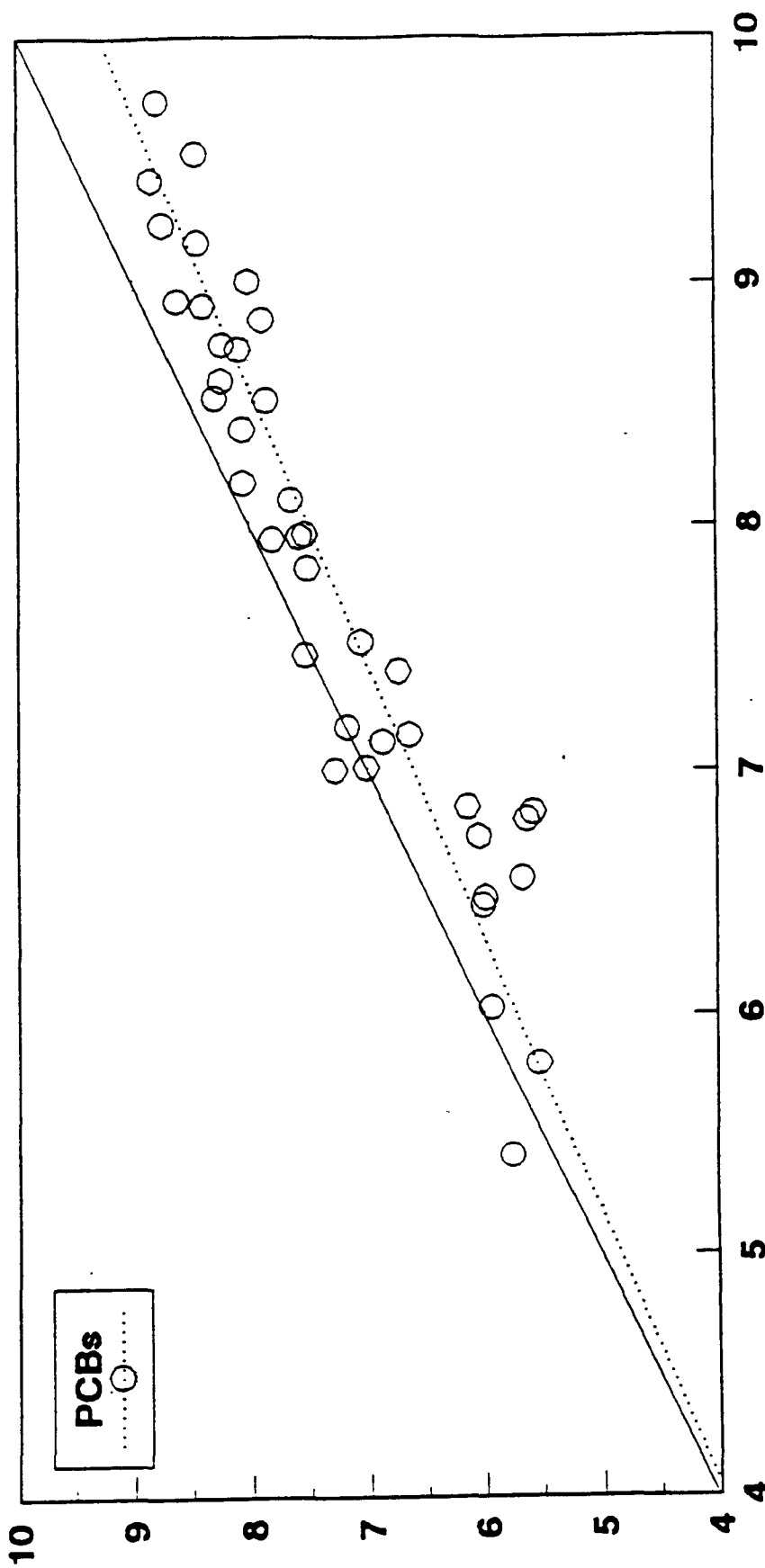
ERLD GB B.Trout Region 3A/3B BAFs ref. PCB 52

Doc=2.5mg/L & Koc=Kow/10

# Figure 9. Correlation of EPA BAFs from BSAFs

Lake Ontario Lake Trout vs. Green Bay B. Trout

G. Bay Brown Trout log BAFs



Lake Ont. Lake Trout log BAFs

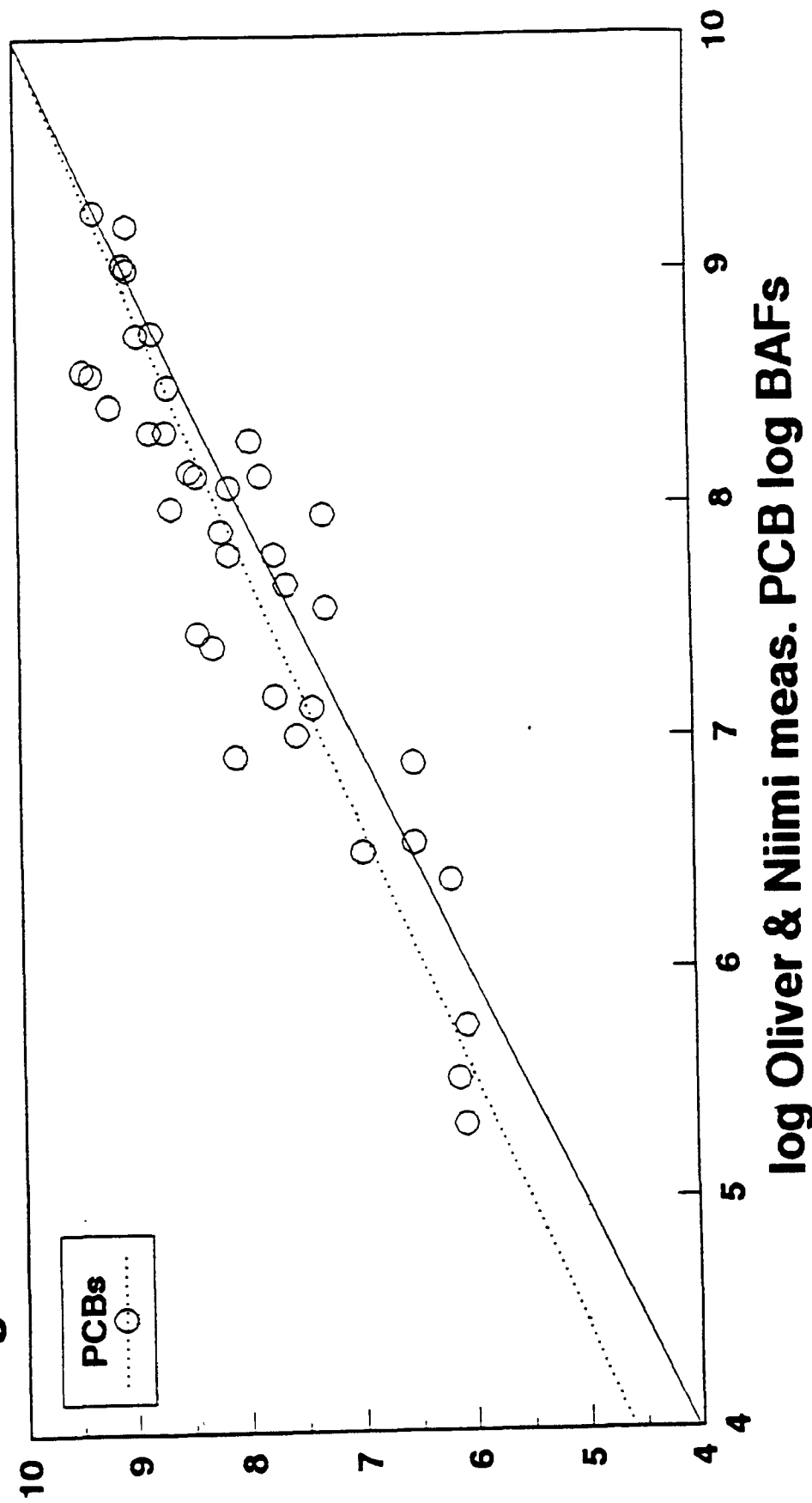
BAFs referenced to PCB 52; Green Bay Region 3A/B

Doc=2.5mg/L & Koc=Kow/10

# Fig. 10. Correlation of L.Ont. & G.Bay log BAFs

Oliver & Niimi Meas./EPA est. from B.Trout BSAFs

EPA log BAFs from G. Bay BT BSAFs



ERLD GB B.Trout Region 3A/3B BAFs ref. PCB 118

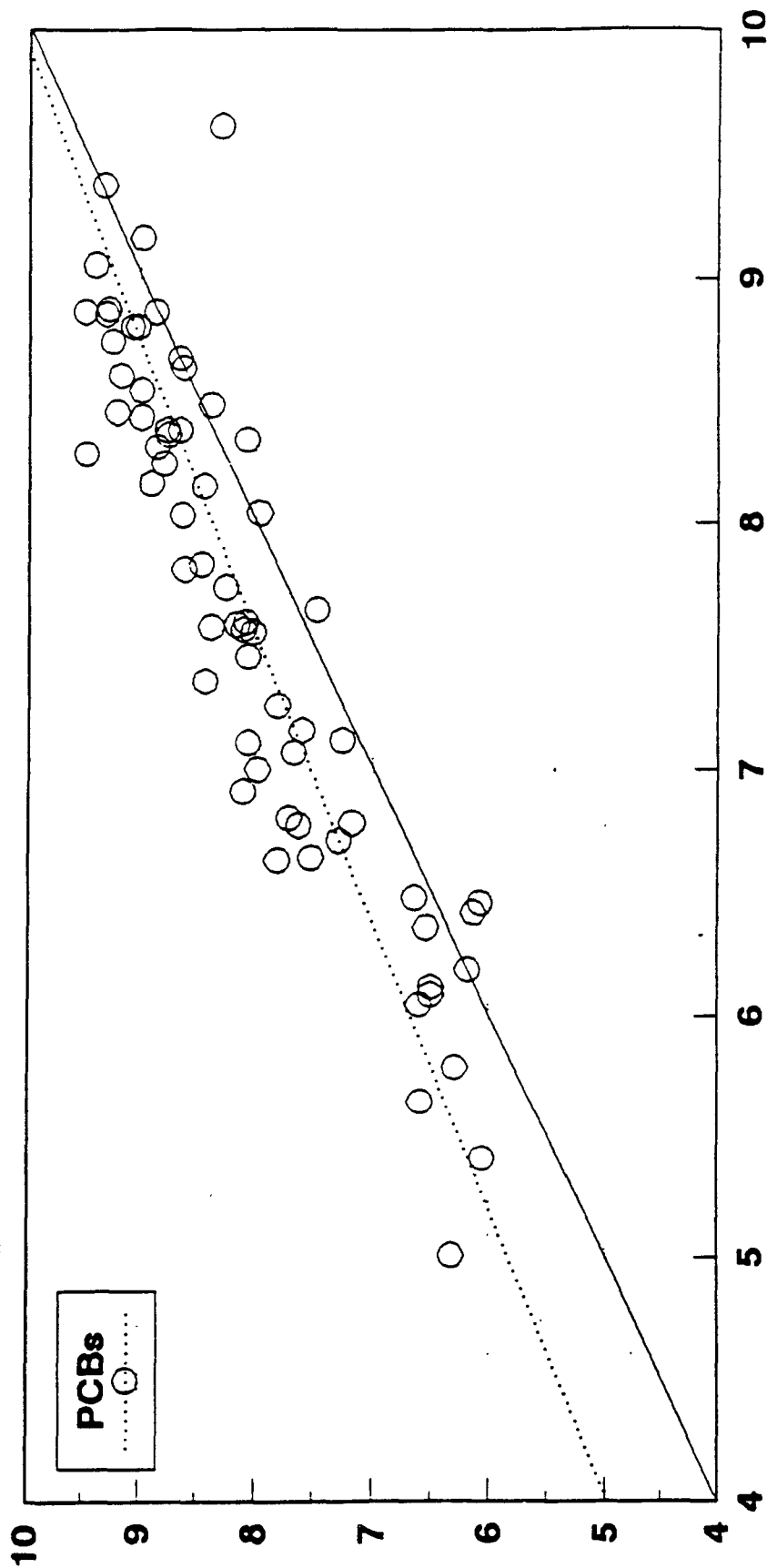
Doc=2-5mg/L & Koc=Kow/10



# Fig. 11. Correlation of BAFs from BSAFs

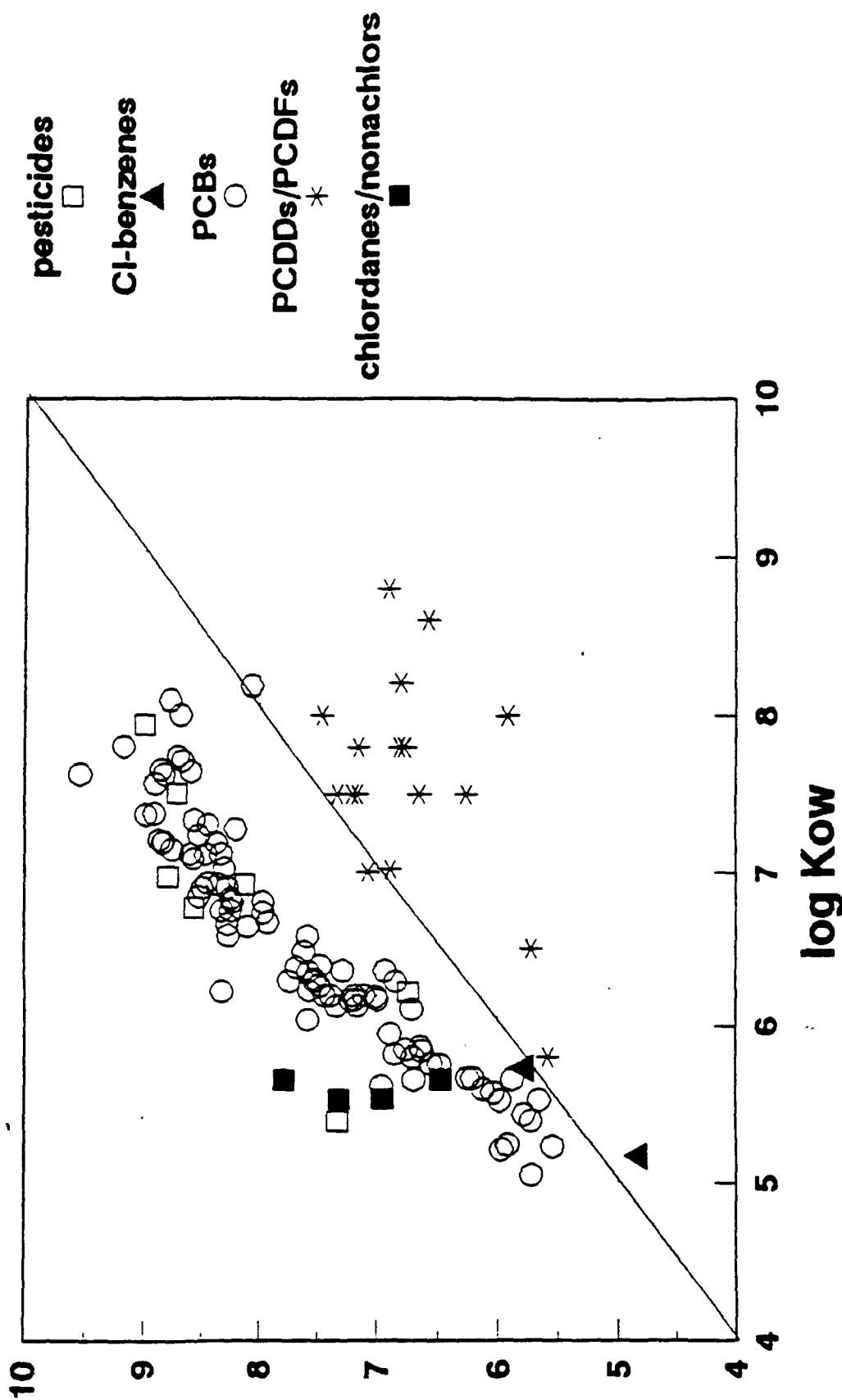
Lake Ont. LT vs. G. Bay BT BSAF-predictions

G. Bay BT log BAFs



GB B.Trout Region 3A/3B; all BAFs ref. PCB 118  
Doc=2.5mg/L & Koc=Kow/10

**Figure 12. Mean log BAFs from Lake Ontario BSAFs**

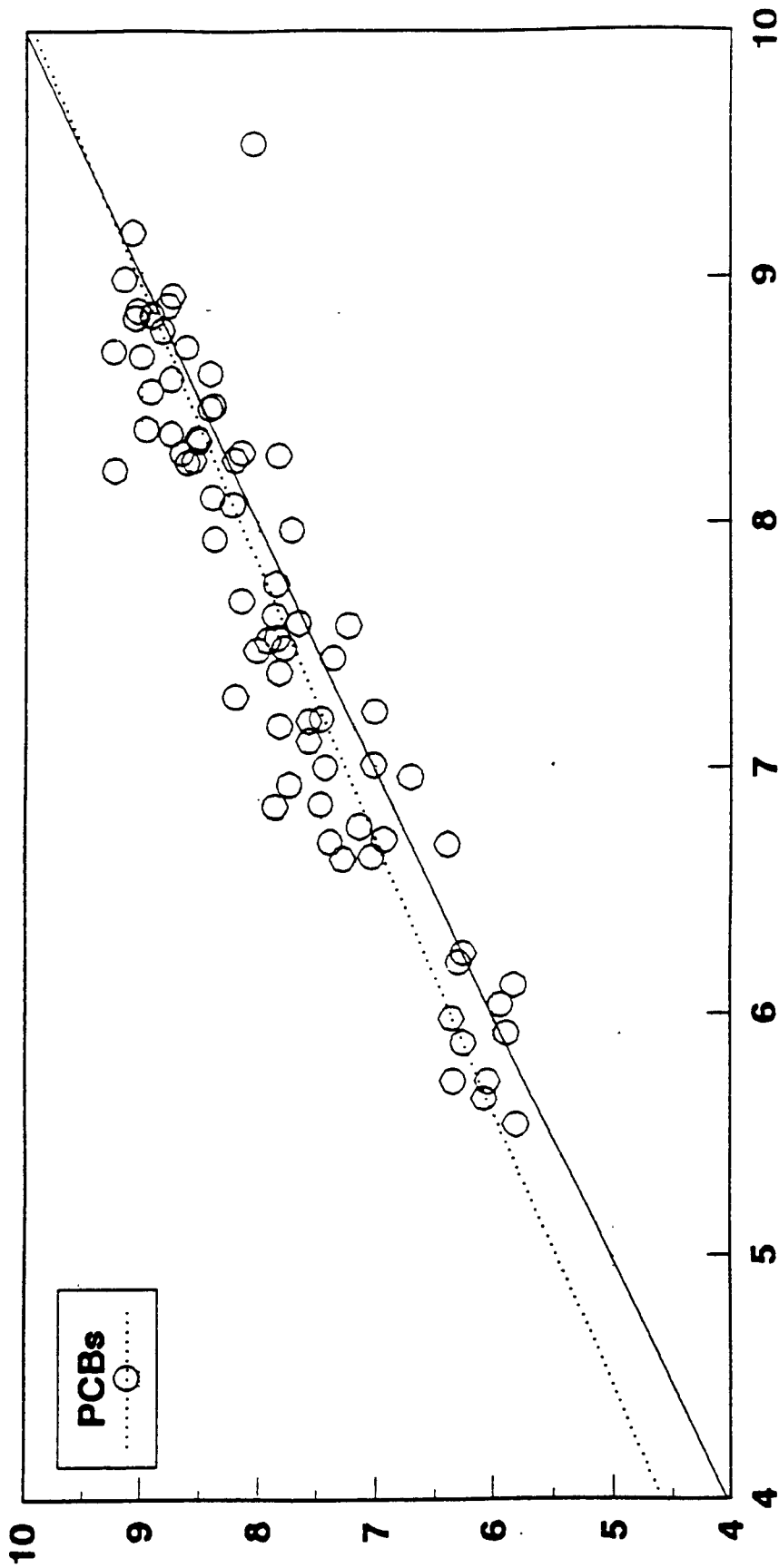


BAFs ref. to BAFs from Oliver & Niliml (1988)  
 Doc=2mg/L & Kdoc=K<sub>ow</sub>/10

# Fig. 13. Correlation of L.Ont. & G.Bay log BAFs

Mean L. Ontario/EPA est. from GB B. Trout BSAFs

EPA log BAFs from G. Bay BT BSAFs



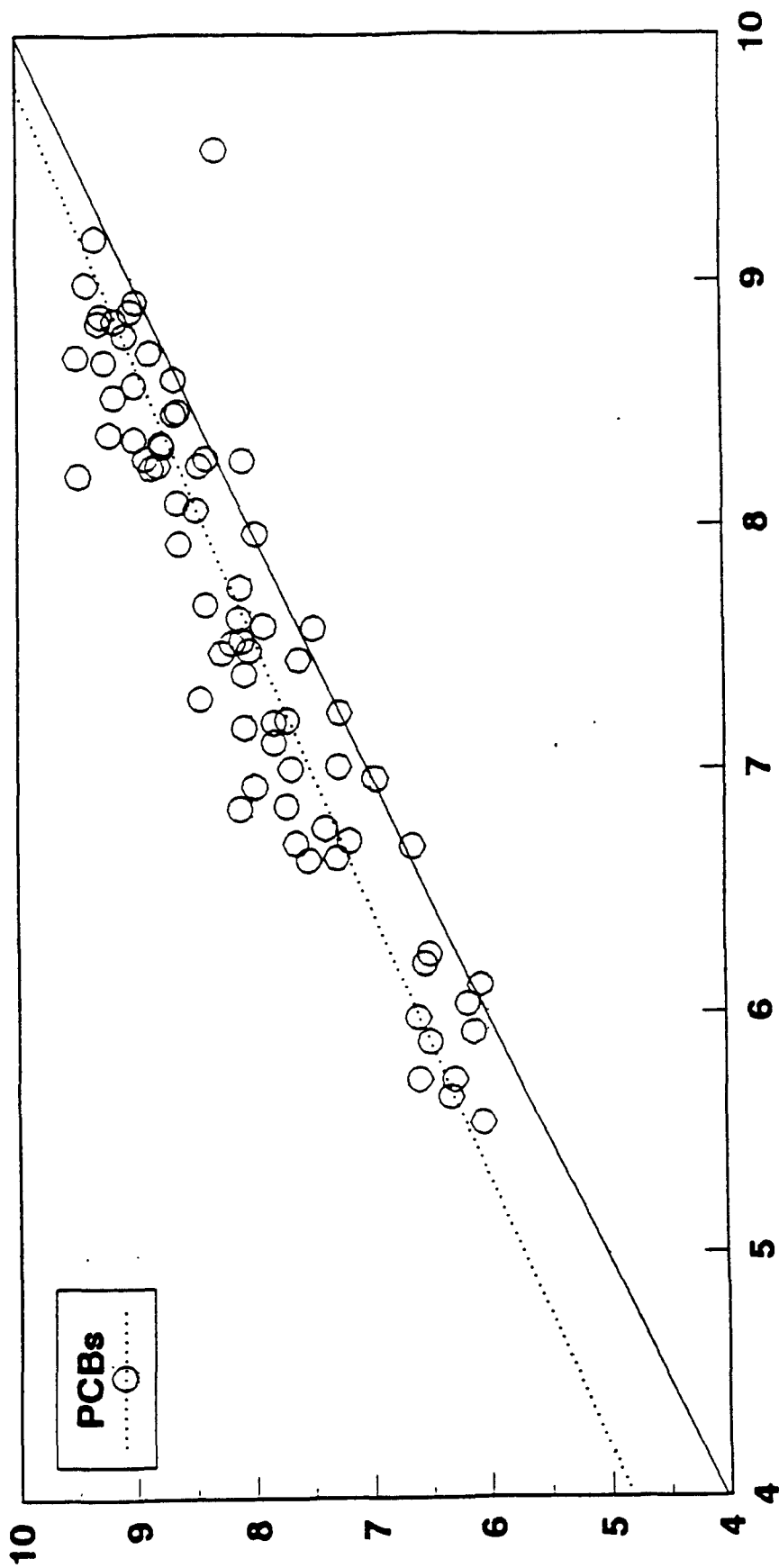
Mean Lake Ontario log BAFs from BSAFs

ERLID GB B.Trout Region 3A/3B BAFs ref. PCB 52  
Doc=2-5mg/L & Koc=Kow/10

# Fig. 14. Correlation of L.Ont. & G.Bay log BAFs

Mean L. Ontario/EPA est. from GB B. Trout BSAFs

EPA log BAFs from G. Bay BT BSAFs



Mean Lake Ontario log BAFs from BSAFs

ERLID GB B.Trout Region 3A/3B BAFs ref. PCB 118

Doc=2-5mg/L & Koc=Kow/10

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## VI. BIOACCUMULATION EQUIVALENCY FACTORS (BEFs)

The use of 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) toxicity equivalency factors (TEFs) for assessing the total TCDD toxicity risk from complex mixtures of polychlorinated dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) in aquatic environments is complicated by the wide range of bioaccumulation potentials associated with these chemicals. Human and wildlife exposures are related to residues of each chemical in fish and other aquatic organisms ingested as food. Each congener's TCDD equivalent risk is proportional to the product of the congener's TEF times the concentration of the chemical in the food. The sum of all the products provides a TCDD equivalence concentration (TEC) for the food exposure. When it is necessary to relate water or effluent concentrations of PCDDs and PCDFs to risk estimates for food exposure, the TEC equals the sum of the products of the water concentration, bioaccumulation factor (BAF) and TEF for each congener present. Note that the BAFs and water concentrations have to be based either on freely dissolved chemical ( $C_w^{fd}$ ) or on total chemical ( $C_w^t$ ) in water (i.e., consistent definition).

$$TEC = \sum_i [(C_w^t)_i (BAF^t)_i (TEF)_i] = \sum_i [(C_w^{fd})_i (BAF^{fd})_i (TEF)_i]$$

BAFs for PCDDs and PCDFs have not been measured due to the very small water concentrations present in contaminated ecosystems. Concentrations of these chemicals can be measured in surface sediments to provide a measure of the relative amounts of each chemical present in association with organic carbon of the ecosystem. Furthermore, the relative activities of each chemical and TCDD should be similar for both sediment organic carbon and organic carbon suspended in water. The fugacity gradients of each chemical between sediment and water may or may not be similar, depending on differences in chemical loading to the water which are not near steady-state with surface sediment. The biota-sediment accumulation factor (BSAF) is a direct measure of each chemical's distribution between sediment organic carbon and lipid of associated aquatic organisms. When PCDDs and PCDFs have similar sources and distribution patterns between water and sediment, the BSAFs at a site will provide good measures of the bioaccumulation potentials relative to TCDD or any other chemical for which a BAF has been estimated (Cook et al., 1994). Systems with steady-state distributions of the chemicals between sediment and water are most appropriate for these measurements of relative bioaccumulation potential.

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## A. Definitions/Symbols

The following bioaccumulation terms and symbols are used to derive and apply TCDD bioaccumulation equivalency factors (BEFs). "C" is used for concentration and "f" for fraction. Subscripts are used to indicate the mass basis for "C" or "f" (w = water, *l* = lipid in tissue, t = whole tissue wet weight, s = dry sediment, soc = sediment organic carbon, and ssoc = suspended solids organic carbon); superscripts are used to indicate the water phase of the chemical (fd = freely dissolved, b = bound to organic carbon in water, and t = total chemical = fd + b; and subscripts following parentheses indicate the chemical (tcdd = 2,3,7,8-TCDD and i = the ith chemical).

### bioaccumulation factors

$$BAF_i^t = C_i/C_w^t, \quad BAF_i^t = C_i/C_w^t = f_i * BAF_i^t \quad (2)$$

$$BAF_i^{fd} = C_i/C_w^{fd}, \quad BAF_i^{fd} = C_i/C_w^{fd} = f_i * BAF_i^{fd} \quad (3)$$

$$BAF_i^b = C_i/C_w^b, \quad BAF_i^b = C_i/C_w^b = f_i * BAF_i^b \quad (4)$$

### biota-sediment accumulation factor

$$BSAF = C_i/C_{soc} = \frac{C_i * f_{soc}}{C_s * f_i} \quad (5)$$

### organic carbon - water partitioning

$$\text{fraction dissolved } f_{fd} = (1 + DOC * K_{ow}/10 + POC * K_{ow})^{-1} \quad (6)$$

$$\text{fraction bound to oc in water } f_b = 1 - f_{fd}$$

TCDD bioaccumulation equivalency factor

$$(BEF)_i = \frac{(BSAF)_i}{(BSAF)_{tcdd}} = \frac{(BAF_i^b)_i}{(BAF_i^b)_{tcdd}} \quad (7)$$

**B. Calculation of BAFs and TEC from BEFs**

The ratio (equation 7) between each PCDD and PCDF congener's BSAF to that of TCDD will be called the TCDD bioaccumulation equivalency factor (BEF). Because BAFs based on freely dissolved chemical in water ( $BAF_i^{fd}$ ) are directly proportional to  $K_{ow}$  which varies among PCDDs and PCDFs, the BEF describes only the BAF relative to TCDD on the basis of organic carbon bound chemical concentration in water ( $BAF_i^b$ ). This assumes that the relative amounts of each PCDD and PCDF congener in the organic carbon of surface sediments are the same as in suspended organic carbon. The relationship between particulate organic carbon (POC), dissolved organic carbon (DOC),  $K_{ow}$  and  $f_{fd}$  is presented in equation 6. the importance of each chemical's  $K_{ow}$  should be evident. The BEF can be used to calculate  $(BAF_i^f)_i$  and  $(BAF_i^{fd})_i$ .  $(BAF_i^f)_i$ s estimated from BEFs, under the condition of similar sediment/water fugacity ratios for each chemical, may be used to predict bioaccumulation by pelagic fish from estimated  $C_w^{fd}$ s regardless of site-specific differences in chemical distribution between sediment and water.

$$BAF_i^b = BAF_i^f / f_b \quad (8)$$

$$(BEF)_i = \frac{(BAF_i^b)_i}{(BAF_i^b)_{tcdd}} = \frac{(BAF_i^f)_i (f_b)_{tcdd}}{(BAF_i^f)_{tcdd} (f_b)_i} \quad (9)$$

so,

$$(BAF_i^f)_i = \frac{(BEF)_i (BAF_i^f)_{tcdd} (f_b)_i}{(f_b)_{tcdd}} \quad (10)$$

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and,

$$(BAF_i^{fd}) = \frac{(BAF_i^t)}{(f_{fd})_i} = \frac{(BEF)_i (BAF_{tcdd}^{fd}) (f_b)_i (f_{fd})_{tcdd}}{(f_{fd})_i (f_b)_{tcdd}} \quad (11)$$

because  $(f_b)_i (f_{fd})_{tcdd} / (f_{fd})_i (f_b)_{tcdd} = (K_{ow})_i / (K_{ow})_{tcdd}$  :

$$(BAF_i^{fd}) = \frac{(BEF)_i (BAF_{tcdd}^{fd}) (K_{ow})_i}{(K_{ow})_{tcdd}} \quad (12)$$

A TCDD TEC can be calculated on the basis of wet tissue residue ( $TEC_t$ ) or lipid normalized residue ( $TEC_l$ ); water concentration of total chemical ( $TEC^t$ ) or freely dissolved chemical ( $TEC^{fd}$ ). When bioaccumulation is to be predicted on the basis of freely dissolved chemical ( $C_w^{fd}$ ), the relative differences in  $BAF^{fd}$ s for PCDD and PCDF congeners will be less than for their  $BAF$ s. This is because  $f_{fd}$ s for the higher chlorinated, more hydrophobic congeners are less than  $f_{fd}$  for TCDD. Since the TEC is based on tissue concentration,  $TEC_t^t = TEC_t^{fd}$  and  $TEC_l^t = TEC_l^{fd}$ . Thus if  $(BAF_{tcdd}^{fd})$  is the reference bioaccumulation factor:

$$TEC_t = \sum_i \left[ \frac{(C_w^{fd})_i (BEF)_i (BAF_{tcdd}^{fd}) (K_{ow})_i (TEF)_i}{(K_{ow})_{tcdd}} \right] \quad (13)$$

$$TEC_l = \sum_i \left[ \frac{(C_w^{fd})_i (BEF)_i (BAF_{tcdd}^{fd}) (K_{ow})_i (TEF)_i}{(K_{ow})_{tcdd}} \right] \quad (14)$$

$$TEC_t = TEC_l * f_l \quad (15)$$

### C. Great Lakes BEFs

Lake Ontario sediment and fish residue data (Lodge et al., 1994) provide a basis for calculation of BEFs. However, very few PCDDs and PCDFs measured as sediment contaminants are detectable in fish tissue. The table below provides estimated BEFs calculated from lake-wide average concentrations of toxicologically important PCDDs and PCDFs in surface sediment and lake trout samples collected



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in 1987 for the EPA Region II Lake Ontario TCDD Bioaccumulation Study. Lake Ontario conditions in 1987 involve sediment as the principal source of these chemicals to the water and food chain. The BSAFs if measured under conditions of steady-state between external chemical loading, water, food chain and surface sediment would be somewhat larger but BEFs should be similar. Lake Ontario sediment cores also demonstrate that all PCDD and PCDF congener concentrations have similar temporal trends during the past four decades and all have water column concentrations that are strongly controlled by sediment resuspension due to large declines in loading from sources external to the lake. Limited comparison to BEFs calculated from data obtained for other ecosystems confirms these bioaccumulation potential differences and suggests that this BEF set would be predictive of bioaccumulation differences for PCDDs and PCDFs for fish in ecosystems outside the Great Lakes. Similar results are likely for other persistent bioaccumulative organic chemicals such as PCBs and chlorinated pesticides.

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Table 1. TCDD Bioaccumulation equivalency factors (BEFs) derived for toxicologically important PCDDs and PCDFs from lakewide averages of concentrations in Lake Ontario lake trout and surface sediment in depositional areas.

Congener	log K <sub>ow</sub> <sup>a</sup>	BSAF	TCDD BEF
2,3,7,8-TCDD	7.02	0.059	1.0
1,2,3,7,8-PeCDD	7.50	0.054	0.92
1,2,3,4,7,8-HxCDD	7.80	0.018	0.3
1,2,3,6,7,8-HxCDD	7.80	0.0073	0.12
1,2,3,7,8,9-HxCDD	7.80	0.0081	0.14
1,2,3,4,6,7,8-HpCDD	8.20	0.0031	0.051
OCDD	8.60	0.00074	0.0013
2,3,7,8-TCDF	5.80	0.047	0.80
1,2,3,7,8-PeCDF	6.5 <sup>b</sup>	0.013	0.22
2,3,4,7,8-PeCDF	7.0 <sup>b</sup>	0.095	1.6
1,2,3,4,7,8-PeCDF	7.5 <sup>b</sup>	0.0045	0.076
1,2,3,6,7,8-HxCDF	7.5 <sup>b</sup>	0.011	0.19
2,3,4,6,7,8-HxCDF	7.5 <sup>b</sup>	0.040	0.67
1,2,3,7,8,9-HxCDF	7.5 <sup>b</sup>	0.037	0.63
1,2,3,4,6,7,8-HpCDF	8.0 <sup>b</sup>	0.00065	0.011
1,2,3,4,7,8,9-HpCDF	8.0 <sup>b</sup>	0.023	0.39
OCDF	8.80	0.001	0.016

<sup>a</sup> Burkhard and Kuehl, 1987.

<sup>b</sup> Estimated based on degree of chlorination and Burkhard and Kuehl, 1987.

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#### D. Example of TEC Calculation Using the BEF Method

Projected PCDD and PCDF loadings to a Great Lake result in estimated water concentrations ( $C_w^t$ ) of 0.0001, 0.0008, 0.0002, 0.0008 and 0.02 pg/ml for 2,3,7,8-TCDD, 2,3,7,8-TCDF, 1,2,3,7,8-PeCDD, 2,3,4,7,8-PeCDF and 1,2,3,4,6,7,8-HpCDD, respectively. The concentration of POC is 0.2 mg/L, DOC is 2.0 mg/L, so the  $C_w^d$ s for each congener are 0.00002, 0.0006, 0.000015, 0.00016, and 0.0003 pg/L, respectively. The  $BAF_i^d$  for TCDD is estimated to be  $7.85 \times 10^6$  and TEFs are 1.0, 0.1, 0.5 0.5 and 0.01 for each congener, respectively. At 9% lipid ( $f_l = 0.09$ ), the 2,3,7,8-TCDD  $BAF_{0.09}^d = 7.07 \times 10^5$ . The toxicity equivalency concentration (TEC) for fish with  $f_l = 0.09$  is approximately:

$$\begin{aligned} TEC_{0.09} &= (7.07 \times 10^5)[(0.00002)(1.0)(10.5 \times 10^6)(1.0)/10.5 \times 10^6 + \\ &(0.0006)(0.8)(0.63 \times 10^6)(0.1)/10.5 \times 10^6 + \\ &(0.000015)(0.92)(31.6 \times 10^6)(0.5)/10.5 \times 10^6 + \\ &(0.00016)(1.6)(10 \times 10^6)(0.5)/10.5 \times 10^6 + \\ &(0.0003)(0.05)(158 \times 10^6)(0.01)/10.5 \times 10^6] = 14.4 + 20.4 + 1.5 + 0.86 + 1.6 \\ &= 38.8 \text{ pg TCDD eq./g wet fish.} \end{aligned}$$

In this hypothetical example 2,3,7,8-TCDD contributes 37% of the TEC. Without use of the BEF approach (all  $BAF_{0.09}^d$ s =  $7.07 \times 10^5$ ), the TEC is calculated to be  $14.4 + 42.4 + 0.5 + 5.7 + 21.2 = 84.2$  pg TCDD eq./g wet fish with TCDD contributing only 17%. The overestimation of bioaccumulation for TCDF, PeCDF and HpCDD leads to a greater TEC estimate. Since there appears to be a correlation between TEFs and BEFs (i.e. the more toxic congeners are the most bioaccumulative, primarily due to slower rates of biotransformation), additional data suitable for validating the BSAFs used to calculate the BEFs are needed.

#### References

- Burkhard, L.P. and D.W. Kuehl. 1986. N-octanol water partition coefficients by reverse phase liquid chromatography/mass spectrometry for eight tetrachlorinated planar molecules. *Chemosphere* 15:163-167.
- Cook, P.M., G.T. Ankley, R.J. Erickson, B.C. Butterworth, S.W. Kohlbray, P. Marquis and H. Corcoran. 1994. The biota-sediment accumulation factor (BSAF) evaluation and application to assessment of organic chemical bioaccumulation in the Great Lakes. In preparation.

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Lodge, K., P.M. Cook, D.R. Marklund, S.W. Kohlbry, J. Libal, C. Harper, B.C. Butterworth and A.G. Kizlauskas. 1994. Accumulation of polychlorinated dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs) in sediments and fishes of Lake Ontario. In preparation.

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## VII. DERIVATION OF BAFs FOR TWENTY TWO CHEMICALS

Literature searches were conducted for data concerning  $K_{ow}$ , laboratory-measured BCFs, and field-measured BAFs for the chemicals. Additional information was obtained from Burkhard (1994) and Cook (1994).

### $K_{ow}$

For most chemicals, the values that were found for  $K_{ow}$  were interpreted as described in Appendix A, but for a few chemicals the values used by Burkhard (1994) and Cook (1994) were used to allow comparison of results that were calculated based on the same value for  $K_{ow}$ . The derivation of the best value of  $K_{ow}$  for each chemical is described in Appendix B.

### FCM

Values for the Food Chain Multipliers (FCMs) were obtained by rounding the best value for  $\log K_{ow}$  to one decimal digit and then using the FCM given by Burkhard (1994) for trophic level 4.

### BCF

Baseline BAFs were calculated from total BCFs given by Stephan (1993) using the following equation (see Appendix C):

$$\text{Baseline BAF} = [FCM] \left[ \frac{1}{(f_{td})} \right] \left[ \frac{BCF_T^t - 1}{(f_l)} \right]$$

where

$BCF_T^t$  = a total BCF, i.e., a measured BCF that is based on the total concentration of the chemical in the water and has not been lipid-normalized.

$f_{td}$  = the fraction of the chemical in the water that is freely dissolved.

$$= \frac{1}{1 + \frac{(DOC)(K_{ow})}{10} + (POC)(K_{ow})}$$

$f_l$  = the fraction of the biota (with which the BCF was determined) that is lipid.

Because POC and DOC were not measured in the bioconcentration tests, plausible worst-case concentrations were assumed. The concentrations of POC and DOC

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were assumed to be 1 mg/L (0.000001 Kg/L) and 10 mg/L (0.00001 Kg/L), respectively. When these values are used,  $f_{fd}$  can be calculated as:

$$f_{fd} = \frac{1}{1 + 2(K_{ow})(10^{-6})}$$

### BSAF

Calculations based on BSAFs directly result in baseline BAFs; the values used were calculated by Cook (1994).

### Field-measured BAFs

Most of the field-measured BAFs were calculated from the data of Oliver and Niimi (1988) by Burkhard (1994); these calculations directly result in a baseline BAF. When possible for other chemicals, baseline BAFs were calculated from field-measured total BAFs given by Stephan (1993) using the following equation (see Appendix C):

$$\text{Baseline BAF} = \left[ \frac{1}{(f_{fd})} \right] \left[ \frac{BAF_T^t - 1}{(f_l)} \right]$$

where

$BAF_T^t$  = a total BAF, i.e., a measured BAF that is based on the total concentration of the chemical in water and has not been lipid-normalized.

$f_{fd}$  = the fraction of the chemical in the water that is freely dissolved.

$$= \frac{1}{1 + \frac{(DOC)(K_{ow})}{10} + (POC)(K_{ow})}$$

$f_l$  = the fraction of the biota (with which the BAF was determined) that is lipid.

The concentrations of POC and DOC were assumed to be 0.000000075 Kg/L and 0.000002 Kg/L, respectively, for Lake Ontario, based on data presented by Eadie et al. (1990). Concentrations of POC and DOC in Lake Siskiwit were assumed to be similar to those in Lake Superior, which were assumed to be 0.00000004 Kg/L and 0.000002 Kg/L, respectively, based on data presented by Eadie et al. (1990).

The order of preference of the resulting baseline BAFs, from most preferred to least preferred, is:

1. A measured BAF that was calculated from field data.
2. A predicted BAF that was obtained using BSAFs.

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3. A predicted BAF that was obtained by multiplying a measured BCF by a FCM.
4. A predicted BAF that was obtained by multiplying a predicted BCF by a FCM, where  $K_{ow}$  is used as the predicted BCF.

For some chemicals, Burkhard (1994) calculated field-measured baseline BAFs for trophic level 3 (T. L. 3), but could not calculate field-measured baseline BAFs for trophic level 4 (T. L. 4) because the necessary data were not reported by Oliver and Niimi (1988). For these chemicals a value for the baseline BAF for trophic level 4 can be calculated as:

$$\text{Baseline BAF for T. L. 4} = \frac{(\text{Baseline BAF for T. L. 3})(\text{FCM for T. L. 4})}{(\text{FCM for T. L. 3})}$$

If more than one equally preferred value is available for a baseline BAF using the same method, the geometric mean of the values is the preferred value. The available baseline BAFs are given in Table 1.

After sufficient baseline BAFs were calculated for a chemical, the preferred baseline BAF was used to calculate a desired human health or wildlife  $BAF_{i\%}^{fd}$  using the equation (see Appendix C):

$$BAF_{i\%}^{fd} = 1 + (f_i)(\text{baseline BAF})$$

where  $i = f_i \times 100$  and values of 0.05 and 0.079 were used for  $f_i$  for human health and wildlife, respectively.

To calculate a plausible worst-case value for  $BAF_{i\%}^t$  for each chemical, the  $K_{ow}$  of the chemical was used with estimated concentrations of POC and DOC in Lake Superior (0.00000004 Kg/L and 0.000002 Kg/L, respectively, based on data presented by Eadie et al. 1990) to calculate  $f_{fd}$ , which was then used in the following equation:

$$BAF_{i\%}^t = (BAF_{i\%}^{fd})(f_{fd})$$

$BAF_{i\%}^t$  is the BAF that is appropriate for derivation of the criterion.

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For mercury, the derivation of values for  $BAF_{i\%1}^t$  for trophic levels 3 and 4 for human health and wildlife is described in Appendix D.

The resulting values of  $BAF_{i\%1}^{fd}$  and  $BAF_{i\%1}^t$  are given in Table 2.

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## Appendix A. Derivation of the Value of Log $K_{ow}$ for an Organic Chemical

A valid  $K_{ow}$  can be experimentally determined only for an individual chemical; it is not possible to experimentally determine a valid  $K_{ow}$  for a substance that is a mixture, such as toxaphene, PCBs, and chlordane. A value for  $K_{ow}$  can be assigned to a mixture either by assigning the value for a major component or by assigning an average of the values for several major components. The arithmetic average of values of log  $K_{ow}$  can be used, or the geometric mean of values of  $K_{ow}$  can be used.

Values were used only if they were obtained from the original authors or from a critical review that supplied sufficient information. A Med-Chem Star value was only of concern if the original reference for the value had not been obtained.

Because of potential interference due to radioactivity associated with impurities, values that were determined by measuring radioactivity in water and/or octanol were considered less reliable and were moved down one step in the priority below values that were determined using the same technique but were quantified using other methods.

The shake-flask technique has been reported to be acceptable only for chemicals whose  $K_{ows}$  are less than 4 (Karickhoff et al. 1979; Konemann et al. 1979; Braumann and Grimme 1981; Harnisch et al. 1983; Brooke et al. 1990). Brooke et al. (1986) compared techniques and decided that the shake-flask technique is acceptable for chemicals whose  $K_{ows}$  are less than 5, whereas Chessells et al. (1991) stated that this technique is acceptable for values of log  $K_{ow}$  up to about 5.5.

Values of  $K_{ow}$  were given priority based on the technique used as follows:

$K_{ow} < 4$ :	<u>Priority</u>	<u>Technique</u>
	1	Slow-stir
	1	Generator-column
	1	Shake-flask
	2	Med-Chem Star value
	3	Reverse-phase liquid chromatography on C18 with extrapolation to zero percent solvent
	4	Reverse-phase liquid chromatography on C18 without extrapolation to zero percent solvent
	5	Predicted by the Med-Chem program

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$K_{ow} > 4$ :	<u>Priority</u>	<u>Technique</u>
	1	Slow-stir
	1	Generator-column
	2	Reverse-phase liquid chromatography on C18 with extrapolation to zero percent solvent
	3	Reverse-phase liquid chromatography on C18 without extrapolation to zero percent solvent
	4	Shake-flask
	5	Med-Chem Star value
	6	Predicted by the Med-Chem program

Values that seemed to be different from the rest were considered outliers and were not used.

For each chemical the available value of Log  $K_{ow}$  with the highest priority was considered the best value, except that if more than one such value was available, the arithmetic mean of those values was used as the best value.

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## **Appendix B. Derivation of Values of Log $K_{ow}$ for Twenty-two Chemicals**

The priorities of the methods for determining log  $K_{ow}$  are presented in Appendix A.

### **BENZENE**

The values that have the highest priorities are:

2.11 Shake-flask Karickhoff et al. 1979

2.13 Generator-column Miller et al. 1985

2.19 Slow-stir de Bruijn et al. 1989

The mean is 2.14 and is the best value.

### **CHLORDANE**

The value that has the highest priority is:

6.00 RPLC Veith et al. 1979

The value of 5.54 was used because it was used by Burkhard (1994) and Cook (1994).

### **CHLOROBENZENE**

The values that have the highest priorities are:

2.90 Slow-stir Brooke et al. 1990

2.78 Slow-stir Brooke et al. 1990

2.98 Generator-column Miller et al. 1985

2.80 Shake-flask Voice et al. 1983

2.90 Slow-stir de Bruijn et al. 1989

The mean is 2.87 and is the best value.

### **CYANIDE**

A value of log  $K_{ow}$  was not used for cyanide.

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#### DDT

The values that have the highest priorities are:

6.20	Slow-stir	Brooke et al. 1986
6.31	Slow-stir	Brooke et al. 1990
6.91	Slow-stir	Brooke et al. 1990
6.38	Slow-stir	Stancil 1994
6.91	Slow-stir	de Bruijn et al. 1989

The value of 6.91 was used because it was used by Burkhard (1994) and Cook (1994).

#### DEHP

The values that have the highest priorities are:

7.14	Slow-stir	Brooke et al. 1990
7.45	Slow-stir	Brooke et al. 1990
7.45	Slow-stir	de Bruijn et al. 1989

The mean is 7.35 and is the best value.

#### DIELDRIN

The values that have the highest priorities are:

4.54	Slow-stir	Brooke et al. 1986
5.34	Slow-stir	Stancil 1994
5.40	Slow-stir	de Bruijn et al. 1989

The value of 5.4 was used because it was used by Burkhard (1994) and Cook (1994).

#### 2,4-DIMETHYLPHENOL

The value that has the highest priority is:

2.42	Shake-flask	Banerjee et al. 1980
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This is the best value.

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### 2,4-DINITROPHENOL

The value that has the highest priority is:

1.50 Consensus Klein et al. 1988

This is the best value.

### HEPTACHLOR

The values that have the highest priorities are:

5.27 RPLC McDuffie 1981

5.44 RPLC Veith et al. 1979

The mean is 5.36 and is the best value.

### HEXACHLOROENZENE

The values that have the highest priorities are:

5.47 Generator-column Miller et al. 1985

5.73 Slow-stir de Bruijn et al. 1989

The value of 5.73 was used because it was used by Burkhard (1994) and Cook (1994).

### HEXACHLOROETHANE

The values that have the highest priorities are:

4.04 RPLC McDuffie 1981

4.05 RPLC Veith et al. 1980

4.14 Shake-flask Chiou 1985

3.93 Shake-flask Veith et al. 1980

These values are close to 4, and the range of the four values is small. The mean of the four values is 4.04 and is the best value.

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### LINDANE

The values that have the highest priorities are:

3.69 Slow-stir de Bruijn et al. 1989

3.32 Shake-flask Platford 1981

The value of 3.69 was used because it was used by Burkhard (1994) and Cook (1994).

### MERCURY

A value for log  $K_{ow}$  was not used for mercury.

### METHYLENE CHLORIDE

The value that has the highest priority is:

1.25 Calculated Med-Chem

This is the best value.

### PCBs

Based on data reported by Schulz et al. (1989), congeners 8, 18, 28, 31, 52, 95, 101, 118, 149, and 153 were selected as being the most prevalent.

Burkhard (1994) calculated field-measured BAFs for nine of these, but field data were not available for congener 8. The arithmetic average of the values of log  $K_{ow}$  given by Burkhard (1994) for the nine congeners is 6.14 and is the best value.

### PENTACHLOROPHENOL

The values that have the highest priorities are:

5.08 RPLC Miyake and Terada 1982

5.01 RPLC Veith et al. 1979

The mean of these is 5.04 and is the best value.

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### 2,3,7,8-TCDD

The value that has the highest priority is:

7.02 RPLC Burkhard and Kuehl 1986

This is the best value.

### TOLUENE

The values that have the highest priorities are:

2.65 Generator-column Miller et al. 1985

2.79 Slow-stir de Bruijn et al. 1989

2.63 Slow-stir Brooke et al. 1990

2.79 Slow-stir Brooke et al. 1990

The mean of these is 2.72 and is the best value.

### TOXAPHENE

The value that has the highest priority is:

4.33 Calculated Med-Chem

This is the best value.

### 1,2,4-TRICHLOROBENZENE

The values that have the highest priorities are:

3.98 Generator-column Miller et al. 1985

4.05 Slow-stir de Bruijn et al. 1989

3.93 Shake-flask Konemann et al. 1979

4.02 Shake-flask Chiou et al. 1982

These values are close to 4 and the range of the four values is small. The mean of the four values is 4.00 and is the best value.



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### TRICHLOROETHYLENE

The values that have the highest priority are:

2.42 Shake-flask Banerjee et al. 1980

2.53 Generator-column Miller et al. 1985

3.14 Shake-flask Harnisch et al. 1983

The last value is considered an outlier. The mean of the other two is 2.48 and is the best value.

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## Appendix C. Derivation of BAFs for Organic Chemicals

### PREDICTING BCFs FOR LOW $K_{ow}$ CHEMICALS

The procedures discussed above for estimating bioaccumulation factors were developed for highly lipophilic organic chemicals for which accumulation is closely associated with the lipid of an organism. In order to extend these methods to less lipophilic chemicals, it is necessary to accommodate cases in which accumulation is not dominated by partitioning into lipid. Because weakly lipophilic chemicals are not significantly accumulated via food, bioaccumulation factors are equal to bioconcentration factors. Thus, this discussion can be restricted to the question of predicting steady-state bioconcentration factors based on  $K_{ow}$  or extrapolations from other organisms.

An organic chemical accumulated by an organism associates with various components of the organism; some chemical in the organism is dissolved in its water; some is partitioned into membranes, fat deposits, and other lipid material; and some may be bound to various nonlipid organic material. An organic chemical with  $K_{ow} \approx 1$  will distribute among water and different organic phases with similar concentrations, so that a steady-state bioconcentration factor will be approximately 1 in the absence of metabolism and significant growth dilution. More hydrophilic chemicals will also have bioconcentration factors of the order of one because water is the predominant component in an organism. More lipophilic chemicals will have larger bioconcentration factors because there would be an increased concentration in the organic components relative to water. Bioconcentration factors should therefore be described in terms of two components: an aqueous portion that is approximately 1 and an organic portion which is the product of the amount of organic components and the affinity of the chemical for organic matter relative to water. Lipid will be the most important organic component unless there are important specific binding reactions or very low lipid content. An approximate general equation for bioconcentration factors is therefore:

$$BCF = 1 + f_l \cdot A$$

where 1 represents the contribution of the organisms aqueous phase to the BCF and  $f_l \cdot A$  represents the contribution of the organic components, the fraction lipid  $f_l$  being the quantity of the dominant organic component and  $A$  being a measure of the affinity of the chemical for lipid relative to water.

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#### Prediction of BCF from $K_{ow}$

A predicted equilibrium BCF that is applicable to weakly lipophilic hydrophobic chemicals as well as strongly lipophilic chemicals can therefore be based on the two-term equation:

$$BCF = 1 + f_l \cdot K_{ow}$$

where the octanol:water partition coefficient  $K_{ow}$  is the prediction for the affinity of the chemical to the lipid. For the methods for highly lipophilic chemicals discussed above, the aqueous term in this equation ("1") can be ignored because it is so much smaller than the organic term, but for weakly lipophilic chemicals it cannot be ignored. This equation omits the finer details of chemical distribution within an organism, but it provides a useful approximation that can be applied to a range of chemicals. Because exposure via fish consumption contributes little to the overall risk from weakly lipophilic chemicals, the errors in this approximation are of little real consequence for these chemicals.

#### Extrapolation of BCF among organisms

For highly lipophilic chemicals the aqueous portion of accumulation is usually negligible. Therefore, for these chemicals lipid-normalization of a bioconcentration factor provides an estimate for the affinity of the chemical for the lipid fraction:

$$A \approx \frac{BCF_1 - 1}{f_{l,1}}$$

A BCF for organism "2" can then be estimated by multiplying this lipid affinity by its lipid content and then adding 1:

$$BCF_2 \approx 1 + f_{l,2} \cdot A$$

Again, this treatment is approximate and ignores various aspects of accumulation, but for weakly lipophilic chemicals approximate values should suffice because exposure via fish consumption is an unimportant source of risk.

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#### Appendix D. Derivation of Values for BAF for Mercury

The following rationale is a revision of that used in the derivation of the GLI BAF for mercury dated 3-3-93.

- a. In the Gobas model, which is used in the derivation of BAFs and FCMs for organic chemicals, only bioconcentration applies to trophic levels 1 and 2, whereas biomagnification occurs between trophic levels 2 and 3 and between trophic levels 3 and 4. Watras and Bloom (1992) found that with mercury, biomagnification occurred between trophic levels 1 and 2 and between trophic levels 2 and 3. Watras and Bloom (1992) only studied trophic levels 1, 2, and 3, but a substantial amount of data from other investigators shows a consistent predator-prey factor between fishes. Thus the model used here will provide for bioconcentration at trophic level 1, and biomagnification at trophic levels 2, 3, and 4.
- b. The BCFs for inorganic mercury and methylmercury will remain at 2,998 and 52,175, respectively.
- c. Based on the data of Gill and Bruland (1990), it will be assumed that, on the average, 17 percent of the total mercury in the Great Lakes is methylmercury and that 83 percent is inorganic mercury. Thus the weighted average BCF is:  $(0.17)(52,175) + (.83)(2,998) = 11,358$ . Based on data for phytoplankton, Watras and Bloom (1992) obtained a BCF of about 25,000 for total mercury at a pH of 6.1.
- d. The data of Watras and Bloom (1992) show an increase of about a factor of 2 from trophic level 1 to trophic level 2, and an increase of about a factor of 1.26 from trophic level 2 to trophic level 3.
- e. A variety of studies have found predator-prey factor increases in total mercury in fish from 1.2 to 15, with a mean of about 5.
- f. Use of these factors results in:  
 $(11,358)(2.00) = 22,716$   
 $(22,716)(1.26) = 28,622$   
 $(28,622)(5.00) = 143,110$
- g. Bloom (1992) concluded that "for all species studied, virtually all (>95%) of the mercury present is as  $\text{CH}_3\text{Hg}$  and that past reports of substantially lower  $\text{CH}_3\text{Hg}$  fractions may have been biased by analytical and homogeneity variability". Therefore, it will be assumed that 97.5 percent of the mercury in fish in the Great Lakes is methylmercury:  
 $(28,622)(0.975) = 27,906$   
 $(143,110)(0.975) = 139,532$
- h. It appears that BCFs and BAFs based on whole body and edible portion should be similar for mercury. Thus for a specific trophic level, the human health and wildlife BAFs will be the same.

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- i. This derivation indicates that for total mercury in the water column the values of  $BAF_i$  for human health and wildlife should be:

<u>Trophic level</u>	<u>BAF</u>
3	27,900
4	140,000

The difference between trophic levels 3 and 4 is important.

- A. Comparison of field-measured BAFs for mercury with the BAFs derived above must properly identify the trophic level of the aquatic biota used in the determination of the field-measured BAF. If field-measured BAFs are compared to the BAF derived for trophic level 4, the field-measured BAFs must have been determined with aquatic biota that are in trophic level 4. Many of the field-measured BAFs for mercury have been determined with aquatic biota that is in trophic level 3. It might also be necessary to account for a different percent methylmercury in the water column. In addition, the age of the fish is probably important because the concentration of mercury in fish seems to increase consistently with age without showing signs of leveling off.
- B. If the aquatic biota consumed by humans and wildlife is incorrectly assigned to too high a trophic level on the average, the resulting criteria will be unnecessarily low, but not because the derived BAFs for mercury are too high. For example, if all the consumed food is assumed to be trophic level 4, the BAF used to derive the criterion will be 139,532. If, however, the consumed food is actually a 1:1 combination of trophic levels 3 and 4, the BAF used to derive the criterion will be 62,400.
- C. Identification of the trophic level of some species of fish must take into account the age and/or size of the specific organisms of concern. Some species of fish are in trophic level 3 when they are young, but are in trophic level 4 when they are older. The trophic level might also vary from one body of water to another, depending on the food chain. With both humans and wildlife, knowing the species consumed is not necessarily sufficient to allow an accurate identification of the trophic level of the consumed food.

## References

- Bloom, N.S. 1992. On the Chemical Form of Mercury in Edible Fish and Marine Invertebrate Tissue. *Can. J. Fish. Aquat. Sci.* 49:1010-1017.

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**TABLE 1: BASELINE BAFs FOR TROPHIC LEVEL 4 BY VARIOUS METHODS**

The BAFs in this table are for trophic level 4, are based on 100% lipid, and are based on the concentration of freely dissolved chemical in the water, i.e., these are "baseline BAFs" for trophic level 4. The baseline BAF, i.e.,  $BAF_{ld}^0$ , for trophic level 4 is the value that best characterizes the bioaccumulation of a chemical in regards to water quality criteria for human health, but this does not imply that humans only consume aquatic biota that is in trophic level 4.

All values in this draft of this table have been updated as of the date of the draft.

This table gives the baseline BAFs for trophic level 4 that could be obtained for each chemical by the four procedures described in the GLI BAF methodology:

1. A measured BAF that was calculated from field data.
  2. A predicted BAF that was obtained using BSAFs.
  3. A predicted BAF that was obtained by multiplying a measured BCF by a Food Chain Multiplier (FCM); the FCM was derived from  $\log K_{ow}$ .
  4. A predicted BAF by multiplying a predicted BCF by a FCM, with both the predicted BCF and the FCM being derived from  $\log K_{ow}$ .
- (A few values were derived using other procedures and these are footnoted.) Method 1 gives the most preferred BAF, whereas method 4 gives the least preferred. Sometimes measured or predicted BCFs and BAFs are geometric means of two or more values. The most preferred available value for a chemical is the one farthest to the right in the table. BAFs for most metals were obtained by multiplying a measured BCF by a FCM of 1.0. A BAF was not obtained for one chemical.

BAFs less than 10 are rounded to one decimal digit; BAFs between 10 and 1000 are rounded to whole numbers; BAFs greater than 1000 are rounded to three significant digits; this does not imply anything about the precision or accuracy of the values.

The  $\log K_{ows}$  are the "best" values derived in Appendix B using the procedure described in Appendix A.

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The FCMs for all organic chemicals were derived by rounding the Log  $K_{ow}$  to one decimal digit and then using the FCM given by Burkhard (1994) for trophic level 4.

pBCF = predicted BCF. The value of pBCF for a chemical equals the value of the  $K_{ow}$  for that chemical. The value of "pBCF x FCM" is the same as the BAF that is predicted by the Gobas model for that value of  $K_{ow}$ , except for roundoff error.

mBCF = measured BCF, where the measured BCF is a  $BCF_1$  and the equation used is:

$$\text{Baseline BAF} = BAF_t^M = (FCM) (BCF_t^M) = [FCM] \left( \frac{1}{f^M} \right) \left[ \frac{BCF_1^1 \cdot 1}{(f_1)} \right]$$

The BAFs predicted based on BSAFs are from Table 2 by Cook (1994). Predicted BAFs based on BSAFs are given for all of the chemicals for which they are available.

Most of the measured BAFs were calculated by Burkhard (1994) from data reported by Oliver and Niimi (1988).

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Chemical	Log K <sub>OW</sub>	FCM	Predicted BAFs			Measured BAF
			pBCF x FCM	mBCF x FCM	(BSAF)	
Benzene	2.14	1.0	138	---	----	---
Chlordane gamma trans cis	5.54	7.1	2,460,000	---	----	---
	5.54	7.1	2,460,000	---	9,070,000	5,500,000
	5.54	7.1	2,460,000	---	8,810,000	---
	5.54	7.1	2,460,000	---	21,000,000	---
Chlorobenzene	2.87	1.0	741	---	----	---
Cyanide	----	---	---	---	----	---
4,4'-DDT	6.91	26.7	217,000,000	---	134,000,000	100,000,000
Dieldrin	5.4	5.8	1,460,000	---	21,200,000	---
2,4-Dimethylphenol	2.42	1.0	263	3,110	----	---
2,4-Dinitrophenol	1.50	1.0	32	---	----	---
Heptachlor	5.36	5.8	1,330,000	1,230,000	----	---
Hexachlorobenzene	5.73	10.2	5,480,000	---	590,000	2,570,000
Hexachloroethane	4.04	1.1	12,100	5,812	----	19,000 <sup>b</sup>
Lindane (gamma HCCH)	3.69	1.0	4,900	---	39,600	85,100
Mercury	----	---	---	139,532	----	---
Methylene chloride	1.25	1.0	18	---	----	---

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PCBs	6.14 <sup>c</sup>	17.8	24,600,000	---	----	12,000,000 <sup>c</sup>
Pentachlorophenol	5.04	2.6	285,000	12,900	----	---
2,3,7,8-TCDD	7.02	26.2	274,000,000	---	7,850,000	---
Toluene	2.72	1.0	525	30,900	----	---
Toxaphene	4.33	1.2	25,700	---	----	42,600,000 <sup>b</sup>
1,2,4-Trichlorobenzene	4.00	1.1	11,000	---	----	31,400 <sup>d</sup>
Trichloroethylene	2.48	1.0	302	333	----	---

# Explanations of codes:

<sup>a</sup> Metabolism would probably cause a field-measured BAF to be much lower. Burkhard (manuscript) demonstrated this for PAHs.

<sup>b</sup> This value was calculated from a field-measured  $BAF'_T$  using the equation

$$BAF'^d_T = \left( \frac{1}{f_d} \right) \frac{BAF'_T - 1}{(f_t)}$$

<sup>c</sup> These values are geometric means of values for the more prevalent PCB congeners for  $K_{OWS}$  and measured BAFs calculated by Burkhard (1994), respectively.

<sup>d</sup> Burkhard (1994) calculated a field-measured  $BAF'^d_T$  of 37,154 for 1,2,4-trichlorobenzene in sculpin, which is at trophic level 3. The  $\log K_{OW}$  for 124TCB is 4.00, and so the FCM for trophic level 3 is 1.3 and the FCM for trophic level 4 is 1.1. This results in a predicted/measured  $BAF'^d_T$  of  $(37,154)(1.1)/(1.3) = 31,438$  for trophic level 4.

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TABLE 2: RECOMMENDED BAFs FOR THE DERIVATION OF GLI CRITERIA

The BAFs given in the table are recommended for use in derivation of human health criteria. BAFs recommended for use in the derivation of wildlife criteria are given on the next page. All BAFs given for human health and for wildlife are based on wet weight of the tissue of the aquatic biota.

For an organic chemical, "Baseline BAFs" are based on 100% lipid and on the concentration of freely dissolved chemical in the water. For each chemical, the baseline BAF for trophic level 4 given in this table is the most preferred value available for the chemical in Table 1, i.e., the value farthest to the right for the chemical in Table 1. A BAF is not given in Table 1 for one chemical. The log  $K_{OW}$ s in Table 2 are also from Table 1.

All BAFs given for human health are for trophic level 4. BAFs in the table that are not baseline BAFs are based on 5 percent lipid. The GLI human health guidelines currently specify that humans only consume aquatic biota that are in trophic level 4 and that the applicable percent lipid is 5 percent.

The freely dissolved BAF for 5 percent lipid at trophic level 4 was calculated using the equation:

$$BAF_{5\%l}^{fd} = 1 + (f_l) (BAF_l^{fd})$$

The total BAF for 5 percent lipid at trophic level 4 was calculated using estimated values for Lake Superior of DOC = 2 mg/L and POC = 0.075 mg/L and the equation:

$$BAF_{5\%l}^t = (BAF_{5\%l}^{fd}) (f_{fd})$$

BAFs less than 1 are rounded to one significant digit; BAFs between 1 and 1000 are rounded to whole numbers; BAFs greater than 1000 are rounded to three significant digits; this does not imply anything about the precision or accuracy of the values.

## Wildlife

Water quality criteria are currently being derived for wildlife for only four chemicals and so the BAFs are presented here. Although it is possible that wildlife consume some aquatic biota that are in trophic levels 2, BAFs for the derivation of wildlife criteria are given here only for trophic levels 3 and 4. Note that the trophic level refers to an organism, not to a species, genus, or family, because individuals of some species are not in the same trophic level for their whole life span. For example, many species that are in trophic level 4 as adults are in trophic level 3 when they are young.

Wildlife BAFs are given for 7.9 percent lipid because the GLI wildlife guidelines currently specify 7.9 percent for both trophic level 3 and trophic level 4.

Chemical	Trophic Level 3 BAFs		Trophic Level 4 BAFs			
	Baseline	<div>7.9 percent lipid fr. diss.      total<sup>b</sup></div>	Baseline <sup>a</sup>	<div>7.9 percent lipid fr. diss.      total<sup>b</sup></div>		
DDT	53,700,000 <sup>c</sup>	4,240,000	2,170,000	100,000,000	7,900,000	4,040,000
Mercury	27,900	---	27,900	140,000	---	140,000
PCBs	11,500,000 <sup>d</sup>	908,000	658,000	12,000,000	948,000	687,000
2,3,7,8-TCDD	15,700,000 <sup>e</sup>	1,240,000	320,000	7,850,000	620,000	160,000

<sup>a</sup> From table 1.

<sup>b</sup>  $BAF' = (BAF^{ld})(f_{ld})$ , where  $f_{ld}$  is the fraction that is freely dissolved (see the table).

<sup>c</sup> Burkhard calculated measured log BAFs of 7.70, 7.84, and 7.65 for DDT for sculpin, alewives, and small smelt, respectively, in tables 4, 5, and 6. These are lipid-normalized, freely dissolved log BAFs and the arithmetic mean is 7.73, which gives a BAF of 53,700,000. The measured BAF of 100,000,000 calculated by Burkhard for trophic level 4 for DDT would correspond to a log  $K_{ow}$  of 6.59 in Table 2. A measured BAF of 53,700,000 would correspond to a FCM of 13.8 for trophic level 3 at a  $K_{ow}$  of 6.59; this

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FCM of 13.8 is between the FCMS of 17.3 and 11.3 that Burkhard reported in Table 2 for sculpin and alewives at trophic level 3 for  $\log K_{ow} = 6.6$ .

<sup>d</sup> Geometric mean of measured BAFs for the more prevalent PCB congeners calculated by Burkhard for sculpin and alewives, which are in trophic level 3.

<sup>e</sup> For 2,3,7,8-TCDD, Cook (1994) recommends that the baseline BAF for trophic level 3 be a factor of two higher than that for trophic level 4.

#### Reference

Cook, P.M. 1994. Memorandum to C.E. Stephan. July 7.

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Chemical

Chemical	Log Kow	Baseline BAF for trophic level 4 (BAF <sub>t</sub> )	5 % lipid at trophic level 4 freely diss. (BAF <sub>5%</sub> )	total (BAF <sub>5%</sub> )	fraction freely diss.
Benzene	2.14	138	8	8	1.000
Chlordane	5.54	5,500,000	275,000	250,000	0.909
gamma	5.54	5,500,000	275,000	250,000	0.909
trans	5.54	5,500,000	275,000	250,000	0.909
cis	5.54	5,500,000	275,000	250,000	0.909
Chlorobenzene	2.87	741	38	38	1.000
Cyanide	----	0	0	0	----
4,4'-DDT	6.91	100,000,000	5,000,000	1,550,000	0.310
Dieldrin	5.4	21,200,000	1,060,000	997,000	0.941
2,4-Dimethylphenol	2.42	3,110	157	157	1.000
2,4-Dinitrophenol	1.50	32	3	3	1.000
Heptachlor	5.36	1,230,000	61,500	57,900	0.941
Hexachlorobenzene	5.73	2,570,000	128,000	111,000	0.867
Hexachloroethane	4.04	19,000	950	947	0.997
Lindane (gamma HCCH)	3.69	85,100	4,260	4,260	0.999
Mercury	----	140,000	----	140,000	----
Methylene chloride	1.25	18	2	2	1.000



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PCBs	6.14	12,000,000	600,000	435,000	0.725
Pentachlorophenol	5.04	12,900	646	627	0.971
2,3,7,8-TCDD	7.02	7,850,000	392,000	101,000	0.258
Toluene	2.72	30,900	1,550	1,550	1.000
Toxaphene	4.33	42,600,000	2,130,000	2,120,000	0.994
1,2,4-Trichlorobenzene	4.00	31,400	1,570	1,570	0.997
Trichloroethylene	2.48	333	18	18	1.000

\* Metabolism would probably cause a field-measured BAF to be much lower. Burkhard (manuscript) demonstrated this for PAHs.

$$b \quad BAF'_{5\%t} = (BAF'_{5\%t}) (f_H)$$

where for Lake Ontario:

$$f_H = \frac{1}{1 + \frac{(DOC) (K_{ow})}{10} + (POC) (K_{ow})}$$

$$= \frac{1}{1 + \frac{(0.000002 \text{ kg/L}) (K_{ow})}{10} + (0.000000075 \text{ kg/L}) (K_{ow})}$$

$$= \frac{1}{1 + (0.000000275 \text{ kg/L}) (K_{ow})}$$