Environment Agency

Evidence

Depuration rate constant: growth correction and use as an indicator of bioaccumulation potential

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Miranda Kavanagh

Director of Evidence

Executive summary

Previous work by the Environment Agency has investigated methods for estimating a bioconcentration factor (BCF) from the data generated in the dietary exposure bioaccumulation method. This is a follow-up report to investigate further the following two aspects:

- an alternative mathematical method to correct for fish growth in bioconcentration factor (BCF) and biomagnification factor (BMF) studies;
- the use of the depuration (elimination) rate constant (or depuration half-life) as a direct measure of bioaccumulation and an alternative metric for indirect comparison against regulatory criteria for bioaccumulative (B) or very bioaccumulative (vB) substances.

This work was conducted in the context of the revision of the Organisation for Economic Co-operation and Development (OECD) 305 Test Guideline in which the Environment Agency is involved on behalf of the UK.

The alternative method for estimating the growth-corrected depuration rate constant is based on the amount of substance per fish rather than the normal concentration units (that is, mass of substance per unit mass of fish). The report describes the theory behind the approach and presents several examples from studies using both rapidly growing and slowly growing fish.

Overall, the analysis has shown that the alternative method for obtaining the growth-corrected rate constant is a viable and appropriate method that can provide useful information in cases where the more normal rate constant subtraction method is difficult to apply, or where there are uncertainties over whether growth dilution is following first-order kinetics.

The use of the depuration rate constant as an alternative metric for assessment of the B (BCF >2,000 l kg^{-1}) or vB (BCF >5,000 l kg^{-1}) properties of a substance has been investigated using a data set of available BCF values. The analysis here resulted in a number of regression equations from which the following critical values identifying B or vB substances were derived.

	Critical value
BCF ≥2,000 l kg^{-1}	$k_2 \leq 0.178$ day^{-1}
BCF ≥5,000 l kg^{-1}	$k_2 \leq 0.085$ day^{-1}
$BCF_{lipid\ normalised}$ ≥2,000 l kg^{-1}	$k_2 \leq 0.141$ day^{-1}
$BCF_{lipid\ normalised}$ ≥5,000 l kg^{-1}	$k_2 \leq 0.065$ day^{-1}
$BCF_{lipid\ normalised}$ ≥2,000 l kg^{-1}	$k_{2\ (lipid\ normalised)} \leq 0.181$ day^{-1}
$BCF_{lipid\ normalised}$ ≥5,000 l kg^{-1}	$k_{2\ (lipid\ normalised)} \leq 0.085$ day^{-1}

This approach for identifying substances as B or vB based on the depuration rate constant appears to show promise, with a large proportion of the available data set being correctly categorised for the training and validation data sets analysed here. The approach used, however, resulted in a number of false positive and false negative assignments, particularly for esters and substances where the BCF values themselves are not clear cut as to the B or vB status.

It is important to note that the data sets analysed for this study included data for a number of species and fish sizes. Some depuration processes may depend on fish size

(for example, loss at the gills may depend on the gill surface area and respiration rate which may, in relative terms, decrease with increasing fish size (and age)) and the depuration rate constant may also be species dependent (particularly where different species have different metabolic capacities for a given chemical). Therefore, there may be species- and size-related factors that affect the magnitude of k_2. However, these same factors, but especially metabolic capacity, would also be expected to have some impact on the magnitude of the bioconcentration factor itself.

Taking this into account, the approach may be best used as part of a weight of evidence/expert judgement-type approach.

As well as potentially using cut-offs based on the depuration rate constants for identification of substances as B or vB substances, the regression equations derived may themselves provide a useful means for predicting an actual BCF from the results of a feeding study.

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1. Introduction

Bioaccumulation is an important information requirement for chemicals risk assessment and for regulatory regimes such as REACH.[1] Under REACH, bioaccumulation testing could in theory be triggered for more than 3,000 chemicals based on supply tonnages and octanol–water partition coefficient cut-off values. In addition, bioaccumulation testing may be triggered for other substances that meet the PBT (persistent, bioaccumulative and toxic) or vPvB (very persistent and very bioaccumulative) screening criteria.

The main criterion used in REACH to determine bioaccumulation in the PBT or vPvB assessment is currently the fish bioconcentration factor (BCF), which is normally measured using the Organisation for Economic Co-operation and Development (OECD) 305 Test Guideline methodology (OECD 1996). However, the fish BCF can be difficult to determine directly by experiment for certain types of substances, particularly those that are poorly soluble in water, and the OECD 305 Test Guideline is currently being revised to include a dietary exposure method for difficult to test substances. This new method will result in a biomagnification factor (BMF) rather than a BCF.

A previous report (Crookes and Brooke 2011) investigated various methods for estimating a BCF from the data generated using the dietary exposure method and also considered factors such as growth that could potentially affect bioaccumulation studies. This report is a follow-up to investigate further the following two aspects:

- an alternative mathematical method to correct for fish growth in BCF and BMF studies;
- the use of the elimination rate constant (or elimination half-life) as a direct measure of bioaccumulation and an alternative metric for indirect comparison against regulatory PBT and vPvB criteria.

This work is being conducted in the context of the revision of the OECD 305 Test Guideline in which the Environment Agency is involved on behalf of the UK.

[1] Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC.

2. Growth-corrected depuration rate constant

2.1 Background

In a standard fish BCF test, the uptake into and depuration from fish is usually described in terms of two first-order kinetic processes:

Equation 1 $$\text{Rate of uptake} = k_1 \times [C_{water}]$$

Equation 2 $$\text{Rate of depuration} = k_2 \times [C_{fish}]$$

where k_1 = first-order rate constant for uptake into fish (l kg^{-1} day^{-1})

k_2 = first-order rate constant for depuration/elimination from fish (day^{-1})

$[C_{water}]$ = concentration in water (mg l^{-1})

$[C_{fish}]$ = concentration in fish (mg kg^{-1} wet weight).

At steady state, the rate of uptake equals the rate of depuration, and so combining gives the following relationship:

Equation 3 $$BCF = \frac{[C_{fish}] \text{ at steady state (mg kg}^{-1} \text{ wet weight)}}{[C_{water}] \text{ at steady state (mg l}^{-1})} = \frac{k_1}{k_2}$$

The ratio of k_1/k_2 is known as the kinetic BCF and, if first-order kinetics are followed, should be equal to the steady state BCF obtained by the ratio of the steady state concentration in fish to that in water.

The depuration rate constant represents the overall depuration of the substance from the fish. However, in reality this depuration may consist of a number of processes each contributing to the overall removal from the fish. Such processes include loss via respiration across the gills, loss via faecal elimination and loss via metabolism.

A fourth process, growth, can also contribute to the overall depuration rate constant. Unlike the three processes mentioned above, this process does not result in actual loss of mass of substance from the fish. However, it does contribute to a decline in concentration in the fish with time and so can be considered to contribute to the overall rate of depuration measured in an experiment when concentration units of mass of substance per mass of fish are used. For this reason it is often referred to as growth dilution.

The overall depuration rate constant is therefore frequently written in terms of four first-order kinetic processes as follows (Gobas and Morrison 2002).

Equation 4 $$k_2 = k_r + k_m + k_e + k_{growth-dilution}$$

where k_r = first-order rate constant for respiratory elimination via the gills (day^{-1})

k_m = first-order rate constant for metabolic transformation (day^{-1})

k_e = first-order rate constant for elimination via faeces (day^{-1})

$k_{growth-dilution}$ = first-order rate constant for decline in concentration resulting from growth (growth dilution) (day^{-1}).

As long as all four processes follow first-order kinetics in relation to the concentration in the fish then the rate constants will be additive.

2.1.1 Rate constant subtraction method

Most experimental uptake studies (be they from water or food) would usually determine the overall elimination rate constant from the fish (that is, k_2). However, as growth dilution does not in itself lead to loss of substance in the fish, some regulatory regimes (including REACH) require a growth-corrected depuration rate constant to be considered.

In order to correct the overall k_2 value for growth, the rate constant for growth dilution is usually subtracted out. This is referred to as the rate constant subtraction method above and in the remainder of the report.

Equation 5 $$k_{2-\text{growth}-\text{corrected}} = k_2 - k_{\text{growth}-\text{dilution}}$$

where $k_{2\text{-growth-corrected}}$ = growth-corrected depuration rate constant (day^{-1})

k_2 = overall depuration rate constant obtained from the experimental depuration curve (day^{-1})

$k_{\text{growth-dilution}}$ = rate constant for growth dilution (day^{-1}).

For the correction in this form to be valid, both the overall rate of depuration and the rate of growth dilution must follow first-order kinetics in relation to the concentration in fish. For the growth dilution component alone (ignoring the effect of real removal processes on the concentration in the fish), this means that the process should be defined by the following rate equation (Crookes and Brooke 2011):

Equation 6 $$\frac{d[C_{\text{fish}}]}{dt} = -k_{\text{growth}-\text{dilution}}[C_{\text{fish}}]$$

where $d[C_{fish}]/dt$ = rate of change in the concentration in fish (mg kg^{-1} day^{-1})

$[C_{fish}]$ = concentration in fish (mg kg^{-1})

$k_{\text{growth-dilution}}$ = rate constant for growth dilution (day^{-1}).

The integrated form of this rate equation leads to the following solution:

Equation 7 $$\ln[C_{\text{fish}}] = -k_{\text{growth}-\text{dilution}} \times t + \text{constant}$$

where $\ln[C_{fish}]$ = natural logarithm of the fish concentration (mg kg^{-1})

t = time (days)

Constant = a constant.

If it is then assumed that the amount of chemical in the fish is x mg, the concentration in fish at any time (t) can be estimated as $[C_{fish}]$ = x/fish weight (kg). Substituting this into Equation 7 leads to the following:

Equation 8 $$\ln\left(\frac{x}{\text{Fish weight}}\right) = -k_{\text{growth}-\text{dilution}} \times t + \text{constant}$$

As only growth dilution is considered here and as growth dilution itself does not lead to a reduction in the mass (x) in the fish, this will hold at all time points during the depuration (that is, x is effectively constant). This allows Equation 8 to be rewritten as follows (where the constant now also includes the term –ln (x)):

Equation 9 $$\ln\left(\frac{1}{\text{Fish weight}}\right) = -k_{\text{growth}-\text{dilution}} \times t + \text{constant}$$

Thus a plot of ln (1/fish weight) against time should give a straight line with the slope representing the first-order rate constant for growth dilution.[2]

Thus the value of $k_{growth\text{-}dilution}$ is straightforward to estimate provided information is available on the fish weight at various time points during the depuration phase of the study. The growth-corrected BCF value can then be estimated as the ratio of $k_1/k_{2\text{-}growth\text{-}corrected}$.

Although the rate constant subtraction method is straightforward in principle, a potential problem exists for growth correcting the depuration rate constant for studies using relatively rapidly growing fish with substances that are only slowly eliminated via respiration, metabolism and/or faecal egestion. In such a case, the overall depuration rate constant (k_2) can be dominated by the contribution from the growth dilution ($k_{growth\text{-}dilution}$) and so the $k_{2\text{-}growth\text{-}corrected}$ can represent a small difference between two numbers of similar magnitude, both with an inherent uncertainty. This can result in a value of $k_{2\text{-}growth\text{-}corrected}$ that is small compared with the measured overall depuration rate constant and with a high uncertainty (in some cases the error in k_2 and $k_{growth\text{-}dilution}$ may even lead to a negative estimate of $k_{2\text{-}growth\text{-}corrected}$). This is clearly not an ideal situation.

2.1.2 Alternative method

The growth dilution issue arises mainly because, normally in a bioaccumulation test, the concentrations in the fish are defined on a mass of substance per mass of fish basis during the depuration phase. In this form, a change in mass of the fish (that is, growth) can affect the concentration without any actual loss of substance occurring.

A potential alternative method for estimating the value of $k_{2\text{-}growth\text{-}corrected}$ is to define the concentrations in another unit, namely mass of substance per fish. In this case, even if the fish grows, the concentration will not decrease unless a 'true' loss process (respiration, metabolism, faecal elimination) is occurring. This is explained below.

The overall depuration rate constant is usually obtained from the following equation (for overall first-order kinetics):

Equation 10 $$\frac{d[C_{fish}]}{dt} = -k_2 \times [C_{fish}]$$

Equation 11 $$\ln[C_{fish}] = -k_2 \times t + \text{constant}$$

where $\ln[C_{fish}]$ = the natural logarithm of the concentration in fish (mg kg^{-1})

k_2 = overall depuration rate constant (day^{-1})

t = time (days)

Constant = a constant (in this case it is the natural logarithm of the concentration in fish at the start of the depuration phase).

The value of k_2 can then be determined directly from the slope of a plot of $\ln[C_{fish}]$ against time.

[2] This can also be plotted as ln[fish weight] against time. Here the slope is $+k_{growth\text{-}dilution}$.

But as the k_2 value has units of day^{-1} (and does not involve concentration), there is no underlying reason why the concentration in fish has to be defined in terms of mg substance per kg fish *during the depuration phase*.[3] This can be seen below.

Equation 12 $$[A_{fish}] = [C_{fish}] \times W_{fish}$$

where $[A_{fish}]$ = amount of substance per fish (mg $fish^{-1}$)

$[C_{fish}]$ = concentration in fish (mg kg^{-1})

W_{fish} = fish weight (kg).

Substituting for $[C_{fish}]$ in Equation 11 gives:

Equation 13 $$\ln[A_{fish} / W_{fish}] = -k_2 \times t + constant$$

This can also be written as follows:

Equation 14 $$\ln[A_{fish}] - \ln[\frac{1}{W_{fish}}] = -k_2 \times t + constant$$

Combining with Equation 9 and rearranging gives:

Equation 15 $$\ln[A_{fish}] = (-k_2 \times t) + constant + (k_{growth-dlution} \times t) + constant$$

This can be simplified to give Equation 16:

Equation 16 $$\ln[A_{fish}] = (k_{growth-dilution} - k_2) \times t + constant$$

Thus a plot of $\ln[A_{fish}]$ against time should give a slope of ($k_{growth\text{-}dilution}$-$k_2$). From Equation 5 it can be seen that ($k_{growth\text{-}dilution}$-$k_2$) is $-k_{2\text{-}growth\text{-}corrected}$. Thus the slope of such a plot should yield the growth-corrected k_2 value directly (slope = $-k_{2\text{-}growth\text{-}corrected}$). This is referred to as the alternative method both above and in the remainder of the report.

It is also worth noting that this formulation does not require any *a priori* assumptions about the kinetics of growth dilution (that is, it does not require or imply that growth dilution is a first-order process).

2.2 Testing of the alternative method

2.2.1 Test data with rapidly growing fish

In order to test the alternative method for obtaining the growth-corrected depuration rate constant, a number of depuration curves were analysed using the normal rate constant subtraction method and the alternative method.

The main data sets used were obtained as part of a ring test of the new OECD 305 dietary accumulation study. The raw data and the laboratories involved are

[3] This is not the case for the uptake phase where the uptake rate constant (k_1) does include concentration units (l kg^{-1}) and so the value of k_1 obtained is dependent on the concentration units chosen.

confidential.[4] However, this is a very useful data set for this analysis for the following reasons:

- Essentially the same test protocol was used in each test.
- The same chemicals were tested in several laboratories, meaning multiple results are available for a number of chemicals.
- The fish were growing rapidly in most of the tests and this dominated the overall depuration rate constant seen for some substances.
- Crucially, at each time point both the weight of fish and the concentration present were determined in the sample, thus allowing the amount of substance per fish to be determined.

The chemicals involved in the ring test were:

- hexachlorobenzene;
- musk xylene;
- *o*-terphenyl;
- methoxychlor;
- benzo[a]pyrene.

The tests were mainly carried out with rainbow trout, though carp were used in one case.

In general, one concentration of each substance was tested, but for study D, three concentrations of hexachlorobenzene, musk xylene, *o*-terphenyl and methoxychlor were tested.

The data for the depuration phase were analysed as described below for each usable curve.

For this analysis, the concentrations and wet weights used in the various plots were in units of μg g^{-1} (which is equivalent to mg kg^{-1}), μg $fish^{-1}$ and g, as these related more directly to the units in which the raw data were reported.

Rate constant subtraction method

1. The overall rate constant was obtained from a plot of $\ln[C_{fish}]$ against time (days) with the concentration in fish in units of μg g^{-1} fish. The k_2 value was obtained from the slope of this plot.
2. The rate constant for growth dilution was obtained by a plot of $\ln[1/W_{fish}]$ against time with the fish weight in g. The $k_{growth\text{-}dilution}$ was obtained from the slope of this plot.
3. The growth-corrected depuration rate constant, $k_{2\text{-}growth\text{-}corrected}$ was obtained as $k_2\text{-}k_{growth\text{-}dilution}$.

[4] A total of eight data sets (seven with rainbow trout and one with carp) from seven laboratories were available for inclusion in this report. The full OECD 305 ring test will have data sets from a further three laboratories, but these data were not available at the time of carrying out the analysis described here. The data have been anonymised.

Alternative method

1. The amount of substance in the fish [A_{fish}] at each time point in the depuration phase was determined in μg $fish^{-1}$ from the reported concentration data and fish weight data.
2. The $k_{2\text{-growth-corrected}}$ was obtained directly from a plot of the ln[A_{fish}] against time.

The results of the analysis are summarised in Tables 2.1 to 2.11 by substance. Appendix A shows the plots used to derive the various rate constants.

Benzo[a]pyrene was generally found to be depurated very rapidly from the fish and it was not possible to establish the relevant kinetics for depuration of this substance in all cases (the concentration declined rapidly to below the limit of detection in most cases).

As can be seen, agreement between the growth-corrected depuration rate constants obtained by the two methods is generally good.

Notes to Table 2.1 to

Table 2.11

R^2	Correlation coefficient for the linear (least squares) regression of ln [$1/W_{fish}$] against time, ln [C_{fish}].against time or ln [A_{fish}] against time
p	Statistical significance of the slope of the linear regression – the lower the value the higher the probability that the slope (rate constant) is different from zero. Values where *p* >0.05 (that is, where the probability that the slope is not different from zero is above 5 per cent) are shown **bold**.
S.E.	Standard error in the slope (rate constant) of the linear regression
Propagated S.E.	Approximate standard error estimate in the growth-corrected k_2 value by subtraction. This is estimated here as the square root of the sum of the S.E. for the growth rate constant squared and the S.E. for the overall k_2 squared. This assumes that the standard errors in the growth rate constant are independent of those in the k_2 value, which may not necessarily be the case here.
% S.E.	Standard error (or propagated standard error) expressed as a percentage of the $k_{2\text{-growth-corrected}}$
S.D.	Standard deviation
% S.D.	Standard deviation expressed as a percentage of the mean

Table 2.1 Summary of growth kinetics for the OECD ring test data set

Data set	$k_{growth\text{-}dilution}$ (day^{-1})	R^2	S.E.	% S.E.	*p*
Study A	0.037	0.83	0.002	5.4	3.8×10^{-28}
Study B	0.047	0.87	0.002	4.8	5.2×10^{-31}
Study C	0.010	0.08	0.005	45.1	0.030
Study D	0.033	0.79	0.002	5.2	4.3×10^{-35}
Study E	0.034	0.71	0.003	8.1	1.4×10^{-18}
Study F	0.044	0.89	0.002	4.3	3.3×10^{-34}
Study G	0.036	0.70	0.003	7.9	1.6×10^{-19}
Study H	0.018	0.61	0.002	10.5	2.1×10^{-13}

Table 2.2 Summary of depuration kinetics for hexachlorobenzene – rate constant subtraction method

Data set	$k_{growth\text{-}dilution}$ (day^{-1}; from Table 2.1)	Overall depuration kinetics				Derived growth-corrected kinetics		
		k_2 (day^{-1})	R^2	S.E.	*p*	$k_{2\text{-}growth\text{-}corrected}$ (day^{-1})	Propagated S.E.	% S.E.
Study A	0.037	0.063	0.87	0.005	5.8×10^{-13}	0.026	0.005	20.0
Study B	0.047	0.058	0.90	0.004	6.5×10^{-15}	0.011	0.004	40.4
Study C	0.010	0.041	0.36	0.010	4.3×10^{-4}	0.030	0.011	37.0
Study D	0.033	0.060	0.90	0.011	0.013	0.027	0.012	42.8
Study D	0.033	0.056	0.99	0.004	5.9×10^{-4}	0.023	0.004	17.7
Study D	0.033	0.049	0.71	0.018	**0.073**	0.015	0.018	117.8
Study E	0.034	0.051	0.86	0.004	3.1×10^{-11}	0.017	0.005	29.3
Study F	0.044	0.054	0.85	0.004	3.3×10^{-13}	0.010	0.005	45.3
Study G	0.036	0.050	0.78	0.005	1.1×10^{-10}	0.014	0.006	40.8
Study H	0.018	0.040	0.88	0.003	2.3×10^{-14}	0.022	0.003	15.0
Mean	0.033	0.052				0.020		
S.D.	0.011	0.008				0.007		
% S.D.	33.7	14.6				35.8		

Table 2.3 Summary of depuration kinetics for hexachlorobenzene – alternative method

Data set	$k_{2\text{-growth-corrected}}$	R^2	S.E.	% S.E.	*p*
Study A	0.031	0.43	0.007	22.4	1.4×10^{-4}
Study B	0.012	0.18	0.005	40.6	0.020
Study C	0.032	0.30	0.009	28.9	1.7×10^{-3}
Study D	0.030	0.79	0.009	30.0	0.045
Study D	0.024	0.78	0.007	30.7	0.047
Study D	0.015	0.17	0.020	129.4	**0.50**
Study E	0.024	0.37	0.006	26.9	1.1×10^{-3}
Study F	0.010	0.09	0.006	60.1	**0.11**
Study G	0.018	0.23	0.006	35.1	8.1×10^{-3}
Study H	0.025	0.50	0.005	19.1	1.4×10^{-5}
Mean	0.022				
S.D.	0.008				
% S.D.	35.5				

Table 2.4 Summary of depuration kinetics for musk xylene – rate constant subtraction method

Data set	$k_{growth\text{-}dilution}$ (day^{-1}; from Table 2.1)	Overall depuration kinetics				Derived growth-corrected kinetics		
		k_2 (day^{-1})	R^2	S.E.	*p*	$k_{2\text{-}growth\text{-}corrected}$ (day^{-1})	Propagated S.E.	% S.E.
Study A	0.037	0.105	0.92	0.006	3.9×10^{-16}	0.068	0.006	9.1
Study B	0.047	0.095	0.95	0.004	2.5×10^{-19}	0.048	0.005	9.8
Study C	0.010	0.646	0.86	0.073	7.8×10^{-7}	0.636	0.074	11.6
Study D	0.033	0.139	0.98	0.012	1.6×10^{-3}	0.106	0.012	11.7
Study D	0.033	0.131	0.99	0.006	2.5×10^{-4}	0.097	0.007	6.7
Study D	0.033	0.111	0.96	0.013	3.1×10^{-3}	0.078	0.013	16.4
Study E	0.034	0.062	0.70	0.009	2.2×10^{-7}	0.028	0.009	31.6
Study F	0.044	0.083	0.90	0.005	1.6×10^{-15}	0.039	0.006	14.1
Study G	0.036	0.090	0.88	0.006	1.2×10^{-14}	0.054	0.007	12.5
Study H	0.018	0.073	0.93	0.004	8.0×10^{-18}	0.056	0.004	7.5
Mean	0.033	0.154				0.121		
S.D.	0.011	0.175				0.183		
% S.D.	33.7	113.8				150.8		

Table 2.5 Summary of depuration kinetics for musk xylene – alternative method

Data set	$k_{2\text{-growth-corrected}}$	R^2	S.E.	% S.E.	*p*
Study A	0.074	0.80	0.007	10.0	1.9×10^{-10}
Study B	0.049	0.77	0.005	10.5	3.7×10^{-10}
Study C	0.667	0.87	0.072	10.7	4.1×10^{-7}
Study D	0.109	0.98	0.010	9.0	1.6×10^{-3}
Study D	0.099	0.98	0.007	7.2	8.0×10^{-4}
Study D	0.078	0.92	0.013	17.3	0.010
Study E	0.035	0.43	0.008	23.8	3.4×10^{-4}
Study F	0.039	0.55	0.007	17.0	2.4×10^{-6}
Study G	0.059	0.69	0.007	12.5	1.1×10^{-8}
Study H	0.058	0.79	0.006	9.6	4.2×10^{-11}
Mean	0.127				
S.D.	0.191				
% S.D.	151.2				

Table 2.6 Summary of depuration kinetics for *o*-terphenyl – rate constant subtraction method

Data set	$k_{growth\text{-}dilution}$ (day^{-1}; from Table 2.1)	Overall depuration kinetics				Derived growth-corrected kinetics		
		k_2 (day^{-1})	R^2	S.E.	*p*	$k_{2\text{-}growth\text{-}corrected}$ (day^{-1})	Propagated S.E.	% S.E.
Study A	0.037	0.133	0.73	0.016	6.2×10^{-9}	0.097	0.016	16.4
Study B	0.047	0.113	0.75	0.012	1.1×10^{-9}	0.066	0.013	19.2
Study C	0.010	0.044	0.40	0.010	1.7×10^{-4}	0.034	0.011	33.1
Study D	0.033	0.290	1.00	0.010	8.7×10^{-5}	0.257	0.010	3.9
Study D	0.033	0.351	0.98	0.033	8.7×10^{-3}	0.317	0.033	10.4
Study D	0.033	0.297	0.99	0.016	2.8×10^{-3}	0.263	0.016	6.0
Study E	0.034	0.075	0.36	0.021	1.6×10^{3}	0.041	0.021	51.4
Study F	0.044	0.104	0.79	0.010	2.8×10^{-10}	0.060	0.011	17.8
Study G	0.036	0.087	0.82	0.008	5.5×10^{-12}	0.051	0.008	16.0
Study H	0.018	0.069	0.68	0.009	2.6×10^{-8}	0.052	0.009	17.9
Mean	0.033	0.156				0.124		
S.D.	0.011	0.112				0.110		
% S.D.	33.7	71.4				88.5		

Table 2.7 Summary of depuration kinetics for *o*-terphenyl – alternative method

Data set	$k_{2\text{-growth-corrected}}$	R^2	S.E.	% S.E.	*p*
Study A	0.102	0.56	0.018	17.6	5.4×10^{-6}
Study B	0.067	0.48	0.013	19.8	2.7×10^{-5}
Study C	0.035	0.32	0.010	27.7	1.2×10^{-3}
Study D	0.260	1.00	0.008	3.0	6.2×10^{-5}
Study D	0.305	0.97	0.040	13.2	0.017
Study D	0.248	0.99	0.016	6.6	4.3×10^{-3}
Study E	0.047	0.17	0.021	45.3	0.038
Study F	0.060	0.46	0.013	21.1	6.5×10^{-5}
Study G	0.055	0.59	0.009	15.6	6.1×10^{-7}
Study H	0.054	0.52	0.010	18.3	7.7×10^{-6}
Mean	0.123				
S.D.	0.104				
% S.D.	84.5				

Table 2.8 Summary of depuration kinetics for methoxychlor – rate constant subtraction method

Data set	$k_{growth\text{-}dilution}$ (day^{-1}; from Table 2.1)	Overall depuration kinetics				Derived growth-corrected kinetics		
		k_2 (day^{-1})	R^2	S.E.	*p*	$k_{2\text{-}growth\text{-}corrected}$ (day^{-1})	Propagated S.E.	% S.E.
Study A	0.037	0.133	0.44	0.035	1.1×10^{-3}	0.096	0.035	36.0
Study B	0.047	0.110	0.51	0.021	1.2×10^{-5}	0.063	0.021	32.9
Study C	0.010	0.005	0.003	0.017	**0.79**	-0.006	0.017	-297.7
Study D	0.033	0.310	0.97	0.041	0.017	0.277	0.041	15.0
Study D	0.033	0.294	0.97	0.036	0.015	0.261	0.037	14.0
Study D	0.033	0.264	0.89	0.095	**0.22**	0.231	0.095	41.2
Study E	0.034	0.077	0.27	0.028	0.013	0.044	0.028	65.1
Study F	0.044	0.102	0.56	0.018	8.0×10^{-6}	0.058	0.018	31.3
Study G	0.036	0.150	0.66	0.025	7.9×10^{-6}	0.114	0.025	21.9
Study H	0.018	0.116	0.74	0.013	8.9×10^{-10}	0.098	0.013	13.2
Mean	0.033	0.156				0.124		
S.D.	0.011	0.100				0.098		
% S.D.	33.7	64.3				79.2		

Table 2.9 Summary of depuration kinetics for methoxychlor – alternative method

Data set	$k_{2\text{-growth-corrected}}$	R^2	S.E.	% S.E.	*p*
Study A	0.182	0.78	0.022	12.1	9.8×10^{-8}
Study B	0.065	0.26	0.021	32.8	5.1×10^{-3}
Study C	-0.005	0.003	0.017	-362.3	**0.78**
Study D	0.289	0.97	0.037	12.9	0.016
Study D	0.249	0.94	0.044	17.7	0.030
Study D	0.212	0.84	0.092	43.6	**0.26**
Study E	0.051	0.13	0.029	58.1	**0.10**
Study F	0.056	0.26	0.019	33.7	6.6×10^{-3}
Study G	0.114	0.56	0.023	20.4	1.0×10^{-4}
Study H	0.101	0.68	0.013	12.9	2.0×10^{-8}
Mean	0.131				
S.D.	0.097				
% S.D.	73.6				

Table 2.10 Summary of depuration kinetics for benzo(a)pyrene– rate constant subtraction method

Data set	$k_{growth\text{-}dilution}$ (day^{-1}; from Table 2.1)	Overall depuration kinetics				Derived growth-corrected kinetics		
		k_2 (day^{-1})	R^2	S.E.	*p*	$k_{2\text{-}growth\text{-}corrected}$ (day^{-1})	Propagated S.E.	% S.E.
Study A	0.037	1.684	0.92	0.225	6.7×10^{-4}	1.647	0.225	13.6
Study B	0.047	1.179	0.92	0.120	9.7×10^{-6}	1.132	0.120	10.6
Study C	0.010	2.066	0.77	0.398	8.3×10^{-4}	2.056	0.398	19.3
Study G	0.036	0.986	0.81	0.236	0.014	0.950	0.236	24.8
Study H	0.018	2.094	0.93	0.208	8.0×10^{-6}	2.076	0.208	10.0
Mean	0.030	1.602				1.572		
S.D.	0.015	0.505				0.518		
% S.D.	51.1	31.6				33.0		

Table 2.11 Summary of depuration kinetics for benzo(a)pyrene – alternative method

Data set	$k_{2\text{-growth-corrected}}$	R^2	S.E.	% S.E.	*p*
Study A	1.568	0.91	0.221	14.1	8.6×10^{-4}
Study B	1.179	0.87	0.160	13.6	7.9×10^{-5}
Study C	2.029	0.72	0.443	21.8	1.8×10^{-3}
Study G	0.964	0.80	0.240	24.9	0.016
Study H	2.112	0.91	0.235	11.1	1.9×10^{-5}
Mean	1.570				
S.D.	0.506				
% S.D.	32.2				

2.2.2 Test data with fish of different sizes

A confidential data set using fish of two markedly different sizes was made available to the project team. The tests were dietary feeding tests carried out using five related substances. One series of tests involved smaller fish (rainbow trout around 1–2 g in weight at the start of the test) and the second series used larger fish (rainbow trout around 300 g in weight at the start of the test).

The raw data for these tests were kindly made available for analysis here, but the confidential nature of these data means it is not possible to include the various plots used to derive the various rate constants. The method used to analyse the data was the same as used in Section 2.2.1.

The rate constants for growth dilution derived during the depuration phase were:

- 0.0437 day^{-1} (standard error ±0.0031 day^{-1}) for the smaller fish;
- 0.0138 day^{-1} (standard error ±0.0018 day^{-1}) for the larger fish.

The results of analysing the data using the rate constant subtraction method and the alternative method are summarised in Table 2.12 and 2.13. As can be seen from the tables, there is good agreement between the growth-corrected depuration rate constants obtained using the two methods.

Notes to Table 2.12 and Table 2.13

R^2	Correlation coefficient for the linear (least squares) regression of ln $[C_{fish}]$.against time or ln $[A_{fish}]$ against time
p	Statistical significance of the slope of the linear regression. The lower the value the higher the probability that the slope (rate constant) is different from zero. Values where $p > 0.05$ (that is, where the probability that the slope is not different from zero is above 5 per cent) are shown **bold**.
S.E.	Standard error in the slope (rate constant) of the linear regression
Propagated S.E.	Approximate standard error estimate in the growth-corrected k_2 value by subtraction. This is estimated here as the square root of the sum of the S.E. for the growth rate constant squared and the S.E. for the overall k_2 squared. This assumes that the standard errors in the growth rate constant are independent of those in the k_2 value, which may not necessarily be the case here.
% S.E.	Standard error (or propagated standard error) expressed as a percentage of the $k_{2\text{-growth-corrected}}$

Table 2.12 Summary of depuration kinetics for five substances in smaller and larger fish – rate constant subtraction method

Data set	$k_{growth\text{-}dilution}$ (day^{-1})	Overall depuration kinetics				Derived growth-corrected kinetics		
		k_2 (day^{-1})	R^2	S.E.	*p*	$k_{2\text{-}growth\text{-}corrected}$ (day^{-1})	Propagated S.E.	% S.E.
Smaller fish								
Substance A	0.0437	0.195	0.74	0.023	7.1×10^{-9}	0.152	0.023	15.2
Substance B	0.0437	0.168	0.93	0.009	2.3×10^{-17}	0.125	0.010	7.6
Substance C	0.0437	0.215	0.78	0.023	9.0×10^{-10}	0.171	0.023	13.3
Substance D	0.0437	0.142	0.90	0.009	2.2×10^{-15}	0.098	0.010	9.8
Substance E	0.0437	0.196	0.89	0.013	4.8×10^{-15}	0.152	0.013	8.7
Larger fish								
Substance A	0.0138	0.078	0.62	0.014	4.1×10^{-5}	0.064	0.015	22.7
Substance B	0.0138	0.093	0.83	0.010	2.0×10^{-8}	0.079	0.010	12.6
Substance C	0.0138	0.111	0.79	0.013	1.6×10^{-7}	0.097	0.014	13.9
Substance D	0.0138	0.057	0.72	0.008	2.2×10^{-6}	0.043	0.009	19.8
Substance E	0.0138	0.071	0.70	0.011	4.2×10^{-6}	0.057	0.011	19.3

Table 2.13 Summary of depuration kinetics for five substances in smaller and larger fish – alternative method

Data set	$k_{2\text{-growth-corrected}}$ (day^{-1})	R^2	S.E.	% S.E.	*p*
Smaller fish					
Substance A	0.153	0.65	0.022	14.5	3.2×10^{-7}
Substance B	0.125	0.89	0.008	6.7	8.6×10^{-15}
Substance C	0.169	0.68	0.023	13.6	1.1×10^{-7}
Substance D	0.098	0.84	0.008	8.3	1.2×10^{-12}
Substance E	0.152	0.86	0.011	7.5	1.2×10^{-13}
Larger fish					
Substance A	0.064	0.51	0.015	22.9	3.7×10^{-4}
Substance B	0.079	0.77	0.010	12.7	3.1×10^{-7}
Substance C	0.097	0.75	0.013	13.5	7.0×10^{-7}
Substance D	0.043	0.59	0.008	19.5	7.1×10^{-5}
Substance E	0.057	0.61	0.011	18.7	4.4×10^{-5}

2.2.3 Bioconcentration test data with slowly growing fish

As well as being applicable to fish that are growing during the depuration phase, the alternative method should be equally applicable to fish that are not growing rapidly during the depuration phase. This can be seen from a comparison of Equation 11 and Equation 16. When the value of $k_{growth\text{-}dilution}$ is small, the slope of the plot of ln [A_{fish}] against time (Equation 16) should be the same as a plot of ln [C_{fish}] against time (Equation 11), with the slope of both plots being equal to $-k_2$.

To test this is the case, a data set from a study where there was little or no growth of the fish during the depuration phase was analysed using both methods. The data set was from a standard bioconcentration study carried out with a C_{13} chlorinated paraffin. The full study report is only available in Japanese (Mitsubishi 2009) but an English summary (covering mainly the uptake portion of the study) is available (UNEP 2009).

The test was carried out using carp (*Cyprinus carpio*) exposed to two concentrations, 0.01 mg/l (high exposure) and 0.001 mg/l (low exposure) (nominal concentrations), of the chlorinated paraffin over 62 days followed by a 21-day depuration period. The uptake and depuration of the chlorinated paraffin was monitored by analysing the three main constituents of the substance tested ($C_{13}H_{23}Cl_5$, $C_{13}H_{22}Cl_6$ and $C_{13}H_{21}Cl_7$).

The full study report indicates that duplicate samples were analysed at each time point. However, each sample appears to consist of two fish (that were possibly combined for analysis) and, as only one concentration was reported for each sampling point, it is only possible to carry out an analysis of the data based on the average fish weight in each sample rather than the individual fish weight. It is recognised that this is not ideal for the analysis here as some of the information in the data set may have been lost through the averaging process. The relevant data from the depuration phase are summarised in Table 2.14 and 2.15.

Table 2.14 Summary of depuration data for C_{13}-chlorinated paraffin for the higher exposure group

Depuration day	Mean fish weight (g)	Measured concentration in fish (µg/g)			Estimated amount per fish (µg)		
		Cl_5	Cl_6	Cl_7	Cl_5	Cl_6	Cl_7
0[a]	7.59	14.20	18.08	137.14	107.71	26.68	202.37
0[a]	5.73	13.17	16.86	96.61	75.46	25.69	147.20
4	7.40	7.20	10.35	76.54	53.24	17.49	129.34
4	6.98	9.00	14.15	98.77	62.82	24.11	168.29
8	6.67	6.65	12.44	82.91	44.32	21.70	144.63
8	5.32	4.04	6.74	35.86	21.49	12.23	65.06
15	6.78	2.27	4.67	31.66	15.39	10.69	72.48
15	7.17	1.90	4.06	29.11	13.62	8.74	62.67
21	7.83	1.15	2.52	19.73	9.00	6.29	49.25
21	7.09	0.67	1.59	11.27	4.75	4.07	28.86

Notes: The day 0 values are taken from the concentrations measured in the fish at day 62 of the uptake phase (end of the uptake phase). The values are

slightly different to those given in UNEP (2009), as the day 0 values used there were the average concentration measured in the fish over days 28 to 62.

Table 2.15 Summary of depuration data for C_{13}-chlorinated paraffin for the lower exposure group

Depuration day	Mean fish weight (g)	Measured concentration in fish (µg/g)			Estimated amount per fish (µg)		
		Cl_5	Cl_6	Cl_7	Cl_5	Cl_6	Cl_7
0[a]	5.75	1.450	1.463	2.163	8.33	8.40	12.43
0[a]	5.72	0.875	1.202	1.732	5.00	6.87	9.90
4	7.71	0.495	0.75	1.327	3.81	5.78	10.22
4	7.18	0.502	0.762	1.139	3.60	5.47	8.17
8	5.40	0.538	0.623	1.219	2.91	3.36	6.58
8	6.14	0.545	1.099	2.103	3.35	6.75	12.91
15	7.12	<0.240	0.419	1.116		2.98	7.94
15	8.06	<0.240	<0.275	0.595			4.80
21	6.77	<0.240	0.412	0.631		2.79	4.27
21	7.34	<0.240	<0.275	0.386			2.83

Notes: The day 0 values are taken from the concentrations measured in the fish at day 62 of the uptake phase (end of the uptake phase). The values are slightly different to those given in UNEP (2009), as the day 0 values used there were the average concentration measured in the fish over days 28 to 62.

Plots of ln [1/fish weight] against time (plots are given in Appendix B) gave growth rate constants of 0.0048 day^{-1} (high dose group; standard error ±0.0051 day^{-1}) and 0.0084 day^{-1} (low dose group; standard error ±0.0054 day^{-1}). However, the slopes of the plots were not statistically significantly different from 0. This demonstrates that, in this experiment, the fish were growing only relatively slowly compared with those in the OECD ring test examined in Section 2.2.1.

The concentration data were analysed in terms of plots of ln [C_{fish}] against time and ln [A_{fish}] against time (alternative method). The plots are given in Appendix B and the relevant rate constants and statistics derived are summarised in Table 2.16 (normal rate constant subtraction method) and Table 2.17 (alternative method). As before, agreement between the growth-corrected depuration rate constants obtained using the two methods is good.

Notes to Table 2.16 and Table 2.17

R^2 Correlation coefficient for the linear (least squares) regression of ln [C_{fish}].against time or ln [A_{fish}] against time

p Statistical significance of the slope of the linear regression. The lower the value, the higher the probability that the slope (rate constant) is different from zero. Values where *p* >0.05 (that is,

	where the probability that the slope is not different from zero is above 5 per cent) are shown **bold**.
S.E.	Standard error in the slope (rate constant) of the linear regression
Propagated S.E.	Approximate standard error estimate in the growth-corrected k_2 value by subtraction. This is estimated here as the square root of the sum of the S.E. for the growth rate constant squared and the S.E. for the overall k_2 squared. This assumes that the standard errors in the growth rate constant are independent of those in the k_2 value, which may not necessarily be the case here.
% S.E.	Standard error (or propagated standard error) expressed as a percentage of the $k_{2\text{-growth-corrected}}$
S.D.	Standard deviation
% S.D.	Standard deviation expressed as a percentage of the mean

Table 2.16 Summary of depuration kinetics for C_{13} chlorinated paraffin – rate constant subtraction method

Data set	$k_{growth\text{-}dilution}$ (day^{-1}) (see text)	Overall depuration kinetics				Derived growth-corrected kinetics		
		k_2 (day^{-1})	R^2	S.E.	*p*	$k_{2\text{-}growth\text{-}corrected}$ (day^{-1})	Propagated S.E.	% S.E.
Higher exposure group								
Cl_5	0.0048	0.130	0.97	0.008	3.3×10^{-7}	0.125	0.009	7.9
Cl_6	0.0048	0.102	0.93	0.010	5.1×10^{-6}	0.097	0.011	11.1
Cl_7	0.0048	0.077	0.90	0.009	3.1×10^{-5}	0.072	0.011	14.6
Lower exposure group								
Cl_5	0.0084	0.092	0.58	0.039	**0.081**	0.083	0.040	47.8
Cl_6	0.0084	0.056	0.76	0.013	5.0×10^{-3}	0.047	0.014	29.3
Cl_7	0.0084	0.061	0.73	0.013	1.7×10^{-3}	0.053	0.014	27.0

Table 2.17 Summary of depuration kinetics for C_{13} chlorinated paraffin – alternative method

Data set	$k_{2\text{-growth-corrected}}$ (day^{-1})	R^2	S.E.	% S.E.	*p*
Higher exposure group					
Cl_5	0.125	0.94	0.011	9.0	3.7×10^{-6}
Cl_6	0.097	0.89	0.012	12.1	3.5×10^{-5}
Cl_7	0.072	0.83	0.012	15.9	2.4×10^{-4}
Lower exposure group					
Cl_5	0.091	0.74	0.027	30.0	0.029
Cl_6	0.050	0.76	0.012	23.0	4.8×10^{-3}
Cl_7	0.053	0.72	0.012	22.2	2.0×10^{-3}

A further confidential data set from fish bioconcentration tests (OECD 305 methodology) using slowly growing fish was made available for this study. These tests were carried out mainly using zebrafish (*Danio rerio*) of around 0.1 to 1 g in weight and some of the substances were tested at two concentrations. In most cases, the growth of the fish was not significant over the timescale of the experiment.

The data were analysed using the same procedure as outlined in Section 2.2.1, although not all the data provided were in a suitable form to be analysed using the alternative method.

The relevant kinetic parameters derived from the suitable data sets are summarised in Tables 2.18 and 2.19. The confidential nature of the data means it is not possible to include the various plots used to derive the various rate constants. Again agreement between the growth-corrected depuration rate constants obtained using the two methods is good.

Notes to Table 2.18 to Table 2.19

R^2	Correlation coefficient for the linear (least squares) regression of ln $[C_{fish}]$.against time or ln $[A_{fish}]$ against time
p	Statistical significance of the slope of the linear regression. The lower the value the higher the probability that the slope (rate constant) is different from zero. Values where *p* >0.05 (that is, where the probability that the slope is not different from zero is above 5 per cent) are shown **bold**.
S.E.	Standard error in the slope (rate constant) of the linear regression
Propagated S.E.	Approximate standard error estimate in the growth-corrected k_2 value by subtraction. This is estimated here as the square root of the sum of the S.E. for the growth rate constant squared and the S.E. for the overall k_2 squared. This assumes that the standard errors in the growth rate constant are independent of those in the k_2 value, which may not necessarily be the case here.
% S.E.	Standard error (or propagated standard error) expressed as a percentage of the $k_{2\text{-growth-corrected}}$

Table 2.18 Summary of depuration kinetics obtained in bioconcentration tests with zebrafish – rate constant subtraction method

Data set	$k_{growth\text{-}dilution}$ (day^{-1})	Overall depuration kinetics				Derived growth-corrected kinetics		
		k_2 (day^{-1})	R^2	S.E.	*p*	$k_{2\text{-}growth\text{-}corrected}$ (day^{-1})	Propagated S.E.	% S.E.
Substance 1	0.0055	0.019	0.76	0.002	3.4×10^{-9}	0.013	0.002	18.0
Substance 2 (lower concentration)	**0.027***	13.8	0.83	2.6	1.7×10^{-3}	13.8	2.6	18.5
Substance 2 (higher concentration)	**0.027***	10.7	0.82	2.1	2.0×10^{-3}	10.7	2.1	19.2
Substance 3 (lower concentration)	**-0.093***	3.79	0.74	0.78	1.3×10^{-3}	3.79	0.78	20.8
Substance 3 (higher concentration)	**-0.010***	3.02	0.74	0.53	1.4×10^{-4}	3.02	0.53	17.5
Substance 4 (lower concentration)	**-0.007***	0.55	0.24	0.48	**0.32**	0.55	0.48	88.5
Substance 4 (higher concentration)	**-0.012***	1.04	0.25	0.74	**0.21**	1.04	0.74	71.5
Substance 6 (lower concentration)	**0.14***	18.5	0.82	8.8	**0.28**	18.5	8.8	47.6
Substance 6 (higher concentration)	**0.035***	7.81	0.91	1.73	0.045	7.81	1.73	22.1

Notes: *Growth rate constant is not statistically significant (*p* >0.05) from zero.

Table 2.19 Summary of depuration kinetics obtained in bioconcentration tests with zebrafish – alternative method

Data set	$k_{2\text{-growth-corrected}}$ (day^{-1})	R^2	S.E.	% S.E.	*p*
Substance 1	0.013	0.61	0.002	16.1	1.7×10^{-6}
Substance 2 (lower concentration)	13.1	0.83	2.4	18.5	1.7×10^{-3}
Substance 2 (higher concentration)	9.92	0.70	2.64	26.6	9.4×10^{-3}
Substance 3 (lower concentration)	3.66	0.77	0.70	19.2	8.2×10^{-4}
Substance 3 (higher concentration)	2.67	0.70	0.53	19.9	3.9×10^{-4}
Substance 4 (lower concentration)	0.68	0.30	0.52	77.0	**0.26**
Substance 4 (higher concentration)	0.96	0.19	0.80	83.6	**0.28**
Substance 6 (lower concentration)	26.0	0.87	10.1	38.7	**0.23**
Substance 6 (higher concentration)	7.26	0.92	1.54	21.4	0.042

2.2.4 Discussion

Table 2.20 provides a side-by-side comparison of the growth-corrected depuration rate constants obtained by the rate constant subtraction method and the alternative method.

Table 2.20 Comparison of growth-corrected depuration rate constants obtained

Substance	$k_{2\text{-growth-corrected}}$ (day^{-1})	
	Rate constant subtraction method	**Alternative method**
Hexachlorobenzene	0.026	0.031
	0.011	0.012
	0.030	0.032
	0.027	0.030
	0.023	0.024
	0.015[a]	0.015[a]
	0.017	0.024
	0.010	0.010[a]
	0.014	0.018
	0.022	0.025
Musk xylene	0.068	0.074
	0.048	0.049
	0.636	0.667
	0.106	0.109
	0.097	0.099
	0.078	0.078
	0.028	0.035
	0.039	0.039
	0.054	0.059
	0.056	0.058
o-Terphenyl	0.097	0.102
	0.066	0.067
	0.034	0.035
	0.257	0.260
	0.317	0.305
	0.263	0.248
	0.041	0.047
	0.060	0.060
	0.051	0.055
	0.052	0.054

Substance	$k_{2\text{-growth-corrected}}$ (day^{-1})	
	Rate constant subtraction method	**Alternative method**
Methoxychlor	0.096	0.182
	0.063	0.065
	-0.006[a]	-0.005[a]
	0.277	0.289
	0.261	0.249
	0.231[a]	0.212[a]
	0.044	0.051[a]
	0.058	0.056
	0.114	0.114
	0.098	0.101
Benzo(a)pyrene	1.647	1.568
	1.132	1.179
	2.056	2.029
	0.950	0.964
	2.076	2.112
$C_{13}H_{23}Cl_5$	0.125	0.125
	0.083[a]	0.091
$C_{13}H_{22}Cl_6$	0.097	0.097
	0.047	0.050
$C_{13}H_{21}Cl_7$	0.072	0.072
	0.053	0.053
Substance 1	0.013	0.013
Substance 2	13.8	13.1
	10.7	9.92
Substance 3	3.79	3.66
	3.02	2.67
Substance 4	0.55[a]	0.68[a]
	1.04[a]	0.92[a]
Substance 6	18.5[a]	26.0[a]
	7.81	7.26
Substance A	0.152	0.153
	0.064	0.064
Substance B	0.125	0.125
	0.079	0.079
Substance C	0.171	0.169

Substance	$k_{2\text{-growth-corrected}}$ (day^{-1})	
	Rate constant subtraction method	Alternative method
	0.097	0.097
Substance D	0.098	0.098
	0.043	0.043
Substance E	0.152	0.152
	0.057	0.057

Notes: Slope of ln [C_{fish}] or ln [A_{fish}] against time plot is not significantly different from zero.

Figure 2.1 shows a plot of the $k_{2\text{-growth-corrected}}$ obtained using the alternative method against the $k_{2\text{-growth-corrected}}$ obtained using the rate constant subtraction method (this plot does not include the values where the $k_{2\text{-growth-corrected}}$ obtained was not significantly different from zero). The plot gives a straight line with slope of 0.94 and an intercept of 0.01. The intercept is statistically significantly different from zero (p = 0.045).

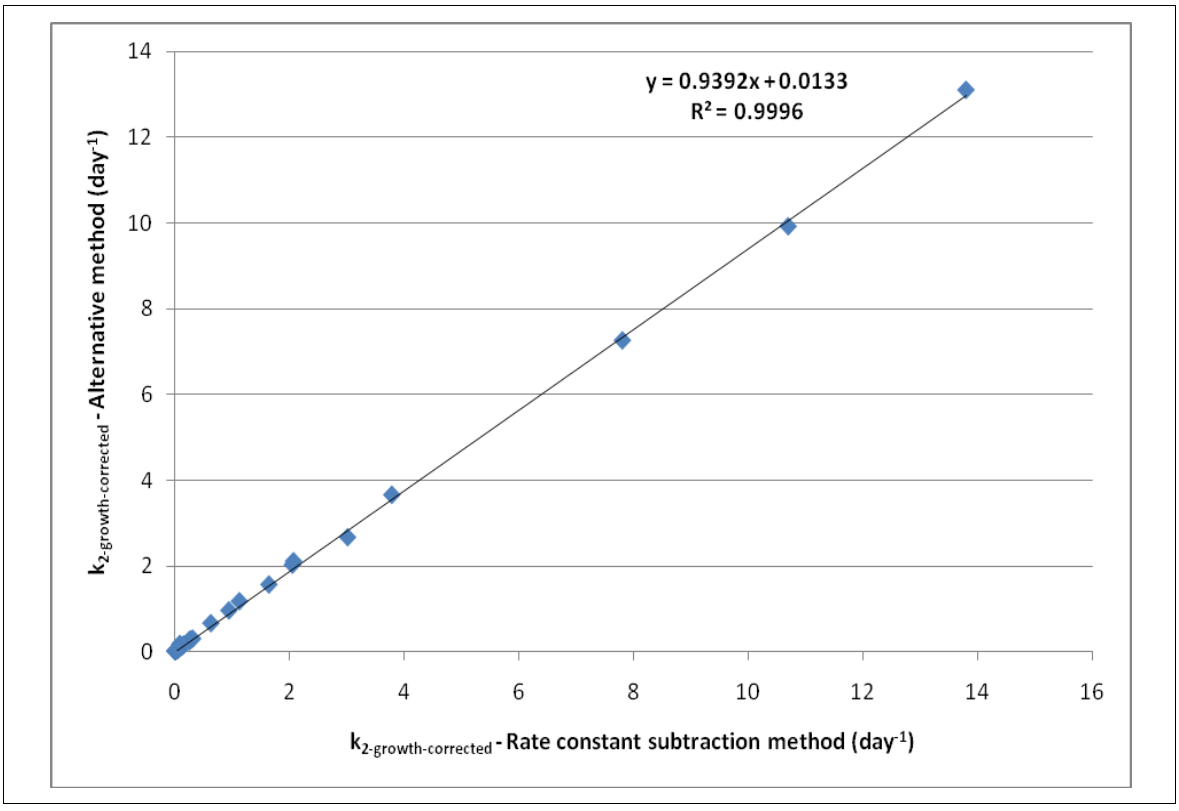

Figure 2.1 Relationship between $k_{2\text{-growth-corrected}}$ values obtained using the two methods

Overall the agreement in the growth-corrected rate constants obtained using the two different approaches is good.

However, the alternative method does appear to show a tendency to estimate a slightly higher value for the rate constant than the rate constant subtraction method in some cases. This tendency can be seen in the mean values for the growth-corrected depuration rate constants generated from the OECD 305 ring test data[5] in

[5] It is also consistent with the small positive intercept seen in Figure 2.1.

Table 2.2 to 2.11, where the mean value obtained using the alternative method is higher than the mean value obtained using the rate constant subtraction method for hexachlorobenzene (mean values 0.022 and 0.020 day^{-1} respectively), musk xylene (mean values 0.127 and 0.121 day^{-1} respectively) and methoxychlor (mean values 0.131 and 0.124 day^{-1} respectively), but not for *o*-terphenyl (mean values 0.123 and 0.124 day^{-1} respectively) or benzo(a)pyrene (mean values 1.570 and 1.572 respectively).

This difference in mean values is statistically significant only for hexachlorobenzene.[6] The reason for this is not entirely clear but could possibly be related to the assumption that growth dilution is a first-order kinetic process. If the kinetics for growth dilution differ from first order then the simple subtraction of the growth rate constant from the overall depuration rate constant may not be appropriate or may represent an approximation.[7] But because growth is effectively factored out of the alternative method before the kinetic analysis is carried out, any deviations from first-order kinetics for growth dilution would not be so important for this method. If this is the case, any difference between the two methods would be expected to be most prevalent for the substances where growth dilution is most important, that is, those where the overall depuration is dominated by growth (which is the case with hexachlorobenzene).

The available analysis also shows that, in many cases, the statistics associated with the regressions are slightly better for the rate constant subtraction method than the alternative method. However, most of the regressions obtained using the alternative method are still statistically significant. The extra uncertainty introduced by the use of the alternative method is, in any case, likely to be much lower than inter- and intra-laboratory variability (as can be seen from Tables 2.2 to 2.11).

It is also important to note that the rate constant subtraction method and the alternative method are both dependent on the fish weight. Therefore any variability introduced by fish weights (either resulting from a wide range of fish sizes at the start of the study or variable growth rates/fish size during the study) will result in increased uncertainty in both methods.

Overall, the analysis shows that the alternative method for obtaining the growth-corrected rate constant is a viable and appropriate method that can provide useful information in cases where the more normal rate constant subtraction method is difficult to apply, or where there are uncertainties over whether growth dilution is following first -order kinetics.

[6] Tested using the two-tail *t*-test for paired two sample means with alpha = 0.05.

[7] Simple subtraction of the rate constants is only strictly valid if both the overall depuration and the growth dilution are both first-order processes in relation to the concentration in fish.

3. Use of depuration rate constant as a measure of bioaccumulation potential

3.1 Background

Many regulatory regimes (for example REACH[1] in the EU) use the BCF as the primary measure of bioaccumulation potential. The proposed OECD 305 feeding study method will result in a dietary BMF rather than a BCF. However, a BCF can be estimated from the depuration rate constant generated in the feeding study provided a value for the rate constant for uptake from water can be estimated for the substance concerned.

A previous report (Crookes and Brooke 2011) investigated various methods that could be used for estimating such an uptake rate constant. However, BCFs obtained in such a way will always be uncertain owing to the need to use an estimate for the uptake rate constant. Such uncertainty may be acceptable in many applications, for example, where it is necessary to determine whether a substance has a high or low bioaccumulation potential in general terms.

However, such uncertainty may be more important when considering the BCF value against precise criteria, such as the current REACH Annex XIII numerical criteria for bioaccumulation. These criteria are used in the identification of persistent, bioaccumulative and toxic (PBT) substances and very persistent and very bioaccumulative (vPvB) substances. The Annex XIII criteria can be summarised as follows:

- A substance fulfils the bioaccumulative criterion (B) when the BCF is higher than 2,000 l/kg.
- A substance fulfils the very bioaccumulative criterion (vB) when the BCF is higher than 5,000 l/kg.

A possible alternative approach to estimating a BCF from the data generated in a feeding study that could be considered in a PBT or vPvB assessment would be to use the depuration rate constant obtained from the study directly as a measure of the bioaccumulation potential. Clearly such an approach would not lead directly to a BCF that could be compared with the Annex XIII criteria but, if such an approach could be 'calibrated' using substances with known BCF values (from studies with similar test organisms), it could potentially be used to identify substances with a bioaccumulation potential that is equivalent to that of having a BCF >2,000 l/kg or >5,000 l/kg. This section considers such a calibration exercise.

There is some logic in an approach based on the depuration rate constant (or depuration half-life) rather than BCF alone, as one of the concerns with PBT or vPvB substances is not necessarily related to a high BCF alone but rather to the fact that accumulation could take a long time to reverse. The depuration rate constant would provide a direct measure of the time taken for the substance to be eliminated from the organism once exposure had ceased and so would be consistent with this concept.

In reality, the depuration rate constant for a given chemical is likely to vary depending on factors such as the fish species and fish size. For example different species of fish may have different metabolic capacities, leading to different elimination kinetics

(although this would be expected to also lead to differences in the BCF between species). Size of the fish may also be important. For example, Sijm et al. (1995) derived the following allometric relationship for hydrophobic organic chemicals relating the uptake rate constant from water into fish to the fish weight.

Equation 17 $$k_1 = 520 \times W^{-0.32}$$

where k_1 = first-order rate constant for uptake into fish (l kg^{-1} day^{-1})

W = fish weight (g).

Equation 17 predicts that the uptake rate constant will decrease as the size of the fish increases. This was explained by Sijm et al. (1995) in terms of uptake occurring via the gills by passive diffusion and the fact that small fish generally have higher ventilation rates and/or larger gill area to body weight ratios relative to larger fish.

Given that elimination of the substance can also occur via the gills (for example, respiration), it is also likely that the depuration rate constant will be dependent on the size of the fish in the same way and so some dependence of the depuration rate constant on the fish weight would be expected (for example, the growth-corrected depuration rate constants obtained for the substances considered in Section 2.2.2 were higher for the smaller fish (1–2 g) than the larger fish (300 g)). However, in this case, elimination via respiration is one of several processes; for example, elimination by faecal elimination and metabolism can also occur. In addition, the metabolic capacity of the fish may also vary with fish age (and hence weight) and dependence on fish weight may be different than for respiration. Therefore the actual dependence of the depuration rate constant on fish weight is difficult to predict and may vary from substance to substance.

Most laboratory bioaccumulation studies are carried out using relatively small fish of a similar size (for example, the OECD 305 Test Guideline specifies the appropriate size of the fish to be tested) and so within this constraint any differences resulting from the use of different size fish would be expected to be relatively small. For example, for the substances considered in Section 2.2.2, the growth-corrected rate constant was lower by a factor of only 2–3 for the 300 g fish than the 1–2 g fish.[8]

3.2 Analysis of depuration rate constant data

Three sets of bioconcentration data were made available for the previous study by Crookes and Brooke (2011). The same data sets were used here to investigate possible relationships between the depuration rate constant and the fish BCF value. The data are summarised in Appendix B.

The first data set was kindly provided by Jon Arnot of Trent University, Canada. This data set contained 169 data points for which both a BCF and a k_2 value were available. The data set was collated for use in validation of bioaccumulation models by Trent University. This data set is referred to as the Arnot data set in Appendix B. In total the data set covered 108 substances. The fish species included in the data set were:

- bluegill sunfish (*Lepomis macrochirus*);
- carp (*Cyprinus carpio*);
- channel catfish (*Ictalurus punctatus*);

[8] The depuration rate constant may also depend on the lipid contents of the fish, and this may be different for fish of different sizes.

- fathead minnow (*Pimephales promelas*);
- flagfish (*Jordanella floridae*);
- goldfish (*Carassius auratus*);
- guppy (*Poecilia reticulata*);
- medaka (*Oryzias latipes*);
- rainbow trout (*Oncorhychus mykiss*);
- sheepshead minnow (*Cyprinodon variegatus*);
- striped mullet (*Mugil cephalus*);
- threespine stickleback (*Gasterosteus aculeatus*)
- willow shiner (*Gnathopogon caerulescens*)
- zebrafish (*Brachydanio rerio*).

The range of fish weights reported in the data sets was from approximately 0.01 g to 700 g, with the majority of values in the 0.1 to 18 g range.[9]

The second data set was data on BCF and k_2 values for pesticides kindly provided by Caren Rauert of the Umweltbundesamt (UBA) in Germany. Many of the details of these studies are confidential but the data have been accepted for regulatory purposes and so are valid for use in this study. This data set is referred to as the UBA data set in Appendix B. The data set contained 18 data points for nine substances. The fish species included in the data set were:

- bluegill sunfish (*Lepomis macrochirus*);
- fathead minnow (*Pimephales promelas*);
- rainbow trout (*Oncorhychus mykiss*);
- zebrafish (*Brachydanio rerio*).

The range of fish weights reported in the data set was from 0.2 to 7 g.

The final data set considered is the EURAS Gold Standard database.[10] As many of the data in the Arnot data set also appeared in the Gold Standard database, the duplicate data were omitted here. This resulted in a further 23 data points. This data set is referred to as the Gold Standard data set in Appendix B. The data set contained 18 substances. The fish species included in the data set were:

- guppy (*Poecilia reticulata*);
- mosquito fish (*Gambusia affinis*);
- sheepshead minnow (*Cyprinodon variegatus*).

The range of fish weights reported in the data set was from 0.19 to 2.5 g.

The three data sets are discussed further in Crookes and Brooke (2011). It should be noted that these data sets report the depuration rate constant without indicating whether the value has been growth corrected. For the analysis here it is assumed that the rate constants reported refer to the overall depuration rate constant (k_2) rather than

[9] The 5th percentile value was 0.09 and the 95th percentile value was 18 g.
[10] See: http://ambit.sourceforge.net/euras/.

growth-corrected depuration rate constants ($k_{2\text{-growth-corrected}}$) as growth correction was generally not routinely carried out until recently.

The following sections effectively utilise the Arnot data set as a training set in order to determine any relationships between the BCF value and the k_2 value. The UBA and EURAS data sets are used as validation data sets to test the relationships derived.

3.2.1 Relationship between BCF and k_2 value

The relationship between the k_2 value and the BCF was initially investigated using the Arnot data set alone.

Figure 3.1 shows a plot of log BCF versus log k_2 (in units of day^{-1}). The two horizontal lines on the plot represent BCFs of 2,000 and 5,000 l kg^{-1}. Fitting a straight line to the data by linear regression yields the following equation:

Equation 18 $$\log[BCF] = -1.2529 \times \log[k_2] + 2.3841$$

$$R^2 = 0.77$$

Using this equation, a BCF of 2,000 l kg^{-1} would correspond to a k_2 value of 0.185 day^{-1} and a BCF of 5,000 l kg^{-1} would correspond to a k_2 value of 0.089 day^{-1}. These k_2 values correspond to overall depuration half-lives of 3.7 and 7.8 days respectively.

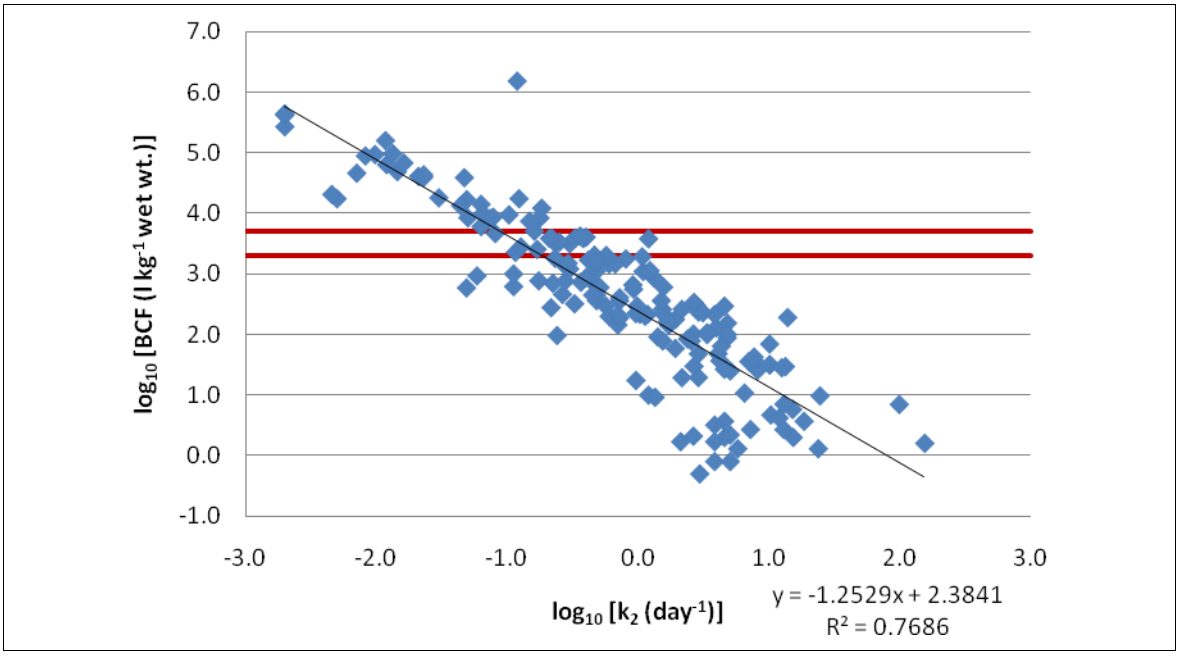

Figure 3.1 Plot of log BCF versus log k_2 for the Arnot data set

The data point for the obvious outlier in Figure 3.1 corresponds to octachlorodibenzo-*p*-dioxin (OCDD), which has a reported BCF of 1.53×10^6 l kg^{-1} (log BCF of 6.18) and a reported k_2 value of 0.119 day^{-1} (log k_2 of -0.92). Omitting this data point from the regression gives the following equation:

Equation 19 $$\log[BCF] = -1.2394 \times \log[k_2] + 2.3706$$

$$R^2 = 0.78$$

Using this equation, a BCF of 2,000 l kg^{-1} would correspond to a k_2 value of 0.178 day^{-1} and a BCF of 5,000 l kg^{-1} would correspond to a k_2 value of 0.085 day^{-1}. These k_2 values correspond to overall depuration half-lives of 3.9 and 8.2 days respectively.

The 95 per cent confidence interval around the slope and intercept of Equation 19 is -1.3396 to -1.1393 for the slope and 2.2748 to 2.4663 for the intercept. Using the lower and upper 95 per cent confidence limits to estimate the limits around the k_2 values that correspond to a BCF of 2,000 or 5,000 l kg^{-1} gives the values shown in Table 3.1.

Table 3.1 Estimated k_2 values for BCF for the Arnot data set

BCF	From regression	Based on lower 95% confidence limit	Based on upper 95% confidence limit
2,000 l kg^{-1}	0.178 day^{-1}	0.171 day^{-1}	0.185 day^{-1}
5,000 l kg^{-1}	0.085 day^{-1}	0.086 day^{-1}	0.083 day^{-1}

3.2.2 Relationship between $BCF_{lipid\ normalised}$ and k_2

To investigate whether some of the uncertainty in the analysis resulted from differences in lipid contents in the fish used in the various tests, the BCF data were normalised to a standard lipid content of 5 per cent by weight (that is, $BCF_{lipid\ normalised} = BCF \times 0.05/f_{lipid}$, where f_{lipid} is the weight fraction of lipid in the fish).

For the Arnot data set, the lipid contents for the fish were reported in the data set. These were either the actual lipid contents reported in the study or were estimated by Arnot. Unfortunately the data set does not appear to distinguish clearly between these two and so the lipid-normalised BCFs can only be considered as approximate.

For the Gold Standard and UBA data sets, the actual lipid contents of the fish were reported in most, but not all, instances (lipid data were missing for one data point from the Gold Standard data set and two data points from the UBA data set). Only the data where the actual lipid contents were available are considered here.

The lipid-normalised data were analysed in the same way as before. First, a plot of $\log_{10}[BCF_{lipid\ normalised}]$ against $\log_{10} k_2$ was constructed (omitting the OCDD data point, which was again an outlier) and the 'best fit' line determined by linear regression (see Figure 3.2). This resulted in the following equation:

Equation 20 $$\log[BCF_{lipid\ normalised}] = -1.1892 \times \log[k_2] + 2.2889$$

$$R^2 = 0.77$$

Using this equation, a $BCF_{lipid\ normalised}$ of 2,000 l kg^{-1} would correspond to a k_2 value of 0.141 day^{-1} and a $BCF_{lipid\ normalised}$ of 5,000 l kg^{-1} would correspond to a k_2 value of 0.065 day^{-1}. These k_2 values correspond to overall depuration half-lives of 4.9 and 10.7 days respectively.

The 95 per cent confidence interval around the slope and intercept of Equation 20 is -1.2879 to -1.0905 for the slope and 2.1945 to 2.3833 for the intercept. Using the lower and upper 95 per cent confidence limits to estimate the limits around the k_2 values that correspond to a $BCF_{lipid\ normalised}$ of 2,000 or 5,000 l kg^{-1} gives the values given in Table 3.2.

Table 3.2 Estimated k_2 values for $BCF_{lipid\ normalised}$ for the Arnot data set

$BCF_{lipid\ normalised}$	From regression	Based on 95% confidence lower limit	Based on 95% confidence upper limit
2,000 l kg^{-1}	0.141 day^{-1}	0.138 day^{-1}	0.144 day^{-1}
5,000 l kg^{-1}	0.065 day^{-1}	0.068 day^{-1}	0.062 day^{-1}

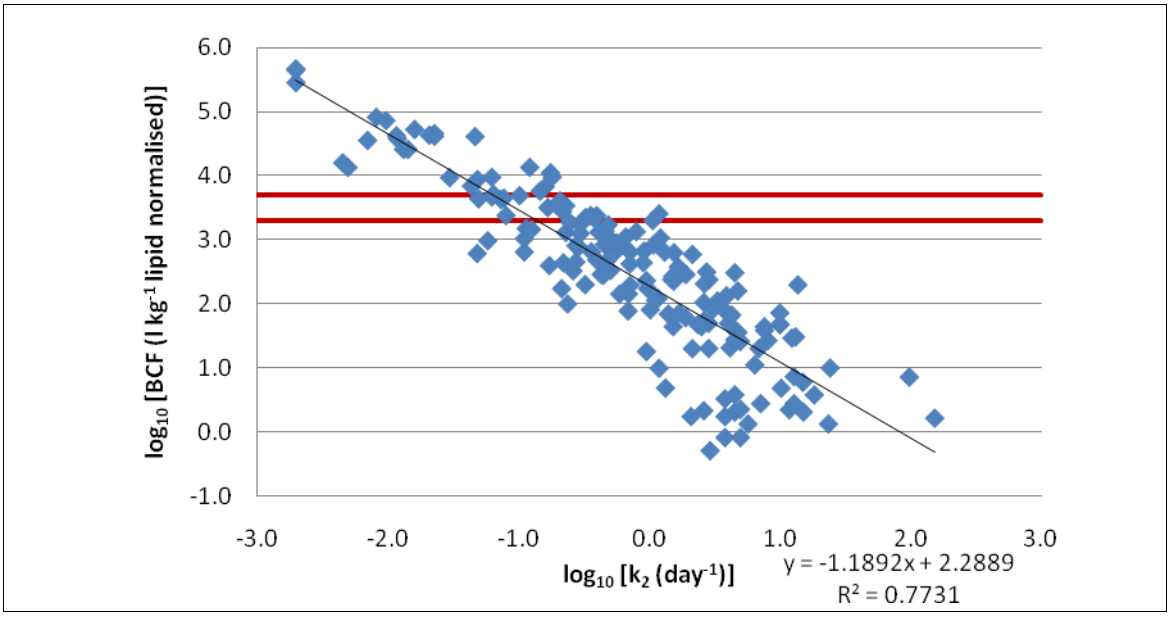

Figure 3.2 Plot of log $BCF_{lipid\ normalised}$ versus log k_2 for the Arnot data set

3.2.3 Relationship between $BCF_{lipid\ normalised}$ and $k_{2\ (lipid\ normalised)}$

As well as lipid normalisation of the BCF, the effect of lipid normalisation of the k_2 on the regression was also investigated. In this case the lipid-normalised k_2 value was determined as $k_{2\ (lipid\ normalised)} = k_2 \times f_{lipid}/0.05$.[11]

The lipid normalised data were analysed in the same way as before. First, a plot of $\log_{10}$ [$BCF_{lipid\ normalised}$] against $\log_{10}$ [$k_{2\ (lipid\ normalised)}$] was constructed (omitting the OCDD data point, which was again an outlier) and the 'best fit' line determined by linear regression (see Figure 3.3). This resulted in the following equation:

Equation 21

$$\log[BCF_{lipid\,normalised}] = -1.2220 \times \log[k_{2\,(lipid\,normalised)}] + 2.3935$$

$$R^2 = 0.76$$

Using this equation, a $BCF_{lipid\ normalised}$ of 2,000 l kg^{-1} would correspond to a k_2 value of 0.181 day^{-1} and a $BCF_{lipid\ normalised}$ of 5,000 l kg^{-1} would correspond to a k_2 value of 0.085 day^{-1}. These k_2 values correspond to overall depuration half-lives of 3.8 and 8.2 days respectively.

The 95 per cent confidence interval around the slope and intercept of Equation 21 is -1.3272 to -1.1169 for the slope and 2.2976 to 2.4894 for the intercept. Using the lower and upper 95 per cent confidence limits to estimate the limits around the k_2 values that correspond to a $BCF_{lipid\ normalised}$ of 2,000 or 5,000 l kg^{-1} gives the values given in Table 3.3.

[11] This is opposite to the way lipid correction is applied to the BCF. The reason for this is that the BCF = k_1/k_2, and there is evidence to suggest that the k_1 may not be dependent on the lipid content of the fish (see Crookes and Brooke 2011). If this is the case then the lipid dependence of the k_2 value should be the inverse of the lipid dependence of the BCF; hence the correction is applied in a different way to that for the BCF.

Table 3.3 Estimated $k_{2(lipid\ normalised)}$ values for $BCF_{lipid\ normalised}$ for the Arnot data set

$BCF_{lipid\ normalised}$	From regression	Based on 95% confidence lower limit	Based on 95% confidence upper limit
2,000 l kg^{-1}	0.181 day^{-1}	0.175 day^{-1}	0.188 day^{-1}
5,000 l kg^{-1}	0.085 day^{-1}	0.088 day^{-1}	0.083 day^{-1}

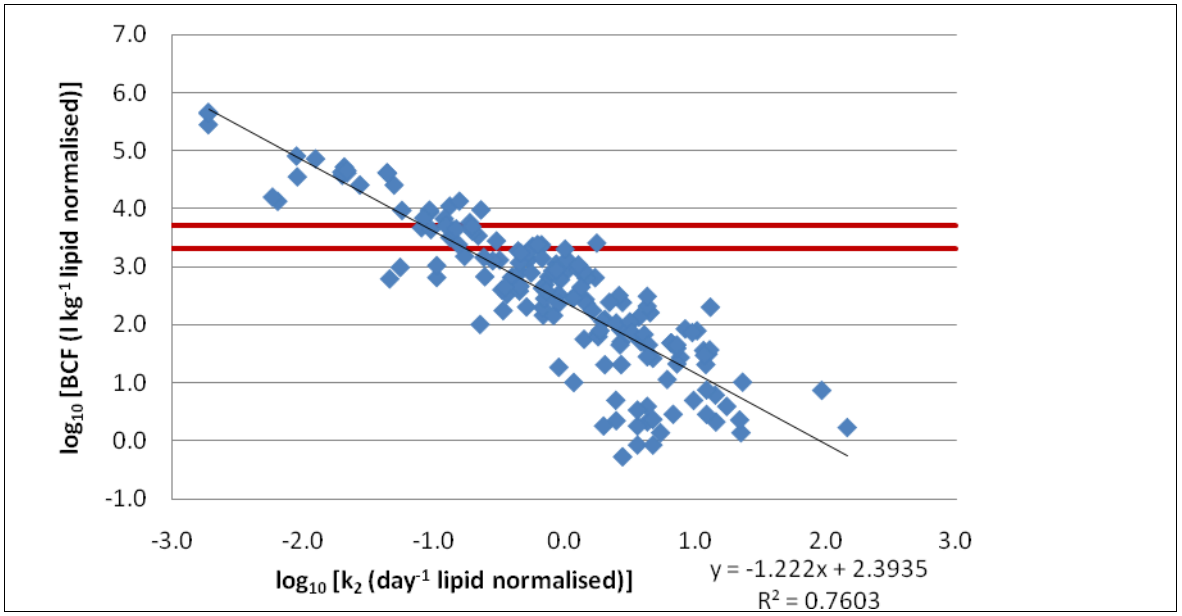

Figure 3.3 Plot of log $BCF_{lipid\ normalised}$ versus log [$k_{2\ (lipid\ normalised)}$] for the Arnot data set

3.2.4 Use of depuration rate constant for identifying potential B and vB substances

To investigate the usefulness of these derived k_2 values in identifying substances with BCFs >2,000 l kg^{-1} or >5,000 l kg^{-1} (as may be required for a PBT or vPvB assessment under REACH), an analysis of the Arnot,[12] UBA and Gold Standard data sets was undertaken to identify the number of substances that would be incorrectly categorised based on the critical k_2 values identified in Sections 3.2.1 to 3.2.3 and summarised in Table 3.4 below.

In this analysis the UBA and Gold Standard data sets are independent validation data sets. However, as the Arnot data set was used as the training set to develop the critical value this is not itself an independent validation set. For this reason, the findings are reported separately for each data set as well as the combined data set.

[12] OCDD was included in the analysis here.

Table 3.4 Summary of critical k_2 values from Sections 3.2.1 to 3.2.3

BCF	Critical value	Summary table of incorrectly categorised substances
BCF ≥2000 l kg^{-1}	$k_2 \leq 0.178$ day^{-1}	Table 3.5
BCF ≥5,000 l kg^{-1}	$k_2 \leq 0.085$ day^{-1}	Table 3.6
$BCF_{lipid\ normalised}$ ≥2,000 l kg^{-1}	$k_2 \leq 0.141$ day^{-1}	Table 3.7
$BCF_{lipid\ normalised}$ ≥5,000 l kg^{-1}	$k_2 \leq 0.065$ day^{-1}	Table 3.8
$BCF_{lipid\ normalised}$ ≥2,000 l kg^{-1}	$k_{2\ (lipid\ normalised)} \leq 0.181$ day^{-1}	Table 3.9
$BCF_{lipid\ normalised}$ ≥5,000 l kg^{-1}	$k_{2\ (lipid\ normalised)} \leq 0.085$ day^{-1}	Table 3.10

As discussed above, it is probable that the k_2 value is dependent on the fish species and the weight of fish. These critical k_2 values have been derived using the Arnot data as the training set and so may not be applicable to species and fish weights outside the range included in the training set.

It is important to recognise that, as well as uncertainty in the predictions, there is also uncertainty in the underlying data base of BCF values. This is particularly relevant when considering the number of potential false positives and false negatives in the following analysis as, in some cases, the BCF data may not always be clear cut as to whether the experimental BCF is itself above or below the cut-off values considered.

Using the substances out of the combined data set, substances that would be mis-identified as having a BCF above or below 2,000 l kg^{-1} or above or below 5,000 l kg^{-1} based on the depuration rate constant compared with the experimental BCF are shown in the relevant table out of Tables 3.5 to 3.10.

For the comparison based on the non-lipid-normalised BCF value of 2,000 l kg^{-1} and the critical k_2 of 0.178 day^{-1}, the number of substances in the data sets with experimental BCFs >2,000 is 49 for the Arnot data set, seven for the Gold Standard data set and two for the UBA data set out of a total of 169 (Arnot), 23 (Gold Standard) and 18 (UBA) data points.

The total number of data points that would be wrongly categorised using the critical k_2 value for a BCF of 2,000 l kg^{-1} compared with the experimental BCF is 30 (18 from the Arnot data set, five from the Gold Standard data set and seven from the UBA data set; see Table 3.5). This corresponds to 14 per cent of the total data points. Of these 30 data points, 12 would result in false negatives (that is, based on the k_2 value the BCF would be expected to be <2,000 l kg^{-1} but the experimental BCF is >2,000) and 18 would result in false positives (that is, based on the k_2 value the BCF would be expected to be >2,000 l kg^{-1} but the experimental BCF is <2,000 l kg^{-1}).

For the comparison based on the non-lipid-normalised BCF value of 5,000 l kg^{-1} and the critical k_2 value of 0.085 day^{-1}, the number of substances in the data sets with experimental BCFs >5,000 is 33 for the Arnot data set, two for the Gold Standard data set and zero for the UBA.

The total number of data points that would be wrongly categorised using the critical k_2 value for a BCF of 5,000 l kg^{-1} compared with the experimental BCF is 13 (ten from the Arnot data set, two from the Gold Standard data set and one from the UBA data set; see Table 3.6). This corresponds to 6 per cent of the total data points. Of these 13 data points, nine would result in false negatives (that is, based on the k_2 value the BCF

would be expected to be <5,000 l kg^{-1} but the experimental BCF is >5,000) and four would result in false positives (that is, based on the k_2 value the BCF would be expected to be >5,000 l kg^{-1} but the experimental BCF is <5,000 l kg^{-1}).

For the comparison based on the $BCF_{lipid\ normalised}$ value of 2,000 l kg^{-1} and the critical k_2 of 0.141 day^{-1}, the number of substances in the data sets with experimental $BCF_{lipid\ normalised}$ >2,000 is 44 for the Arnot data set, six for the Gold Standard data set and zero for the UBA data set out of a the total number of data points of 169 (Arnot), 22 (Gold Standard) and 16 (UBA).

The total number of data points that would be wrongly categorised using the critical k_2 value for a $BCF_{lipid\ normalised}$ of 2,000 l kg^{-1} compared with the experimental $BCF_{lipid\ normalised}$ is 29 (20 from the Arnot data set, five from the Gold Standard data set and four from the UBA data set; see Table 3.7). This corresponds to 14 per cent of the total data points. Of these 29 data points, 19 would result in false negatives (that is, based on the k_2 value the $BCF_{lipid\ normalised}$ would be expected to be <2,000 l kg^{-1} but the experimental $BCF_{lipid\ normalised}$ is >2,000) and ten would result in false positives (that is, based on the k_2 value the $BCF_{lipid\ normalised}$ would be expected to be >2,000 l kg^{-1} but the experimental $BCF_{lipid\ normalised}$ is <2,000 l kg^{-1}).

For the comparison based on the $BCF_{lipid\ normalised}$ value of 5,000 l kg^{-1} and the critical k_2 value of 0.065 day^{-1}, the number of substances in the data sets with experimental $BCF_{lipid\ normalised}$ >5,000 is 28 for the Arnot data set, three for the Gold Standard data set and zero for the UBA.

The total number of data points that would be wrongly categorised using the critical k_2 value for a $BCF_{lipid\ normalised}$ of 5,000 l kg^{-1} compared with the experimental $BCF_{lipid\ normalised}$ is 13 (ten from the Arnot data set, three from the Gold Standard data set and zero from the UBA data set; see Table 3.6). This corresponds to 6 per cent of the total data points. Of these 13 data points, nine would result in false negatives (that is, based on the k_2 value the $BCF_{lipid\ normalised}$ would be expected to be <5,000 l kg^{-1} but the experimental $BCF_{lipid\ normalised}$ is >5,000) and four would result in false positives (that is, based on the k_2 value the $BCF_{lipid\ normalised}$ would be expected to be >5,000 l kg^{-1} but the experimental $BCF_{lipid\ normalised}$ is <5,000 l kg^{-1}).

For the comparison based on the $BCF_{lipid\ normalised}$ value of 2,000 l kg^{-1} and the critical $k_{2\ (lipid\ normalised)}$ of 0.181 day^{-1}, the number of substances in the data sets with experimental $BCF_{lipid\ normalised}$ >2,000 is 44 for the Arnot data set, six for the Gold Standard data set and zero for the UBA data set out of a the total number of data points of 169 (Arnot), 22 (Gold Standard) and 16 (UBA).

The total number of data points that would be wrongly categorised using the critical $k_{2\ (lipid\ normalised)}$ value for a $BCF_{lipid\ normalised}$ of 2,000 l kg^{-1} compared with the experimental $BCF_{lipid\ normalised}$ is 27 (18 from the Arnot data set, five from the Gold Standard data set and four from the UBA data set; see Table 3.9). This corresponds to 13 per cent of the total data points. Of these 27 data points, 18 would result in false negatives (that is, based on the $k_{2\ (lipid\ normalised)}$ value the $BCF_{lipid\ normalised}$ would be expected to be <2,000 l kg^{-1} but the experimental $BCF_{lipid\ normalised}$ is >2,000) and nine would result in false positives (that is, based on the $k_{2\ (lipid\ normalised)}$ value the BCF would be expected to be >2,000 l kg^{-1} but the experimental $BCF_{lipid\ normalised}$ is <2,000 l kg^{-1}).

For the comparison based on the $BCF_{lipid\ normalised}$ value of 5,000 l kg^{-1} and the critical $k_{2\ (lipid\ normalised)}$ value of 0.085 day^{-1}, the number of substances in the data sets with experimental $BCF_{lipid\ normalised}$ >5,000 is 28 for the Arnot data set, three for the Gold Standard data set and zero for the UBA data set.

The total number of data points that would be wrongly categorised using the critical $k_{2\ (lipid\ normalised)}$ value for a $BCF_{lipid\ normalised}$ of 5,000 l kg^{-1} compared with the experimental $BCF_{lipid\ normalised}$ is 17 (12 from the Arnot data set, three from the Gold Standard data set

and two from the UBA data set; see Table 3.10). This corresponds to 8 per cent of the total data points. Of these 17 data points, 12 would result in false negatives (that is, based on the $k_{2\ (lipid\ normalised)}$ value the $BCF_{lipid\ normalised}$ would be expected to be <5,000 l kg^{-1} but the experimental $BCF_{lipid\ normalised}$ is >5,000) and five would result in false positives (that is, based on the $k_{2\ (lipid\ normalised)}$ value the $BCF_{lipid\ normalised}$ would be expected to be >5,000 l kg^{-1} but the experimental $BCF_{lipid\ normalised}$ is <5,000 l kg^{-1}).

It is evident from the analysis here that a similar subset of the data base is wrongly categorised in each case. Furthermore, in some cases multiple data points for the same substance appear within each table indicating that the number of substances wrongly categorised is smaller than the number of data points wrongly categorised. Although it is beyond the scope of this project to look in detail into possible reasons for wrong categorisation in each and every case, the following points are evident from the data base used (by substance).

- NL-63A (Ref No. 8). This substance is an aryl alkylfluoroether with a BCF >5,000 l kg^{-1}. Depending on the method used it would be identified as not B or B rather than vB based on the depuration rate constant.
- NL-63B (Ref No.9). This substance is an aryl alkylfluoroether with a BCF >5,000 l kg^{-1}. Depending on the method used it would be identified as not B or B rather than vB based on the depuration rate constant.
- 4,4'-Dibromobiphenyl (Ref No. 200). This substance is a brominated aromatic substance with a BCF >5,000 l kg^{-1}. Generally identified as B rather than vB based on the depuration rate constant.
- Benzene, 1,2,4,5-tetrachloro- (Ref No. 236). This substance is a chlorinated aromatic substance with a BCF of 4,050 l kg^{-1} or a $BCF_{lipid\ normalised}$ of 2,382 l kg^{-1}. Generally identified as not B rather than B based on the depuration rate constant.
- 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester (Ref No. 394, 395, 396, 397). This is a phthalic acid diester with a BCF of 1,000 l kg^{-1} or less. Depending on the method used would be identified as B or vB rather than not B based on the depuration rate constant.
- Benzene, 1,2,4-trichloro- (Ref No.441). This substance is a chlorinated aromatic with a BCF of 2,026 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 888 l kg^{-1}. Generally identified as not B based on the depuration rate constant which is consistent with the $BCF_{lipid\ normalised}$ but not the non-lipid-normalised BCF.
- Phosphorothioic acid, *O*,*O*-dimethyl *O*-(2,4,5-trichlorophenyl) ester (Ref No. 539). This substance is an ester of phosphorothioic acid with a BCF of 3,841 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 2,183 l kg^{-1}. Generally identified as not B rather than B based on the depuration rate constant.
- Octamethylcyclotetrasiloxane (D4) (Ref No. 606). This is a cyclic siloxane compound with a BCF >5,000 l kg^{-1}. Generally identified as not B rather than vB based on the depuration rate constant.
- Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)- (Ref No. 706, 707, 708, 710, 711, 712). This substance is a fluoroalkyl derivative and an aromatic amine. There are seven results for this substance in the Arnot data set with BCF values ranging from 1,819 to 3,880 l kg^{-1} (and $BCF_{lipid\ normalised}$ values between 1,299 and 3,397). The available experimental data are therefore not clear cut as to whether the BCF for this substance is above or below 2,000 l kg^{-1}. Generally identified as not B based on the

depuration rate constant which is consistent with some, but not all, of the experimental BCF data.

- 2,3,7,8-Tetrachlorodibenzo[b,e][1,4] dioxin (Ref No. 730). This is a chlorinated aromatic compound with a BCF >5,000 l kg^{-1}. This substance is correctly identified as vB based on the k_2 value but would be identified as B using the $k_{2\ (lipid\ normalised)}$ value.

- Bromophos (Ref No. 755). This substance is an ester of phosphorothioic acid with a BCF of 3,931 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 2,234 l kg^{-1}. Generally identified as not B rather than B based on the depuration rate constant.

- Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester (Ref No. 793, 794). This substance is an ester of phosphorothioic acid. There are nine entries in the Arnot data set for this substance. The experimental BCF ranges from 451 to 3,363 l kg^{-1} ($BCF_{lipid\ normalised}$ from 333 to 1,868 l kg^{-1}) and so it is not clear cut whether the BCF for this substance is above or below 2,000 l kg^{-1}. Generally identified as not B rather than B based on the depuration rate constant which is consistent with some, but not all, of the available experimental BCF data.

- 1,2,3,4,5,6,7,8-Octachlorodibenzo-*p*-dioxin (Ref No.808). This substance is a chlorinated aromatic substance with a reported BCF >>5,000 l kg^{-1}. The substance appeared to be an outlier on the regression analysis. Depending on the method used, predicted to be B or not B based on the depuration rate constant.

- 2,4,5-Trichloro-1,1'-biphenyl (Ref No. 871). This substance is a chlorinated aromatic substance with a reported BCF of 6,066 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 4,666 l kg^{-1}. The predictions using the depuration rate constant are consistent with the non-lipid-normalised BCF (predicted to be vB based on k_2) but result in a $BCF_{lipid\ normalised}$ of just over 5,000 l kg^{-1} (based on both k_2 and $k_{2\ (lipid\ normalised)}$. In these cases the actual difference between the predicted $BCF_{lipid\ normalised}$ (5,199 and 5,256 l kg^{-1}) based on the depuration rate constant and the experimental $BCF_{lipid\ normalised}$ of 4,666 l kg^{-1} is small in absolute terms.

- 2,4',5-Trichloro-1,1'-biphenyl (Ref No. 876). This substance is a chlorinated aromatic substance with a BCF >5,000 l kg^{-1}. This is predicted to be vB based on the estimates using the k_2 value but is predicted to be B using the estimate based on the $k_{2\ (lipid\ normalised)}$.

- Phosphorothioic acid, *O*-(2,5-dichloro-4-iodophenyl) *O*,*O*-dimethyl ester (Ref No. 883). This substance is an ester of phosphorothioic acid and has a reported BCF of 4,212 l kg^{-1} and $BCF_{lipid\ normalised}$ of 2,393 l kg^{-1}. The predictions using the depuration rate constant are generally not B rather than B.

- 1,2,3,4-Tetrachlorodibenzo-*p*-dioxin (Ref No. 929). This substance is a chlorinated aromatic substance with a BCF of 3,812 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 2,541 l kg^{-1}. The substance is generally predicted to be not B rather than B based on the depuration rate constant.

- 2,4-Dichloro-1-(3-methoxy-4-nitrophenoxy)benzene (Ref No. 932). This substance is a chlorinated aromatic ether with a BCF of 3,877 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 4,039 l kg^{-1}. The predictions based on the depuration rate constant are generally not B rather than B.

- 1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin (Ref No. 945). This substance is a chlorinated aromatic substance with a BCF of 4,643 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 2,393 l kg^{-1}. The predictions for the $BCF_{lipid\ normalised}$ based on the depuration rate constant are in line with B but the prediction of BCF (not lipid normalised) using the k_2 value results in vB rather than B. However in this case the predicted BCF is 5,290 l kg^{-1}, which is close to the experimental BCF.

Table 3.5 Summary of substances that would be incorrectly categorised as having a BCF above or below 2,000 l kg^{-1} based on a k_2 value of 0.178 day^{-1}

Data set	Ref No.	Substance	Experimental data		BCF estimated using Equation 19	Incorrect classification based on k_2 [a]
			BCF (l kg^{-1})	k_2 (day^{-1})		
Arnot	236	Benzene, 1,2,4,5-tetrachloro-	4,050	0.4	731	Not B rather than B
Arnot	394	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	588	0.049	9,909	B or vB rather than not B
Arnot	395	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	620	0.112	3,548	B rather than not B
Arnot	396	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	930	0.059	7,877	B or vB rather than not B
Arnot	397	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	1,000	0.112	3,548	B rather than not B
Arnot	441	Benzene, 1,2,4-trichloro-	2,026	0.57	471	Not B rather than B
Arnot	539	Phosphorothioic acid, *O*,*O*-dimethyl *O*-(2,4,5-trichlorophenyl)ester	3,841	0.38	779	Not B rather than B
Arnot	606	Octamethylcyclotetrasiloxane (D4)	12,169	0.183	1,926	Not B rather than B or vB
Arnot	707	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	2,050	0.463	609	Not B rather than B
Arnot	711	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	3,880	0.219	1,538	Not B rather than B
Arnot	712	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	3,261	0.232	1,436	Not B rather than B
Arnot	755	Bromophos	3,931	0.33	928	Not B rather than B
Arnot	793	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	3,150	0.3	1,044	Not B rather than B

Data set	Ref No.	Substance	Experimental data		BCF estimated using Equation 19	Incorrect classification based on k_2 [a]
			BCF (l kg^{-1})	k_2 (day^{-1})		
Arnot	794	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	3,363	0.25	1,309	Not B rather than B
Arnot	883	Phosphorothioic acid, *O*-(2,5-dichloro-4-iodophenyl) *O*,*O*-dimethyl ester	4,212	0.360	833	Not B rather than B
Arnot	929	1,2,3,4-Tetrachlorodibenzo-*p*-dioxin	3,812	1.2	187	Not B rather than B
Arnot	932	2,4-Dichloro-1-(3-methoxy-4-nitrophenoxy)benzene	3,877	0.21	1,624	Not B rather than B
Arnot	958	1,2,3,4,5,6,7,8-Octachlorodibenzofuran	771	0.174	2,051	B rather than not B
Gold Standard	GS3	2-Methylnaphthalene	2,921	0.62	425	Not B rather than B
Gold Standard	GS4	2-Methylnaphthalene	2,852	0.60	442	Not B rather than B
Gold Standard	GS45	Hexachlorobenzene	3,730	0.49	568	Not B rather than B
Gold Standard	GS5	1,3-Dimethylnaphthalene	4,761	0.35	862	Not B rather than B
Gold Standard	GS6	1,3-Dimethylnaphthalene	3,426	0.47	598	Not B rather than B
UBA	UBA 13	Substance 13	59	0.126	3,071	B rather than not B
UBA	UBA 14	Substance 14	63	0.125	3,092	B rather than not B
UBA	UBA 14	Substance 14	65	0.12	3,258	B rather than not B
UBA	UBA 4	Substance 4	117	0.097	4,217	B rather than not B
UBA	UBA 4	Substance 4	8	0.077	5,593	B or vB rather than not B
UBA	UBA 6	Substance 6	57	0.102	3,960	B rather than not B
UBA	UBA 6	Substance 6	44	0.119	3,292	B rather than not B

Notes: [a] Comparison of the B or vB classification that would be obtained based on the k_2 value with that that would be obtained using the measured BCF value.

Table 3.6 Summary of substances that would be incorrectly categorised as having a BCF above or below 5,000 l kg^{-1} based on a k_2 value of 0.085 day^{-1}

Data set	Ref No.	Substance	Experimental data		BCF estimated using Equation 19	Incorrect classification based on k_2 [a]
			BCF (l kg^{-1})	k_2 (day^{-1})		
Arnot	8	NL-63A	8,400	0.178	1,997	~B rather than vB
Arnot	9	NL-63B	5,080	0.161	2,254	B rather than vB
Arnot	200	4,4'-Dibromobiphenyl	17,495	0.123	3,151	B rather than vB
Arnot	394	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	588	0.049	9,909	vB rather than not B
Arnot	396	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	930	0.059	7,877	vB rather than not B
Arnot	606	Octamethylcyclotetrasiloxane (D4)	12,169	0.183	1,926	Not B rather than vB
Arnot	945	1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin	4,643	0.081	5,290	vB rather than B
Arnot	986	2,4,6-tribromobiphenyl	7,463	0.148	2,508	B rather than vB
Arnot	991	2,3,4,6,7,8-Hexachlorodibenzofuran	9,479	0.103	3,927	B rather than vB
Arnot	*808*	*1,2,3,4,5,6,7,8-Octachlorodibenzo-p-dioxin*[b]	*1,529,000*	*0.119*	*3,284*	B rather than vB
Gold Standard	GS7	2-Isopropylnaphthalene	12,405	0.09	4,642	B rather than vB
Gold Standard	GS8	2-Isopropylnaphthalene	13,420	0.16	2,275	B rather than vB
UBA	UBA 4	Substance 4	8	0.077	5,593	vB rather than not B

Notes: Comparison of the B or vB classification that would be obtained based on the k_2 value with that that would be obtained using the measured BCF value.

[b] The substance was omitted from the regression as it appeared to be an outlier.

Table 3.7 Summary of substances that would be incorrectly categorised as having a $BCF_{lipid\ normalised}$ above or below 2,000 l kg^{-1} based on a k_2 value of 0.141 day^{-1}

Data set	Ref No.	Substance	Experimental data		$BCF_{lipid\ normalised}$ estimated using Equation 20	Incorrect classification based on k_2 [a]
			$BCF_{lipid\ normalised}$ (l kg^{-1})	k_2 (day^{-1})		
Arnot	8	NL-63A	11,053	0.178	1,517	Not B rather than B or vB
Arnot	9	NL-63B	6,684	0.161	1,704	Not B rather than B or vB
Arnot	236	Benzene, 1,2,4,5-tetrachloro-	2,382	0.4	578	Not B rather than B
Arnot	394	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	613	0.049	7,055	B or vB rather than not B
Arnot	395	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	646	0.112	2,633	B rather than not B
Arnot	396	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	969	0.059	5,661	B or vB rather than not B
Arnot	397	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	1,042	0.112	2,633	B rather than not B
Arnot	539	Phosphorothioic acid, O,O-Dimethyl O-(2,4,5-trichlorophenyl)ester	2,183	0.38	615	Not B rather than B
Arnot	606	Octamethylcyclotetrasiloxane (D4)	9,507	0.183	1,466	Not B rather than B or vB
Arnot	706	Benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-	2,000	1.073	179	Not B rather than B
Arnot	708	Benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-	1,500	0.116	2,533	B rather than not B
Arnot	710	Benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-	3,185	0.169	1,613	Not B rather than B
Arnot	711	Benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-	2,771	0.219	1,181	Not B rather than B

Data set	Ref No.	Substance	Experimental data		$BCF_{lipid\ normalised}$ estimated using Equation 20	Incorrect classification based on k_2 [a]
			$BCF_{lipid\ normalised}$ (l kg^{-1})	k_2 (day^{-1})		
Arnot	712	Benzenamine, 2,6-dinitro-N,N-dipropyl-4-(trifluoromethyl)-	3,397	0.232	1,105	Not B rather than B
Arnot	755	Bromophos	2,234	0.33	727	Not B rather than B
Arnot	883	Phosphorothioic acid, O-(2,5-dichloro-4-iodophenyl) O,O-dimethyl ester	2,393	0.36	655	Not B rather than B
Arnot	929	1,2,3,4-Tetrachlorodibenzo-p-dioxin	2,541	1.2	157	Not B rather than B
Arnot	932	2,4-Dichloro-1-(3-methoxy-4-nitrophenoxy)benzene	4,039	0.21	1,244	Not B rather than B
Arnot	986	2,4,6-tribromobiphenyl	5,741	0.148	1,888	Not B rather than B or vB
Arnot	995	1,2,3,4,6,7,8-Heptachlorodibenzofuran	1,442	0.127	2,263	B rather than not B
Gold Standard	GS43	1,2,3,5-Tetrachlorobenzene	2,129	0.48	466	Not B rather than B
Gold Standard	GS44	1,2,4-Tribromobenzene	2,903	0.58	372	Not B rather than B
Gold Standard	GS45	Hexachlorobenzene	6,016	0.49	454	Not B rather than B or vB
Gold Standard	GS5	1,3-Dimethylnaphthalene	2,454	0.35	678	Not B rather than B
Gold Standard	GS8	2-Isopropylnaphthalene	6,918	0.16	1,719	Not B rather than B or vB
UBA	UBA 14	Substance 14	98	0.125	2,308	B rather than not B
UBA	UBA 14	Substance 14	101	0.12	2,427	B rather than not B
UBA	UBA 6	Substance 6	45	0.102	2,926	B rather than not B
UBA	UBA 6	Substance 6	35	0.119	2,451	B rather than not B

Notes: [a] Comparison of the B or vB classification that would be obtained based on the k_2 value with that that would be obtained using the measured BCF value.

Table 3.8 Summary of substances that would be incorrectly categorised as having a $BCF_{lipid\ normalised}$ above or below 5,000 l kg^{-1} based on a k_2 value of 0.065 day^{-1}

Data set	Ref No.	Substance	Experimental data		$BCF_{lipid\ normalised}$ estimated using Equation 20	Incorrect classification based on k_2 [a]
			$BCF_{lipid\ normalised}$ (l kg^{-1})	k_2 (day^{-1})		
Arnot	8	NL-63A	11,053	0.178	1,517	Not B rather than vB
Arnot	9	NL-63B	6,684	0.161	1,704	Not B rather than vB
Arnot	200	4,4'-Dibromobiphenyl	13,458	0.123	2,350	B rather than vB
Arnot	394	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	613	0.049	7,055	vB rather than not B
Arnot	396	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	969	0.059	5,661	vB rather than not B
Arnot	606	Octamethylcyclotetrasiloxane (D4)	9,507	0.183	1,466	Not B rather than vB
Arnot	871	2,4,5-Trichloro-1,1'-biphenyl	4,666	0.063	5,199	vB rather than B (but marginal)
Arnot	985	1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin	4,355	0.05	6,856	vB rather than B
Arnot	986	2,4,6-tribromobiphenyl	5,741	0.148	1,888	Not B rather than vB
Arnot	*808*	*1,2,3,4,5,6,7,8-Octachlorodibenzo-p-dioxin*[b]	*788,144*	*0.119*	2,445	*B rather than vB*
Gold Standard	GS45	Hexachlorobenzene	6,016	0.49	454	Not B rather than vB
Gold Standard	GS7	2-Isopropylnaphthalene	6,394	0.09	3,408	B rather than vB
Gold Standard	GS8	2-Isopropylnaphthalene	6,918	0.16	1,719	Not B rather than vB

Notes: [a] Comparison of the B or vB classification that would be obtained based on the k_2 value with that that would be obtained using the measured BCF value.

b The substance was omitted from the regression as it appeared to be an outlier.

Table 3.9 Summary of substances that would be incorrectly categorised as having a $BCF_{lipid\ normalised}$ above or below 2,000 l kg^{-1} based on a $k_{2\ (lipid\ normalised)}$ value of 0.181 day^{-1}

Data set	Ref No.	Substance	Experimental data		$BCF_{lipid\ normalised}$ estimated using Equation 21	Incorrect classification based on k_2 [a]
			$BCF_{lipid\ normalised}$ (l kg^{-1})	$k_{2\ (lipid\ normalised)}$ (day^{-1})		
Arnot	236	Benzene, 1,2,4,5-tetrachloro-	2,382	0.68	396	Not B rather than B
Arnot	394	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	613	0.047	10,418	B or vB rather than not B
Arnot	395	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	646	0.107	3,784	B rather than not B
Arnot	396	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	969	0.056	8,308	B or vB rather than not B
Arnot	397	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	1,042	0.107	3,784	B rather than not B
Arnot	539	Phosphorothioic acid, *O*,*O*-dimethyl *O*-(2,4,5-trichlorophenyl)ester	2,183	0.669	405	Not B rather than B
Arnot	606	Octamethylcyclotetrasiloxane (D4)	9,507	0.234	1,458	Not B rather than B or vB
Arnot	706	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	2,000	1.03	239	Not B rather than B
Arnot	708	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	1,500	0.176	2,074	B rather than not B
Arnot	711	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	2,771	0.307	1,047	Not B rather than B
Arnot	712	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	3,397	0.223	1,551	Not B rather than B
Arnot	755	Bromophos	2,234	0.581	481	Not B rather than B
Arnot	883	Phosphorothioic acid, *O*-(2,5-	2,393	0.634	432	Not B rather than B

Data set	Ref No.	Substance	Experimental data		$BCF_{lipid\ normalised}$ estimated using Equation 21	Incorrect classification based on k_2 [a]
			$BCF_{lipid\ normalised}$ ($l\ kg^{-1}$)	$k_{2\ (lipid\ normalised)}$ (day^{-1})		
		dichloro-4-iodophenyl) *O*,*O*-dimethyl ester				
Arnot	929	1,2,3,4-Tetrachlorodibenzo-*p*-dioxin	2,541	1.8	121	Not B rather than B
Arnot	932	2,4-Dichloro-1-(3-methoxy-4-nitrophenoxy)benzene	4,039	0.202	1,752	Not B rather than B
Arnot	986	2,4,6-Tribromobiphenyl	5,741	0.192	1,856	Not B rather than B or vB
Arnot	991	2,3,4,6,7,8-Hexachlorodibenzofuran	4,886	0.20	1,771	Not B rather than B
Arnot	*808*	*1,2,3,4,5,6,7,8-Octachlorodibenzo-p-dioxin* [b]	*788,144*	*0.231*	*1,484*	*Not B rather than B or vB*
Gold Standard	GS43	1,2,3,5-Tetrachlorobenzene	2,129	0.298	1,088	Not B rather than B
Gold Standard	GS44	1,2,4-Tribromobenzene	2,903	0.36	864	Not B rather than B
Gold Standard	GS45	Hexachlorobenzene	6,016	0.304	1,061	Not B rather than B or vB
Gold Standard	GS5	1,3-Dimethylnaphthalene	2,454	0.679	397	Not B rather than B
Gold Standard	GS8	2-Isopropylnaphthalene	6,918	0.31	1,034	Not B rather than B
UBA	UBA 14	Substance 14	98	0.081	5,362	B or vB rather than not B
UBA	UBA 14	Substance 14	101	0.077	5,646	B or vB rather than not B
UBA	UBA 6	Substance 6	45	0.129	3,031	B rather than not B
UBA	UBA 6	Substance 6	35	0.149	2,526	B rather than not B

Notes: [a] Comparison of the B or vB classification that would be obtained based on the k_2 value with that that would be obtained using the measured BCF value.

[b] The substance was omitted from the regression as it appeared to be an outlier.

Table 3.10 Summary of substances that would be incorrectly categorised as having a $BCF_{lipid\ normalised}$ above or below 5,000 l kg^{-1} based on a $k_{2\ (lipid\ normalised)}$ of 0.085 day^{-1}

Data set	Ref No.	Substance	Experimental data		$BCF_{lipid\ normalised}$ estimated using Equation 21	Incorrect classification based on k_2 [a]
			$BCF_{lipid\ normalised}$ (l kg^{-1})	$k_{2\ (lipid\ normalised)}$ (day^{-1})		
Arnot	8	NL-63A	11,053	0.135	2,857	B rather than vB
Arnot	9	NL-63B	6,684	0.123	3,219	B rather than vB
Arnot	200	4,4'-Dibromobiphenyl	13,458	0.16	2,324	B rather than vB
Arnot	394	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	613	0.047	10,418	vB rather than not B
Arnot	396	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	969	0.056	8,308	vB rather than not B
Arnot	606	Octamethylcyclotetrasiloxane (D4)	9,507	0.234	1,458	Not B rather than vB
Arnot	730	2,3,7,8-Tetrachlorodibenzo[b,e][1,4] dioxin	8,689	0.095	4,389	B rather than vB
Arnot	871	2,4,5-Trichloro-1,1'-biphenyl	4,666	0.082	5,256	vB rather than B (but marginal)
Arnot	876	2,4',5-Trichloro-1,1'-biphenyl	9,418	0.095	4,421	B rather than vB
Arnot	959	1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin	5,116	0.126	3,108	B rather than vB
Arnot	986	2,4,6-Tribromobiphenyl	5,741	0.192	1,856	Not B rather than vB
Arnot	*808*	*1,2,3,4,5,6,7,8-Octachlorodibenzo-p-dioxin* [b]	*788,144*	*0.231*	*1,484*	*Not B rather than vB*
Gold Standard	GS45	Hexachlorobenzene	6,016	0.304	1,061	Not B rather than vB
Gold Standard	GS7	2-Isopropylnaphthalene	6,394	0.175	2,088	B rather than vB
Gold Standard	GS8	2-Isopropylnaphthalene	6,918	0.31	1,034	Not B rather than vB

Data set	Ref No.	Substance	Experimental data		$BCF_{lipid\ normalised}$ estimated using Equation 21	Incorrect classification based on k_2[a]
			$BCF_{lipid\ normalised}$ ($l\ kg^{-1}$)	$k_{2\ (lipid\ normalised)}$ (day^{-1})		
UBA	UBA 14	Substance 14	98	0.081	5,362	vB rather than not B
UBA	UBA 14	Substance 14	101	0.077	5,646	vB rather than not B

Notes: [a] Comparison of the B or vB classification that would be obtained based on the k_2 value with that that would be obtained using the measured BCF value.

[b] The substance was omitted from the regression as it appeared to be an outlier.

- 1,2,3,4,5,6,7,8-Octachlorodibenzofuran (Ref No. 958). This substance is a chlorinated aromatic substance with a BCF of 771 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 397 l kg^{-1}. The predictions for the $BCF_{lipid\ normalised}$ based on the depuration rate constant are in line with B but the prediction of BCF (not lipid normalised) using the k_2 value results in B (predicted BCF 2,051 l kg^{-1}) rather than not B.

- 1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin (Ref No. 959). This substance is a chlorinated aromatic substance with a BCF >5,000 l kg^{-1}. The substance is correctly predicted to be vB using the k_2 value (for both the normalised and non-lipid-normalised BCF) but is predicted to be B using the $k_{2\ (lipid\ normalised)}$ value.

- 1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin (Ref No. 985). This substance is a chlorinated aromatic substance with a BCF of 8,448 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 4,355 l kg^{-1}. The predictions for the $BCF_{lipid\ normalised}$ based on the k_2 result in vB (predicted $BCF_{lipid\ normalised}$ 6,856 l kg^{-1}) rather than B but the other predictions are in line with the experimental data.

- 2,4,6-Tribromobiphenyl (Ref No. 986). This is a brominated aromatic substance with a BCF >5,000 l kg^{-1}. The substance is generally predicted to be not B or B rather than vB based on the depuration rate constant depending on the method used.

- 2,3,4,6,7,8-Hexachlorodibenzofuran (Ref No. 991). This substance is a chlorinated aromatic substance with a BCF of 9,479 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 4,886 l kg^{-1}. The prediction for $BCF_{lipid\ normalised}$ using k_2 is in agreement with the measured data (predicted to be B). However, the prediction of non-lipid normalised BCF from k_2 results in B rather than vB and the prediction of the $BCF_{lipid\ normalised}$ from the $k_{2\ (lipid\ normalised)}$ results in not B rather than B.

- 1,2,3,4,6,7,8-Heptachlorodibenzofuran (Ref No. 995). This substance is a chlorinated aromatic substance with a BCF of 2,798 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 1,442 l kg^{-1}. The predictions all lead to not B, which is consistent with the experimental $BCF_{lipid\ normalised}$ but not the non-lipid-normalised BCF.

- 2-Methylnaphthalene (Ref No. GS3, GS4). This substance is an alkyl naphthalene derivative with a measured BCF of 2,852-2,921 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 1,470-1,506 l kg^{-1}. The predictions based on the depuration rate constant generally result in not B rather than B, which is consistent with the experimental $BCF_{lipid\ normalised}$ but not the non-lipid-normalised BCF.

- 1,2,3,5-Tetrachlorobenzene (Ref No. GS43). This substance is a chlorinated aromatic with a measured BCF of 1,320 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 2,129 l kg^{-1}. The predictions based on the depuration rate constant all result in not B, which is consistent with the experimental non-lipid-normalised BCF but not the lipid-normalised BCF.

- 1,2,4-Tribromobenzene (Ref No. GS44). This substance is a brominated aromatic with a measured BCF of 1,800 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 2,903 l kg^{-1}. The predictions based on the depuration rate constant all result in not B, which is consistent with the experimental non-lipid normalised BCF but not the lipid-normalised BCF.

- Hexachlorobenzene (Ref No. GS45). This substance is a chlorinated aromatic with a measured BCF of 3,730 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 6,016

l kg^{-1}. The predictions based on the depuration rate constant all result in not B. The k_2 value reported in the Gold Standard data set for this substance is 0.49 day^{-1}. As seen from the hexachlorobenzene results in Section 2, the observed depuration of hexachlorobenzene can be dominated by growth dilution and the available information from the OECD ring test suggests a growth-corrected depuration rate constant and overall depuration rate constant much lower than the value given in the Gold Standard data set. For example the mean k_2 value from the OECD ring test was 0.052 day^{-1} and the mean value of $k_{2\text{-growth-corrected}}$ was 0.020 or 0.022 (see Table 2.2 and Table 2.3). Based on the k_2 value of 0.052 day^{-1} a BCF of 9,162 l kg^{-1} would be predicted.

- 1,3-Dimethylnaphthalene (Ref No. GS5, GS6). This substance is an alkyl naphthalene derivative with a measured BCF of 3,426-4,761 l kg^{-1} and a $BCF_{lipid\ normalised}$ of 1,766-2,454 l kg^{-1}. The predictions based on the depuration rate constant generally result in not B, which is consistent with one of the experimental $BCF_{lipid\ normalised}$ values but not the remaining three values.
- 2-Isopropylnaphthalene (Ref No. GS7, GS8). This substance is an alkyl naphthalene derivative with a measured BCF >5,000 l kg^{-1}. The predictions based on the depuration rate constant generally result in B or not B rather than vB.
- Substance 13 (Ref No. UBA13). This substance is confidential.
- Substance 14 (Ref No. UBA14). This substance is confidential.
- Substance 4 (Ref No. UBA4). This substance is confidential.
- Substance 6 (Ref No. UBA6). This substance is confidential.

Based on this analysis, the substances whose bioaccumulation potential is incorrectly predicted using the approach based on the depuration rate constant can be tentatively assigned to the following groups.

- Esters. The reason for this may be related to complications in the depuration kinetics resulting from metabolism. For example it is known that 1,2-benzenedicarboxylic acid, bis(2-ethylhexyl) ester undergoes extensive metabolism (ECB 2008).
- Substances where the experimental BCF data themselves are not clear cut (for example several of the chlorinated aromatic substances in the data sets). This may be a function of the inherent variability in experimental BCF data where some of the data are above a given criteria value and some are below. Expert judgement would normally be applied in such cases to decide whether the substance meets the B or vB criteria or not.
- Other miscellaneous substances where no clear pattern is yet evident.

It should be noted that the k_2 values and BCF values used for this analysis have not been growth corrected. There are currently insufficient data available to carry out a similar analysis using growth-corrected data. The effect of growth correction would be to reduce the k_2 value reported and to increase the BCF value reported, although the extent of this would be dependent on the size of the growth rate constant compared with the size of depuration rate constant. This may be more important for substances with depuration rate constants around the critical value for vB rather than B.

One possible way to use this approach with growth-corrected data would be first to use the overall k_2 value to obtain an estimate of the non growth-corrected BCF using Equation 19 and then to estimate the growth-corrected BCF from this value using the ratio of the overall k_2 value to the growth-corrected k_2 value. This is illustrated in the following equation:

$$BCF_{growth\text{-}corrected} = \frac{BCF \times k_2}{k_{2-growth-corrected}}$$

Equation 22

where $BCF_{growth\text{-}corrected}$ = growth-corrected BCF value (l kg^{-1}). This can subsequently be lipid normalised if required.

BCF = BCF value, not growth corrected (l kg^{-1})

k_2 = overall depuration rate constant (day^{-1})

$k_{2\text{-}growth\text{-}corrected}$ = growth-corrected depuration rate constant.

It is also important to consider that the available experimental BCF data will themselves contain variability (as can be seen from some of the substances in the data set used) and, in some cases, conflicting data may be obtained. The approach based on the depuration rate constant therefore should be seen within the context of this variability and uncertainty.

3.2.5 Comparison with other methods for predicting a BCF value from the results of a dietary study

The relationship between BCF and k_2 given in Equation 19 allows a BCF value to be estimated from the data generated in a dietary accumulation study with fish. A previous investigation (Crookes and Brooke 2011) looked at other methods that could be used for predicting a BCF value from a dietary study. This previous study focused on methods for predicting an uptake rate constant (k_1) that could be combined with the k_2 or $k_{2\text{-}growth\text{-}corrected}$ value obtained from a dietary test to estimate the kinetic BCF or growth-corrected BCF.

The methods identified by Crookes and Brooke (2011) have been applied to the full results from the OECD 305 ring test[13] and will be published in the ring test validation report (OECD 2011). The fish species used by the laboratories was rainbow trout (*Oncorhynchus mykiss*), except for Lab 2 which used both rainbow trout and carp (*Cyrpinus carpio*). The methods used for the estimates of k_1 are listed in Table 3.11.

Table 3.11 References for methods used for estimates of k_1

Method	Reference
Method 1	Sijm et al. (1995)
Method 2	Omega/Hendriks et al. (2001)
Method 6	QEAFDCHN/Thomann (1989)
Method 7	BASS/Barber (2001)

[13] Some of these data are included in Section 2.2.1. However, the OECD (2011) uses a different numbering system for the laboratories and so Study A here does not necessarily correspond to Lab 1 in the OECD report.

Method	Reference
Method 8	FGETS/Barber et al. (1991)
Method 9	Erickson and McKim (1990a)
Method 10	Erickson and McKim (1990b)
Method 13	Hayton and Barron (1990)
Method 15	Streit and Siré (1993)
Method 17	Barber (2003 observed)
Method 18	Barber (2003 calibrated)
Method 21	Spacie and Hamelink (1982)
Method 22	Tolls and Sijm (1995)

Notes: See Crookes and Brooke (2011) for further details; method numbering used here is consistent with that report.

The results of these estimates, using the fish weight and depuration data from the ring test, are summarised in Table 3.12. Table 3.13 shows the BCF values that are estimated from the OECD ring test data set using Equation 19. The data for the OECD ring test were again taken from the OECD analysis of the full data sets (OECD 2011).[13] The data for Lab 5 from the OECD report have been omitted (see OECD 2011 for further details).

Visual comparisons of the estimated BCFs obtained using each method are given in Figures 3.4 to 3.8, which show that the BCF estimates obtained using Equation 19 are comparable with those obtained using the methods in Crookes and Brooke (2011).

A comparison of the BCFs predicted using the methods outlined in Crookes and Brooke (2011) with the experimental BCFs in OECD (2011) found that the predictions obtained from the ring test data are reasonably consistent with the available experimental data. The same experimental data are included here to compare with the predicted BCFs using Equation 19.

The available experimental data for hexachlorobenzene in rainbow trout (*Oncorhynchus mykiss*) were in the range 5,370–20,000 l kg^{-1}. The mean predicted BCF using Equation 19 is 9,354 l kg^{-1}, which is consistent with this range. For carp (*Cyprinus carpio*), the experimental BCF values are in the range 19,000–30,000 l kg^{-1}. The mean predicted BCF using Equation 19 is somewhat lower than this range at 8,643 l kg^{-1}.

For musk xylene, the experimental BCF values are in the range 3,230–6,610 l/kg for carp. The mean predicted BCF using Equation 19 is similar at 3,060 l kg^{-1}. No experimental data are available for rainbow trout.

For *o*-terphenyl, the experimental BCF values are in the range 1,000–5,000 l/kg, again with carp. The mean predicted BCF value using mean predicted BCF using Equation 19 is 1,002 l kg^{-1}.

No experimental data with rainbow trout or carp were located for methoxychlor or benzo[a]pyrene and so it is not possible to carry out a comparison of the experimental data with the predicted data for these substances.

Overall the predictions obtained from the ring test data using Equation 19 are reasonably consistent with the available experimental data.

Table 3.12 Summary of BCF values estimated from the OECD 305 ring test depuration data using the methods outlined in Crookes and Brooke (2011) (taken from OECD (2011))

Method for predicting k_1	Estimated BCF (l kg^{-1}; not growth corrected or lipid normalised) [a]									
	Hexachlorobenzene		Musk xylene		*o*-Terphenyl		Methoxychlor		Benzo[a]pyrene	
	Trout [b]	Carp [c]	Trout [b]	Carp [c]	Trout [b]	Carp [c]	Trout [b]	Carp [c]	Trout [b]	Carp [c]
Method 1	8,749 ± 1,218	5,549 ± 619	5,239 ± 1,139	2,401 ± 293	4,970 ± 1,108	975 ± 98	3,610 ± 1,088	1,051 ± 87	343 ± 157	No data
Method 2	6,902 ± 703	4,792 ± 534	3,781 ± 719	1,898 ± 232	3,885 ± 787	834 ± 84	2,699 ± 774	860 ± 71	271 ± 117	No data
Method 6	13,841 ± 1,410	9,610 ± 1,071	8,279 ± 1,575	4,157 ± 507	7,868 ± 1,595	1,689 ± 170	5,713 ± 1,639	1,820 ± 151	538 ± 233	No data
Method 7	12,466 ± 898	9,675 ± 1,079	7,444 ± 1,224	4,185 ± 511	7,092 ± 1,344	1,701 ± 172	5,144 ± 1,403	1,833 ± 152	479 ± 191	No data
Method 8	12,127 ± 913	9,171 ± 1,022	7,245 ± 1,225	3,967 ± 484	6,898 ± 1,317	1,612 ± 163	5,005 ± 1,379	1,737 ± 144	467 ± 190	No data
Method 9	12,119 ± 870	9,453 ± 1,054	7,237 ± 1,184	4,089 ± 499	6,895 ± 1,306	1,662 ± 168	5,001 ± 1,362	1,791 ± 148	465 ± 185	No data
Method 10	9,947 ± 910	7,102 ± 792	5,948 ± 1,086	3,072 ± 375	5,656 ± 1,119	1,248 ± 126	4,106 ± 1,161	1,345 ± 111	385 ± 164	No data
Method 13	8,919 ± 706	6,629 ± 739	5,330 ± 921	2,868 ± 350	5,073 ± 976	1,165 ± 118	3,681 ± 1,022	1,256 ± 104	344 ± 142	No data
Method 15	7,347 ± 528	5,724 ± 638	4,387 ± 719	2,476 ± 302	4,180 ± 792	1,006 ± 102	3,032 ± 826	1,084 ± 90	282 ± 112	No data
Method 17	7,875 ± 626	5,846 ± 652	4,706 ± 815	2,529 ± 309	4,479 ± 863	1,027 ± 104	3,250 ± 903	1,107 ± 92	304 ± 125	No data

Method for predicting k_1	Estimated BCF (l kg^{-1}; not growth corrected or lipid normalised) [a]									
	Hexachlorobenzene		Musk xylene		*o*-Terphenyl		Methoxychlor		Benzo[a]pyrene	
	Trout [b]	Carp [c]	Trout [b]	Carp [c]	Trout [b]	Carp [c]	Trout [b]	Carp [c]	Trout [b]	Carp [c]
Method 18	10,953 ± 2,065	6,166 ± 687	6,560 ± 1,671	2,665 ± 325	6,215 ± 1,583	1,084 ± 109	4,513 ± 1,453	1,167 ± 97	434 ± 211	No data
Method 21	12,960 ± 1,915	12,174 ± 1,357	5,822 ± 1,031	3,976 ± 485	6,877 ± 1,565	1,993 ± 201	4,282 ± 1,170	1,851 ± 153	558 ± 185	No data
Method 22	15,183 ± 2,244	14,262 ± 1,590	7,154 ± 1,267	4,886 ± 596	8,155 ± 1,856	2,363 ± 238	5,207 ± 1,422	2,251 ± 186	639 ± 211	No data

Notes: [a] Values reported as mean ±standard deviation of the estimates for all laboratories for each method. The estimates are based on the fish weight at the start of the uptake phase omitting the results for rainbow trout for one laboratory (see OECD 2011) for further explanation).

[b] Estimates for the rainbow trout (*Oncorhynchus mykiss*) data.

[c] Estimates for the carp (*Cyprinus carpio*) data.

Table 3.13 Summary of the BCF estimates obtained using Equation 19 for the full OECD 305 ring test data set

Laboratory	Species	k_2 (l kg^{-1} day^{-1}) (overall depuration rate constant from ring test)					Estimated BCF (l kg^{-1}) (not growth corrected or lipid normalised)[a]				
		HCB [a]	MX [a]	oTP [a]	MC [a]	BaP	HCB [a]	MX [a]	oTP [a]	MC	BaP
Lab 1	Rainbow trout	0.0502	0.0904	0.0872	0.15	0.986	9,571	4,617	4,828	2,465	239
Lab 2	Rainbow trout	0.0399	0.0734	0.0691	0.116	2.094	12,722	5,977	6,441	3,389	94
Lab 2	Carp	0.0603	0.14	0.29	0.31	[b]	7,626	2,685	1,089	1,002	[b]
Lab 2	Carp	0.0561	0.131	0.351	0.294	[b]	8,339	2,915	859	1,070	[b]
Lab 2	Carp	0.0486	0.111	0.297	0.264	[b]	9,963	3,580	1,057	1,223	[b]
Lab 3	Rainbow trout	0.0537	0.083	0.104	0.102	[b]	8,804	5,132	3,881	3,975	[b]
Lab 4	Rainbow trout	0.0517	0.067	0.077	0.0922	[b]	9,228	6,692	5,632	4,505	[b]
Lab 6	Rainbow trout	0.0625	0.105	0.133	0.225	1.684	7,294	3,835	2,861	1,491	123
Lab 7	Rainbow trout	0.0491	0.105	0.0775	0.148	[b]	9,837	3,835	5,587	2,506	[b]
Lab 8	Rainbow trout	0.0579	0.0948	0.113	0.11	1.179	8,019	4,353	3,501	3,620	191
Mean value	Rainbow trout						9,354	4,920	4,676	3,136	162
SD	Rainbow trout						1,730	1,086	1,303	1,035	66
Mean value	Carp						8,643	3,060	1,002	1,099	
SD	Carp						1,198	465	124	113	

Notes: [a] Estimated using Equation 19.

[b] No estimate possible.

HCB = hexachlorobenzene; MX = musk xylene; oTP = *o*-Terphenyl; MC = methoxychlor; BaP = benzo[a]pyrene

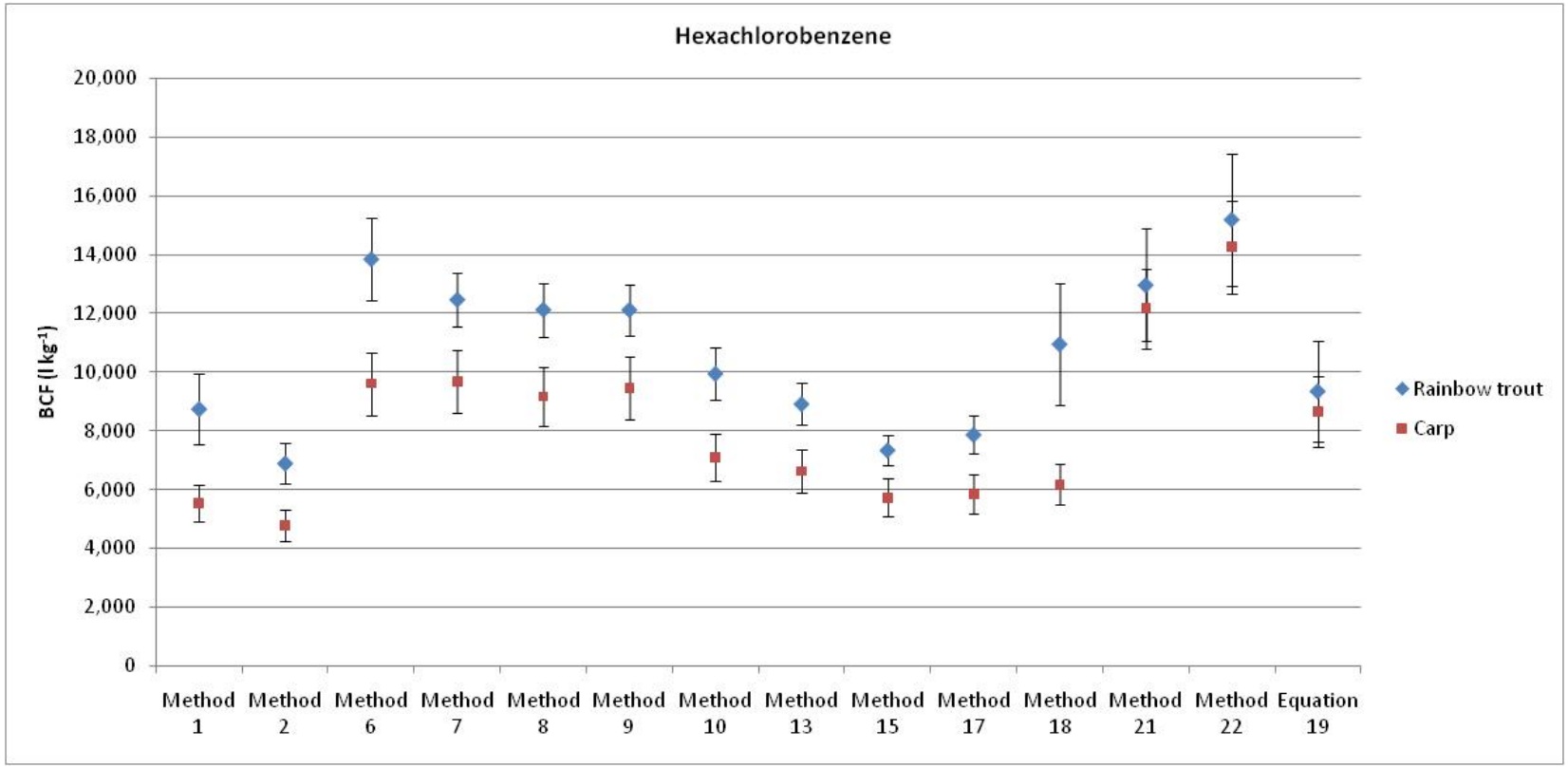

Figure 3.4 Plot showing mean predicted BCF for hexachlorobenzene for the OECD 305 ring test data set using the various methods for calculation (error bars represent the standard deviation)

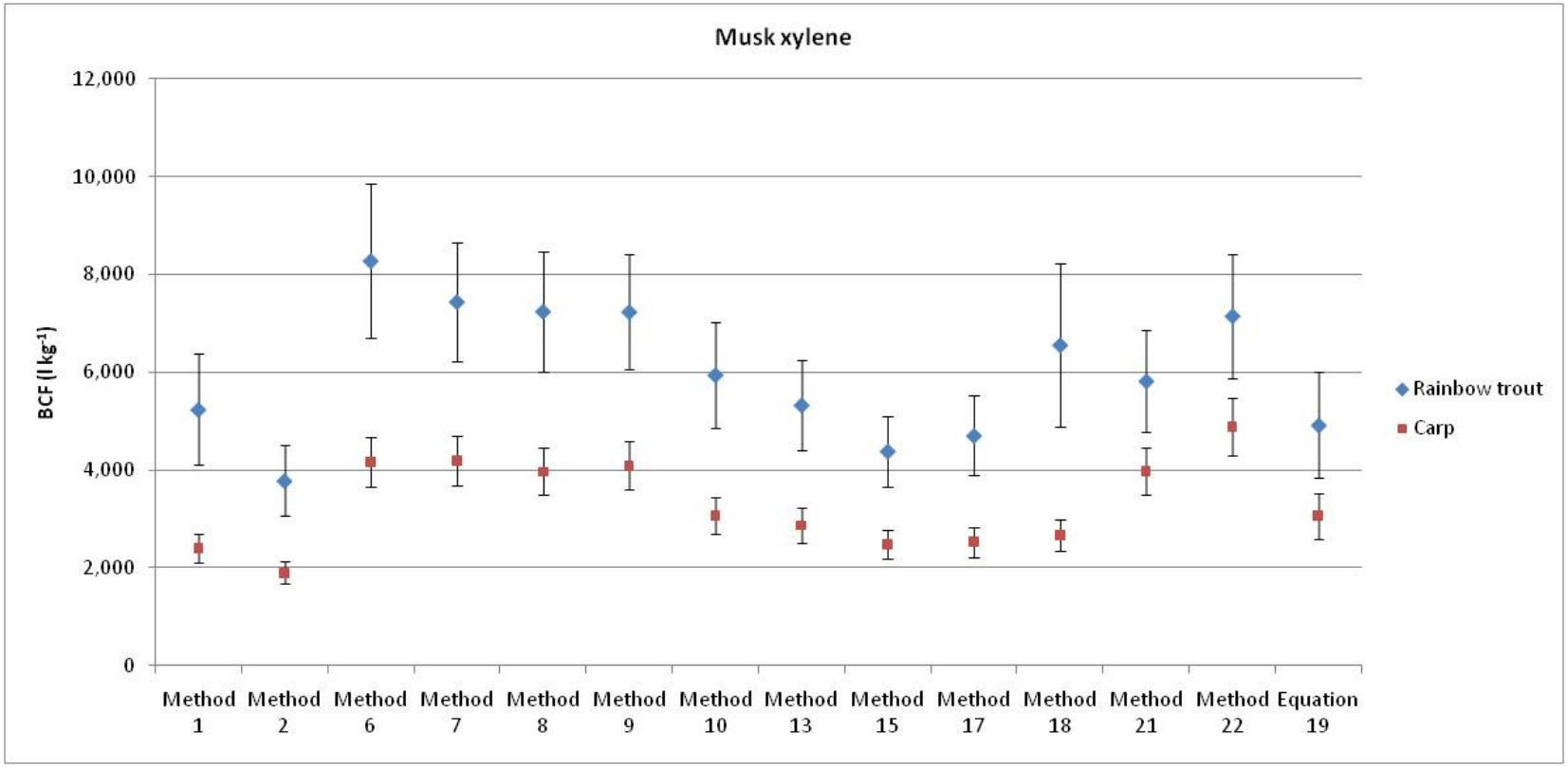

Figure 3.5 Plot showing mean predicted BCF for musk xylene for the OECD 305 ring test data set using the various methods for calculation (error bars represent the standard deviation)

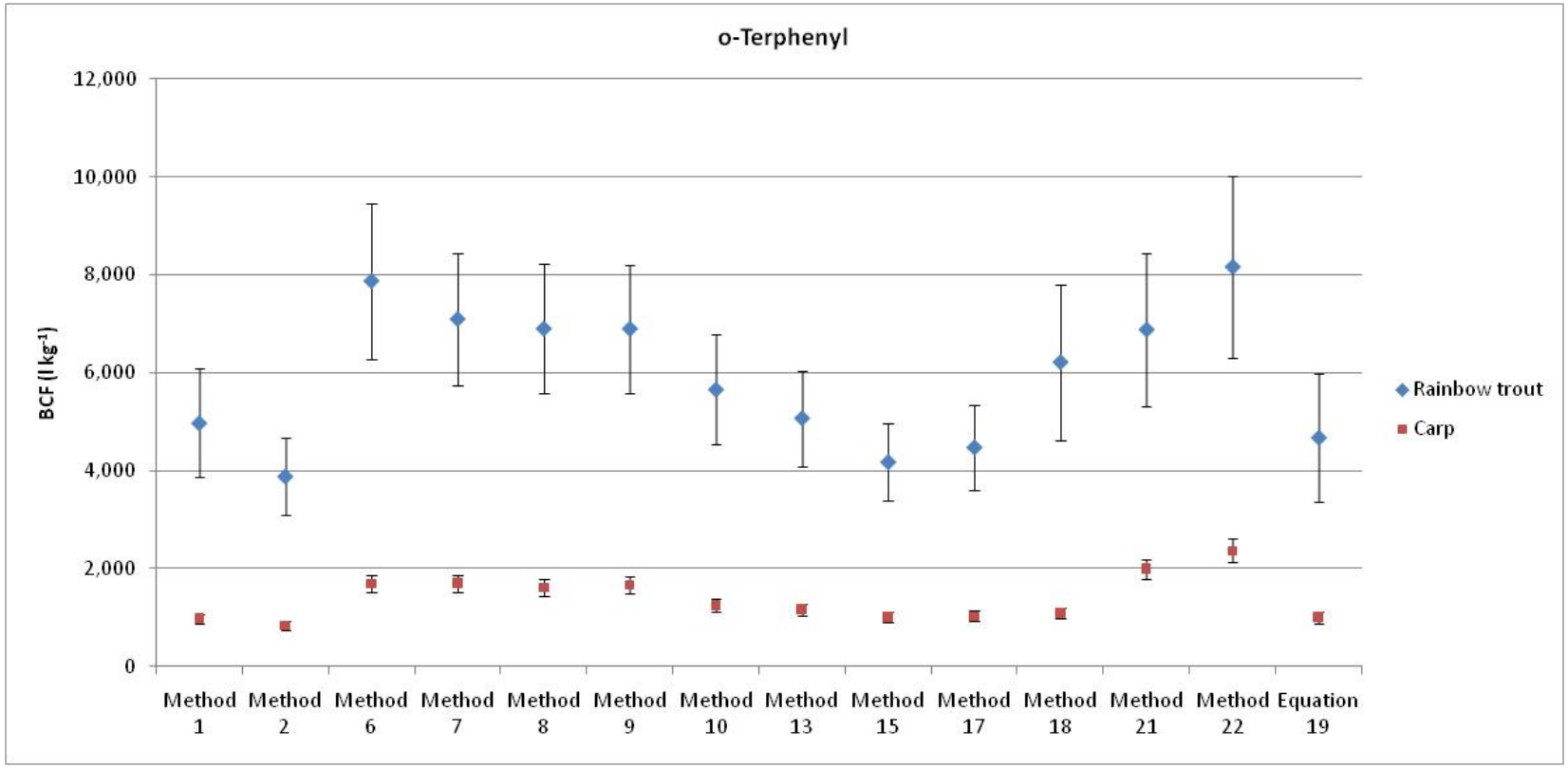

Figure 3.6 Plot showing mean predicted BCF for *o*-terphenyl for the OECD 305 ring test data set using the various methods for calculation (error bars represent the standard deviation)

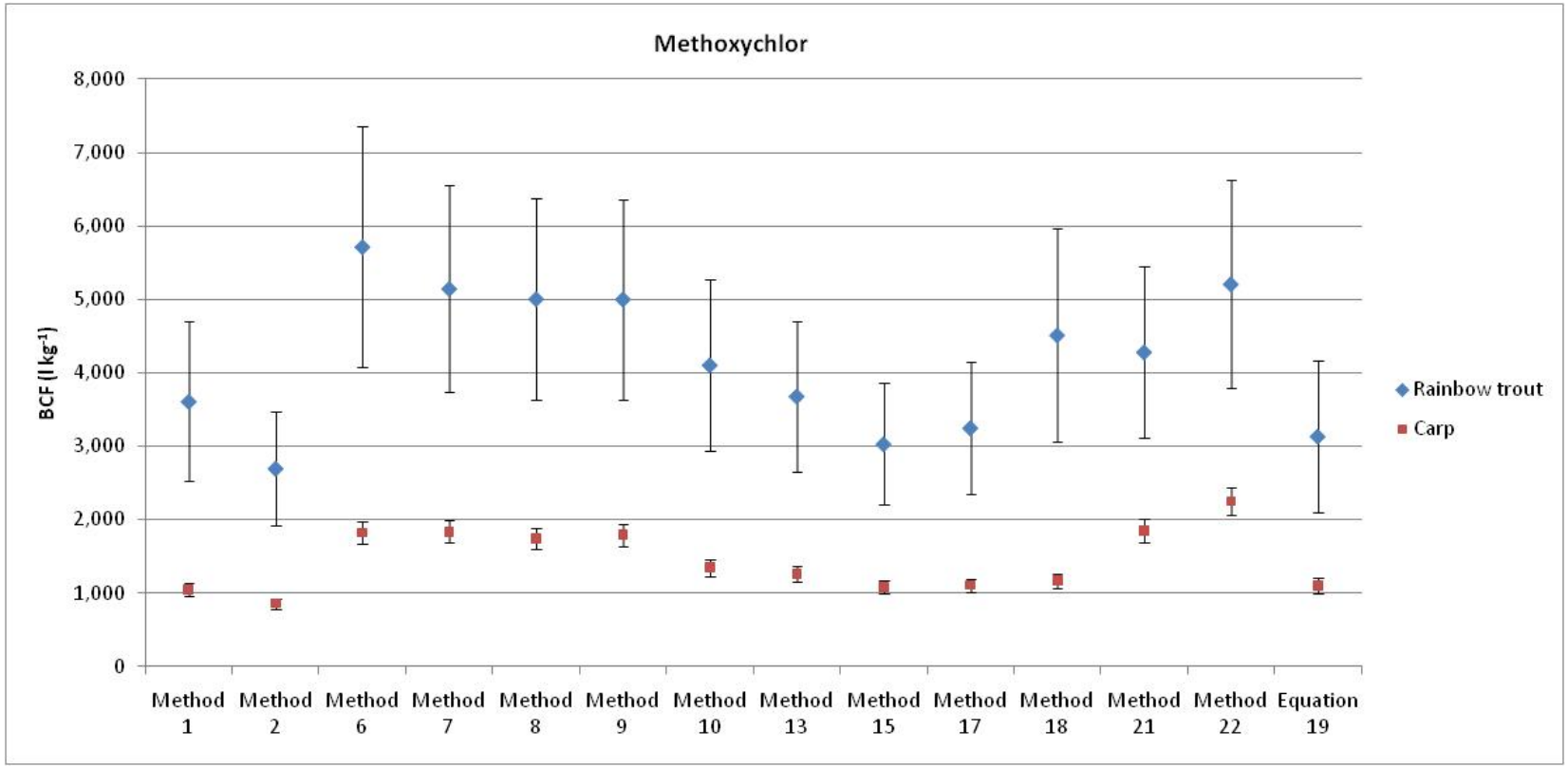

Figure 3.7 Plot showing mean predicted BCF for methoxychlor for the OECD 305 ring test data set using the various methods for calculation (error bars represent the standard deviation)

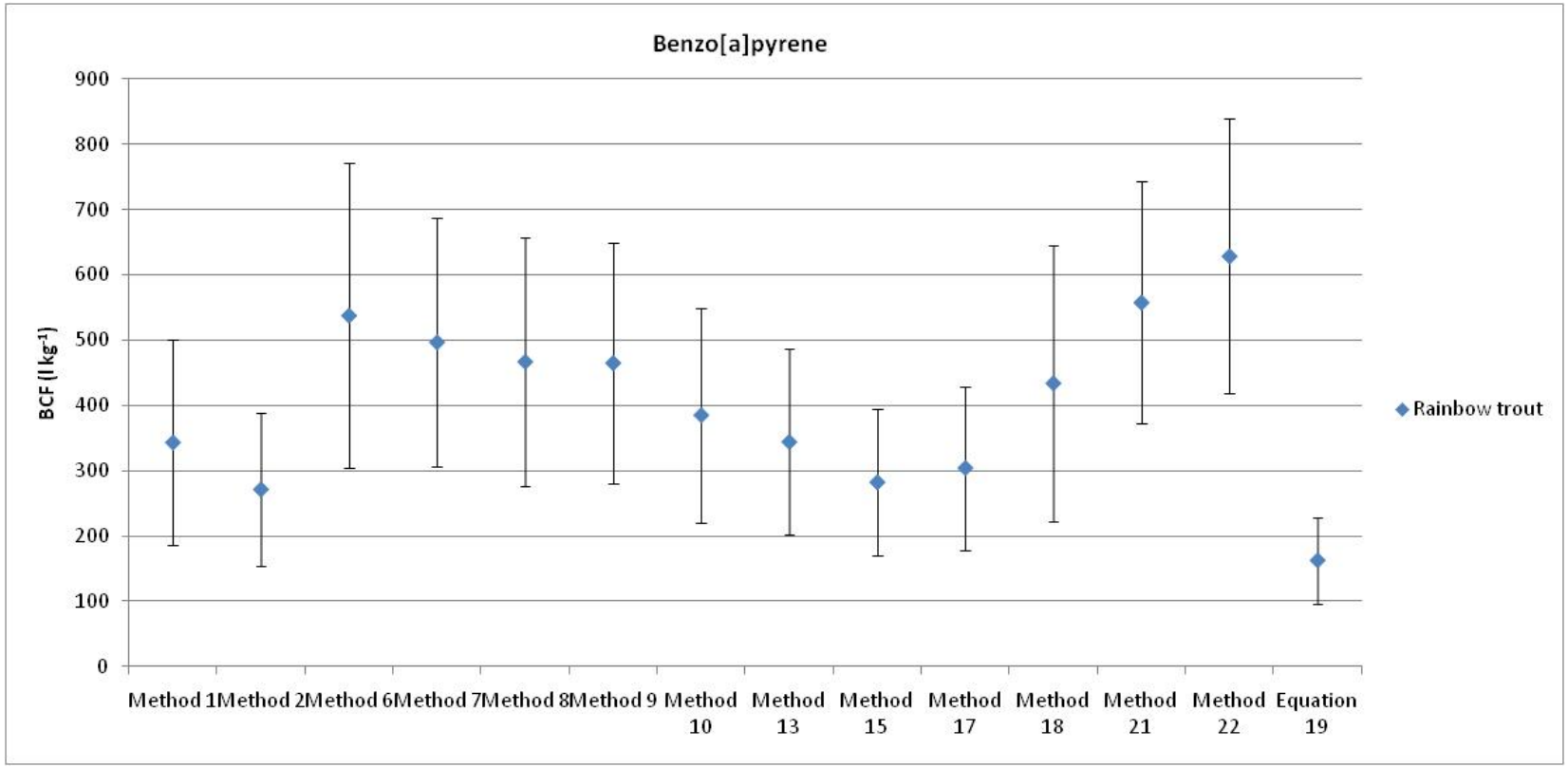

Figure 3.8 Plot showing mean predicted BCF for benzo[a]pyrene for the OECD 305 ring test data set using the various methods for calculation (error bars represent the standard deviation)

3.2.6 Summary

The following critical values have been derived for identifying B or vB substances.

Table 3.14 Critical values for identifying B or vB substances

	Critical value
BCF ≥2000 l kg^{-1}	$k_2 \leq 0.178$ day^{-1}
BCF ≥5,000 l kg^{-1}	$k_2 \leq 0.085$ day^{-1}
$BCF_{lipid\ normalised}$ ≥2,000 l kg^{-1}	$k_2 \leq 0.141$ day^{-1}
$BCF_{lipid\ normalised}$ ≥5,000 l kg^{-1}	$k_2 \leq 0.065$ day^{-1}
$BCF_{lipid\ normalised}$ ≥2,000 l kg^{-1}	$k_{2\ (lipid\ normalised)} \leq 0.181$ day^{-1}
$BCF_{lipid\ normalised}$ ≥5,000 l kg^{-1}	$k_{2\ (lipid\ normalised)} \leq 0.085$ day^{-1}

Overall an approach for identifying substances as B or vB based on the depuration rate constant appears to show promise, with a large proportion of the available data set being correctly categorised based on the criteria derived here. However, the approach used resulted in a number of false positive and false negative assignments, particularly for esters and substances where the BCF values themselves are not clear cut as to B or vB status. The effect of growth correction on the depuration rate constant may also be an important consideration, particularly where the overall depuration rate constant is close to the critical value for a vB substance. Therefore the approach may be best used as part of a weight of evidence/expert judgement-type system.

As well as potentially using cut-offs based on the depuration rate constants for identification of substances as B or vB substances, the regression equations derived may provide useful methods for predicting an actual BCF from the results of a feeding study.

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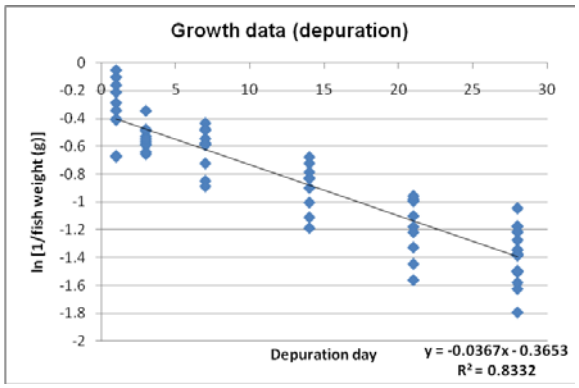
List of abbreviations

B	bioaccumulative criterion [REACH Annex XIII]
BCF	bioconcentration factor
BMF	biomagnification factor
OCDD	octachlorodibenzo-*p*-dioxin (OCDD
OECD	Organisation for Economic Co-operation and Development
PBT	persistent, bioaccumulative and toxic
vB	very bioaccumulative criterion [REACH Annex XIII]
vPvB	very persistent and very bioaccumulative

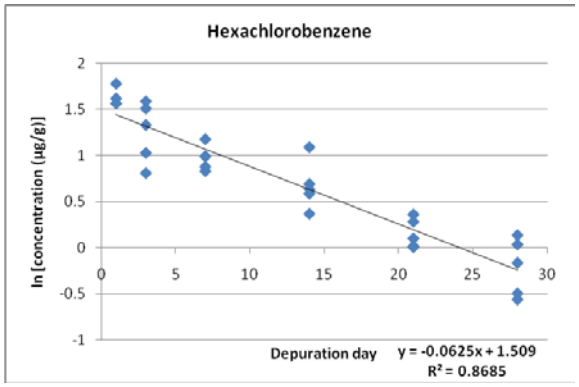
Appendix A: Depuration curves from the OECD 305 ring test

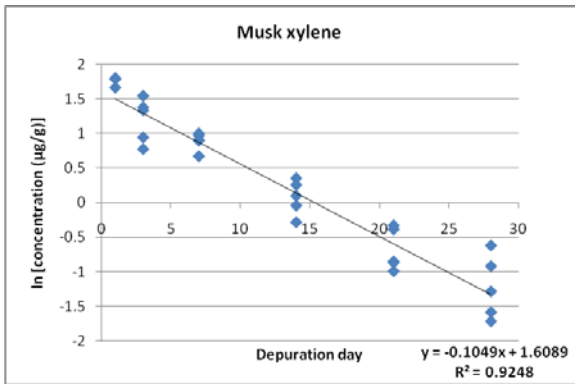
Study A

Growth data

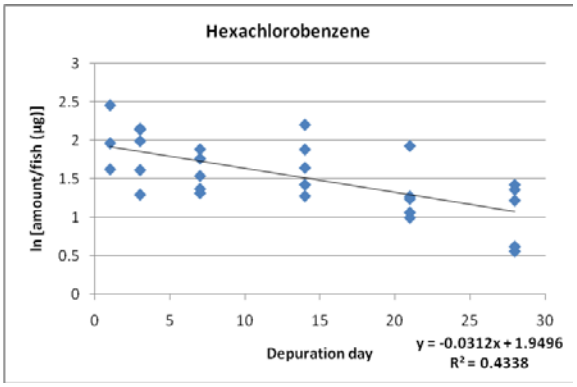


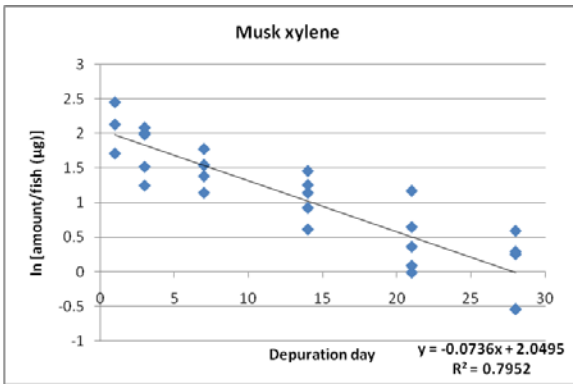
Rate constant subtraction method

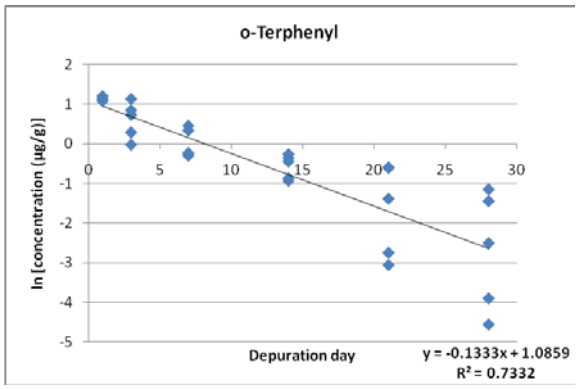


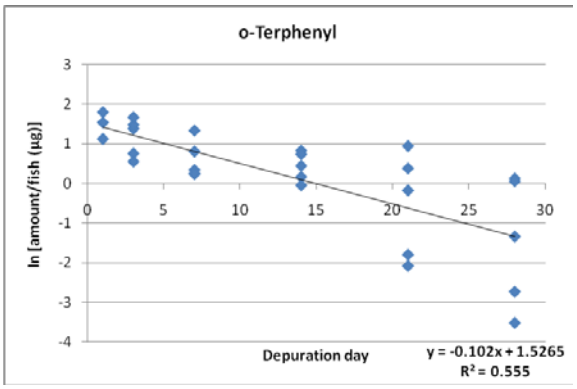


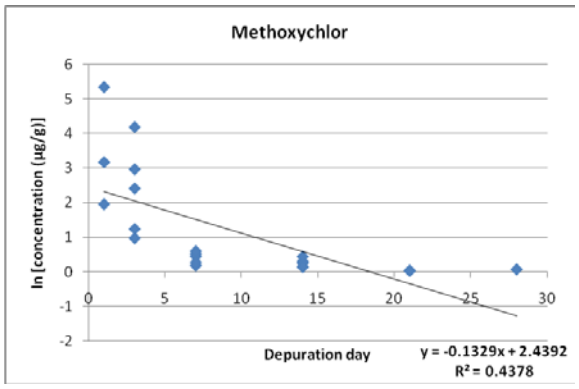
Alternative method






o-Terphenyl
ln [concentration (µg/g)]
Depuration day
y = -0.1333x + 1.0859
R² = 0.7332


o-Terphenyl
ln [amount/fish (µg)]
Depuration day
y = -0.102x + 1.5265
R² = 0.555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Depuration day
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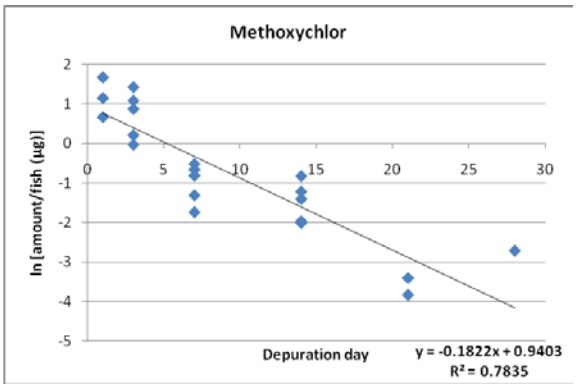
R² = 0.4378


Methoxychlor
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Depuration day
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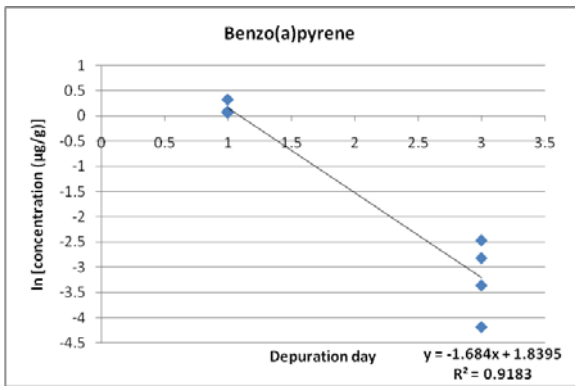
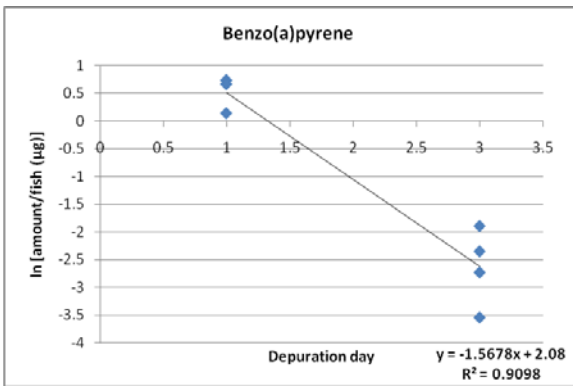
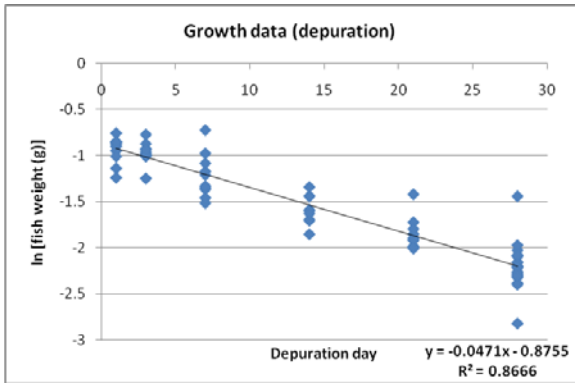
R² = 0.7835


Benzo(a)pyrene
ln [concentration (µg/g)]
Depuration day
y = -1.684x + 1.8395
R² = 0.9183

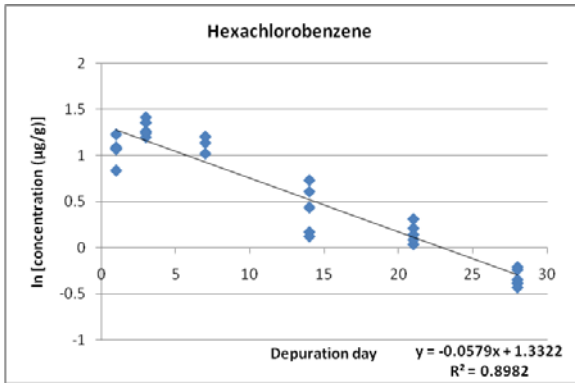

Benzo(a)pyrene
ln [amount/fish (µg)]
Depuration day
y = -1.5678x + 2.08
R² = 0.9098

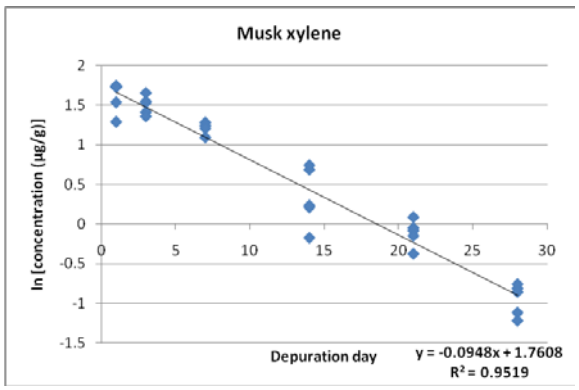
Study B

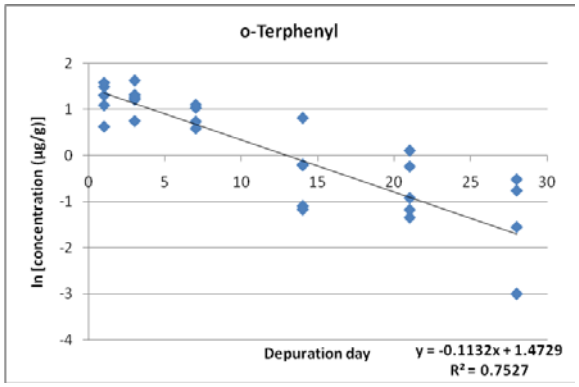
Growth data



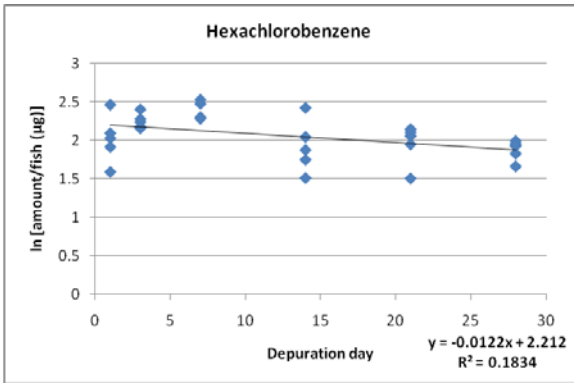
Rate constant subtraction method

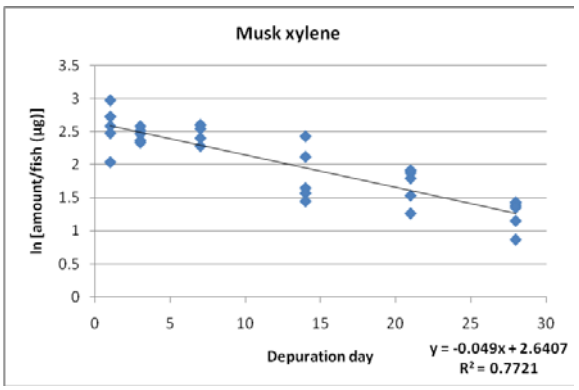


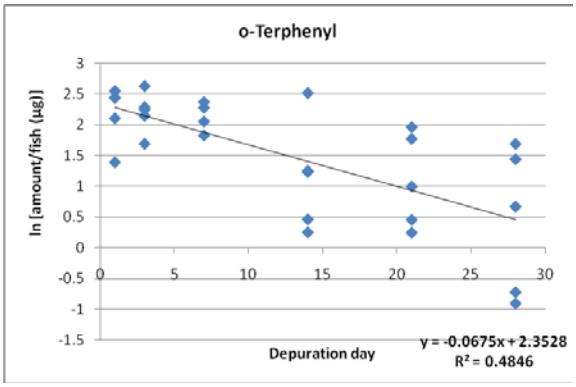


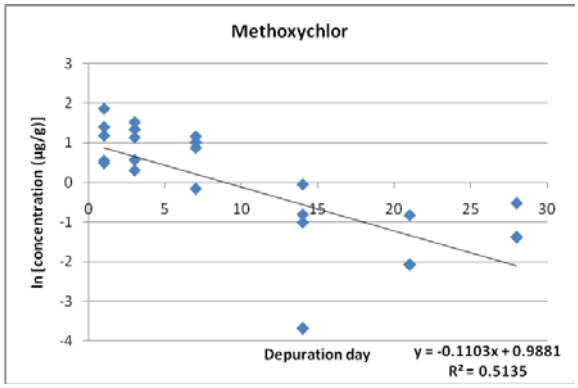


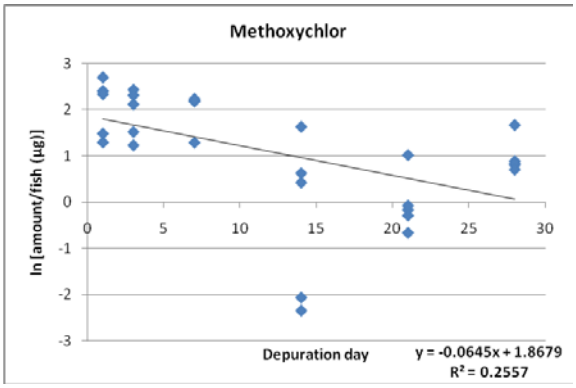
Alternative method

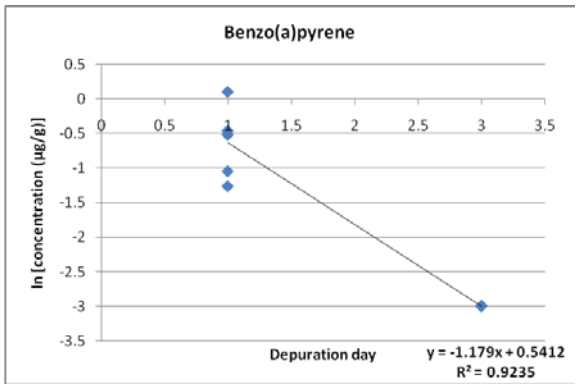


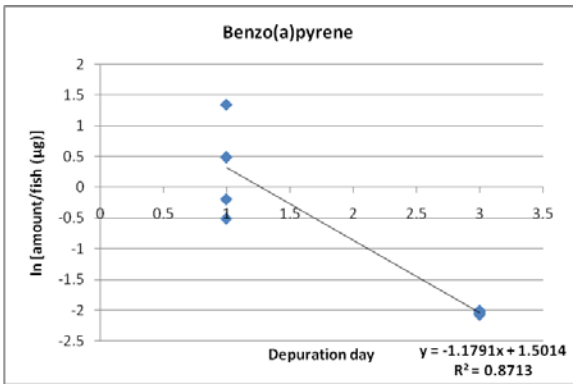





Methoxychlor
ln [concentration (µg/g)]
Depuration day
y = -0.1103x + 0.9881
R² = 0.5135

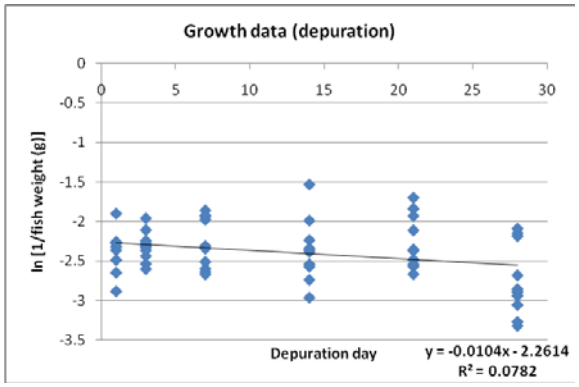

Methoxychlor
ln [amount/fish (µg)]
Depuration day
y = -0.0645x + 1.8679
R² = 0.2557


Benzo(a)pyrene
ln [concentration (µg/g)]
Depuration day
y = -1.179x + 0.5412
R² = 0.9235

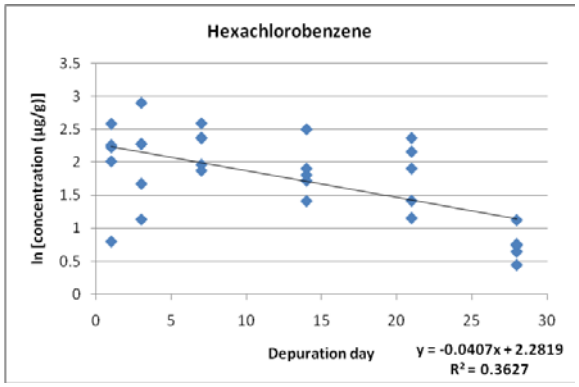

Benzo(a)pyrene
ln [amount/fish (µg)]
Depuration day
y = -1.1791x + 1.5014
R² = 0.8713

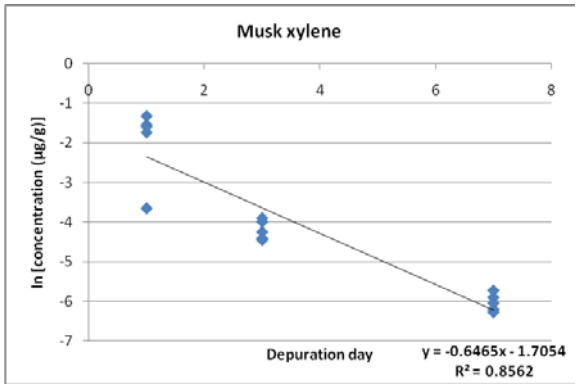
Study C

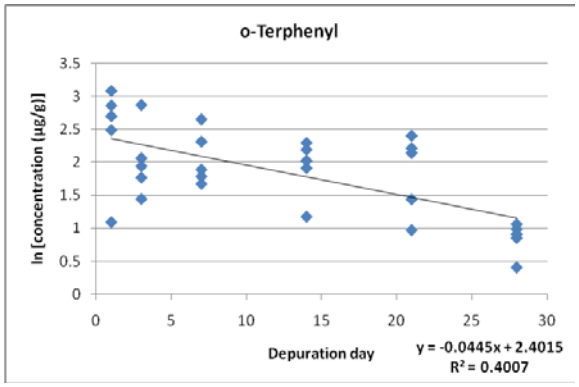
Growth data



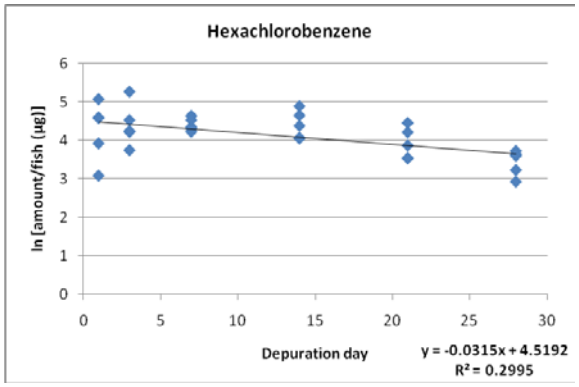
Rate constant subtraction method

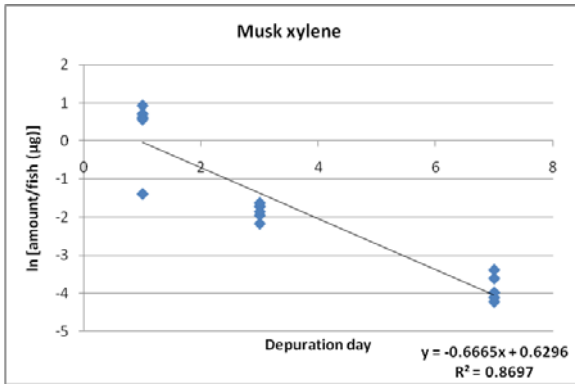


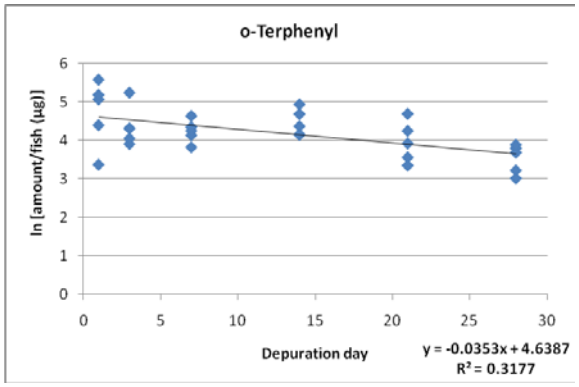


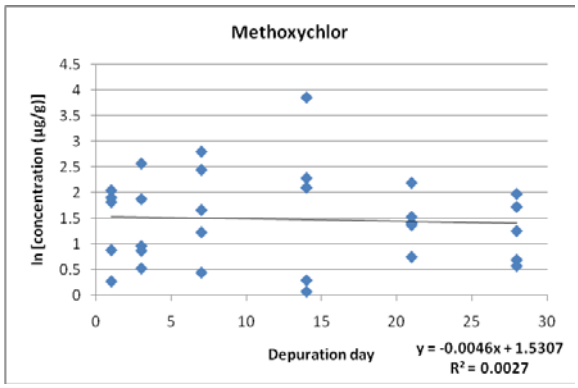


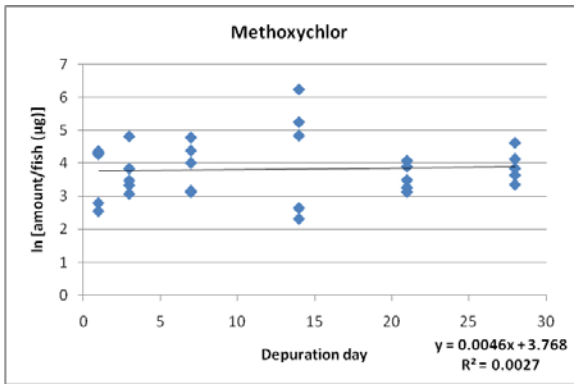
Alternative method

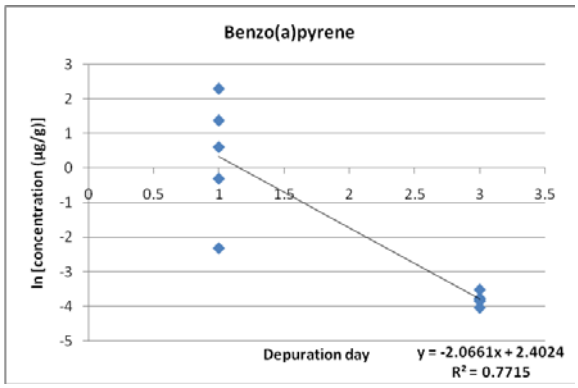


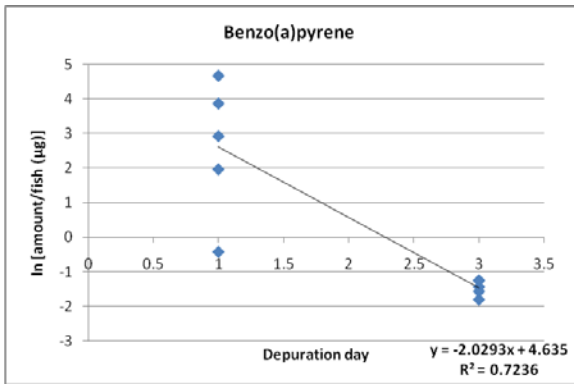





Methoxychlor
ln [concentration (µg/g)]
Depuration day
y = -0.0046x + 1.5307
R² = 0.0027

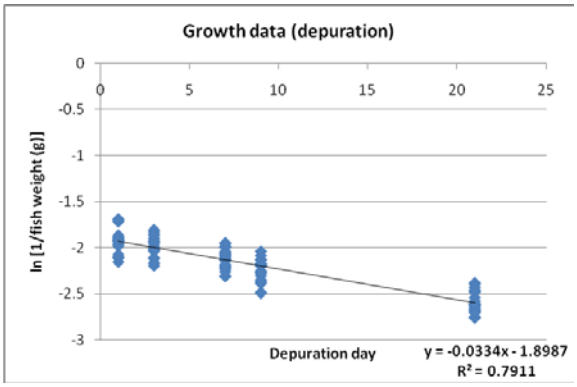

Methoxychlor
ln [amount/fish (µg)]
Depuration day
y = 0.0046x + 3.768
R² = 0.0027


Benzo(a)pyrene
ln [concentration (µg/g)]
Depuration day
y = -2.0661x + 2.4024
R² = 0.7715

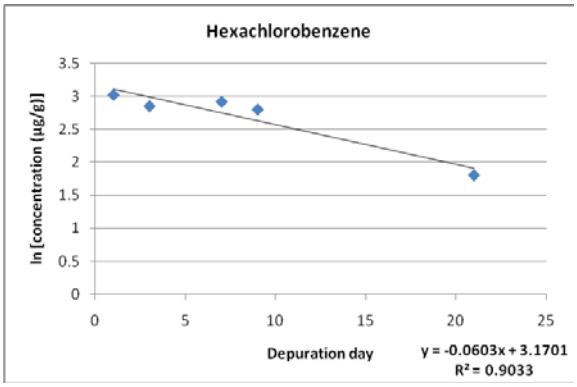

Benzo(a)pyrene
ln [amount/fish (µg)]
Depuration day
y = -2.0293x + 4.635
R² = 0.7236

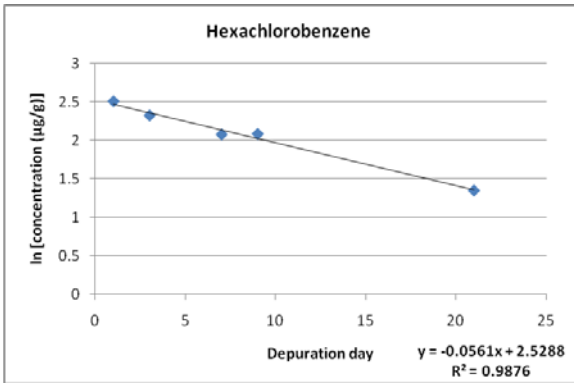
Study D

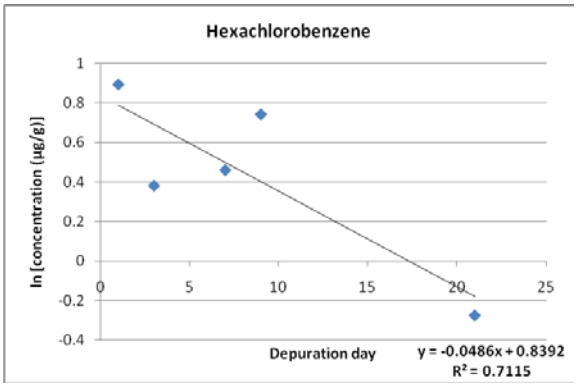
Growth data



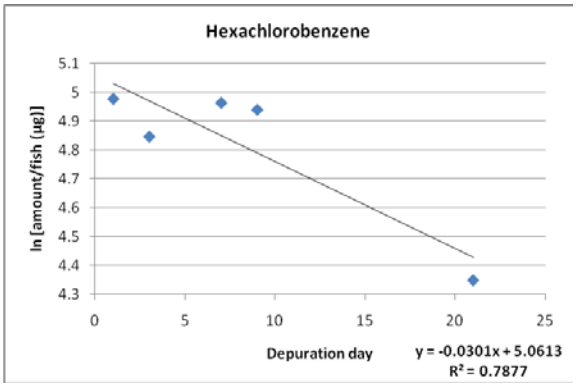
Rate constant subtraction method

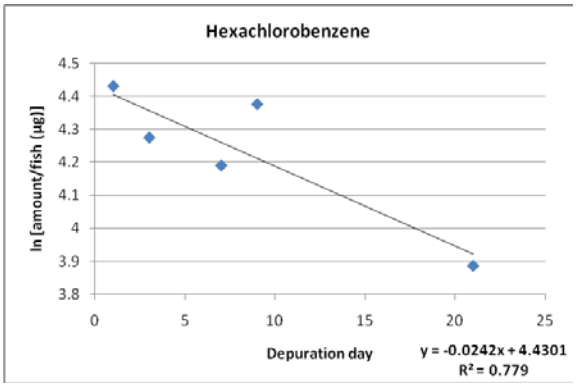


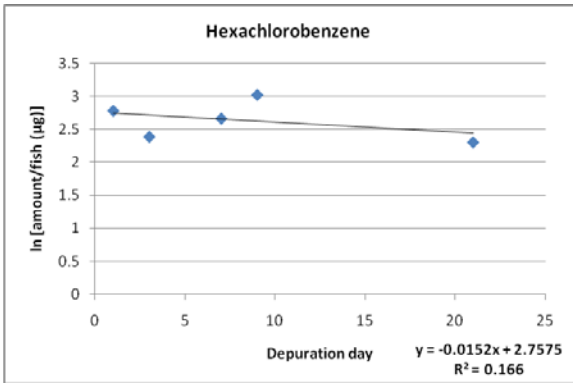


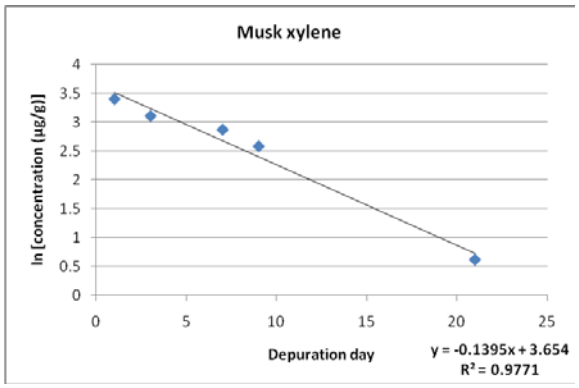


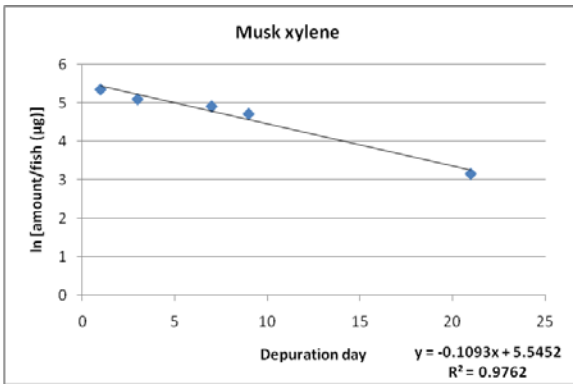
Alternative method

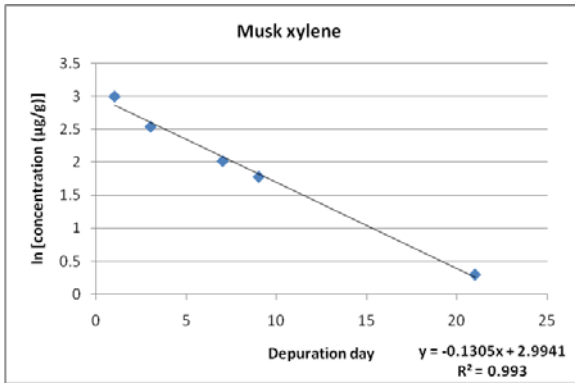


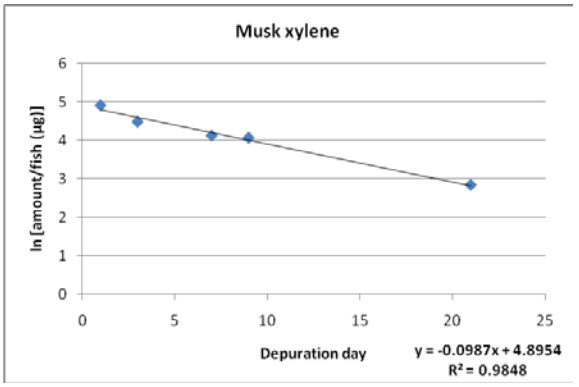


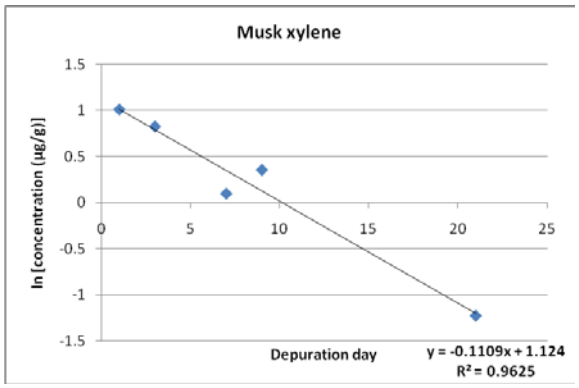


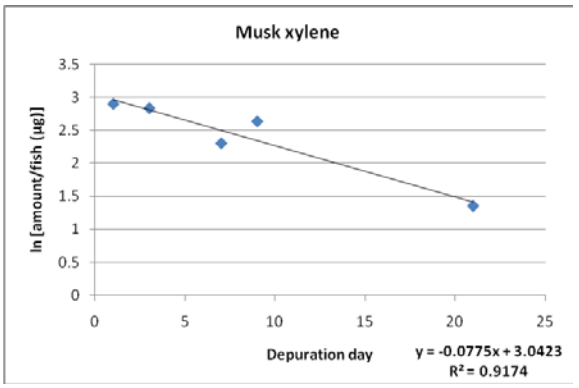

Musk xylene
ln [concentration (µg/g)]
Depuration day
y = -0.1395x + 3.654
R² = 0.9771

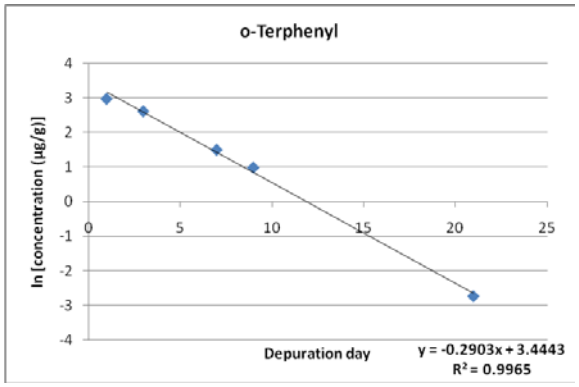

Musk xylene
ln [amount/fish (µg)]
Depuration day
y = -0.1093x + 5.5452
R² = 0.9762

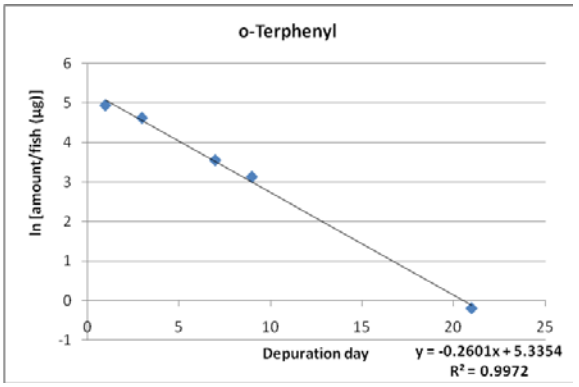

Musk xylene
ln [concentration (µg/g)]
Depuration day
y = -0.1305x + 2.9941
R² = 0.993

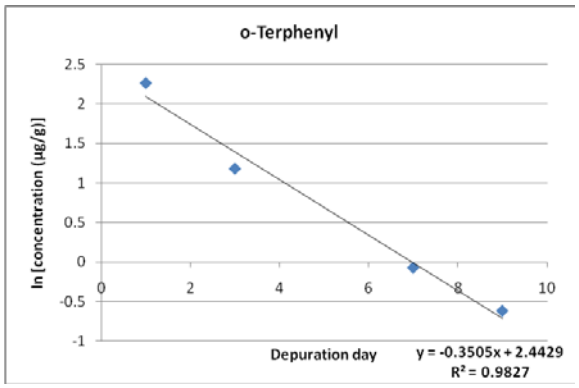

Musk xylene
ln [amount/fish (µg)]
Depuration day
y = -0.0987x + 4.8954
R² = 0.9848

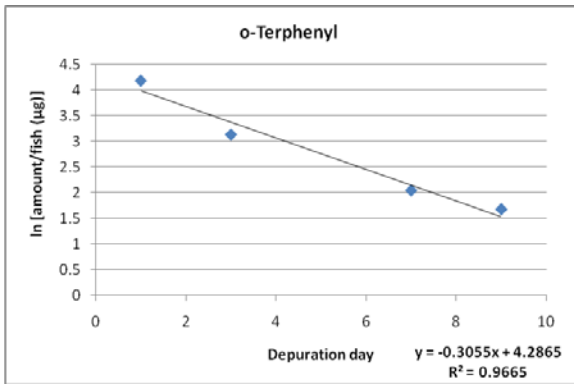

Musk xylene
ln [concentration (µg/g)]
Depuration day
y = -0.1109x + 1.124
R² = 0.9625

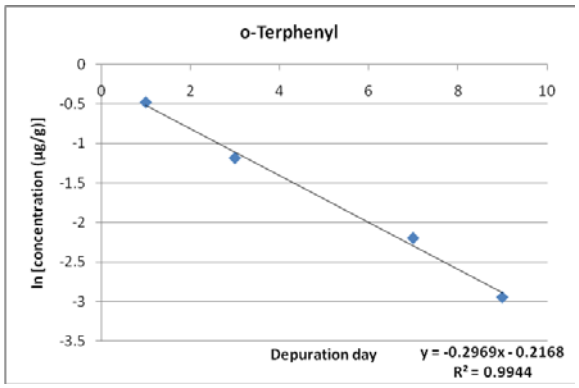

Musk xylene
ln [amount/fish (µg)]
Depuration day
y = -0.0775x + 3.0423
R² = 0.9174

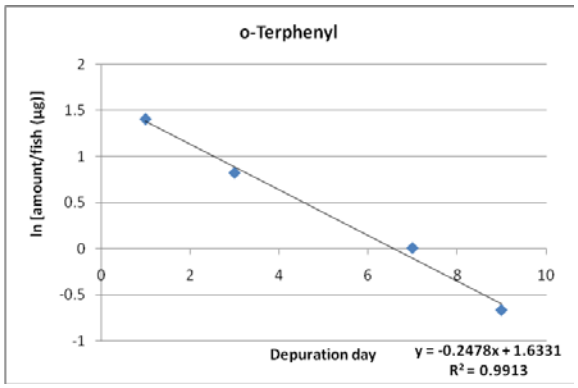

o-Terphenyl
ln [concentration (µg/g)]
Depuration day
y = -0.2903x + 3.4443
R² = 0.9965

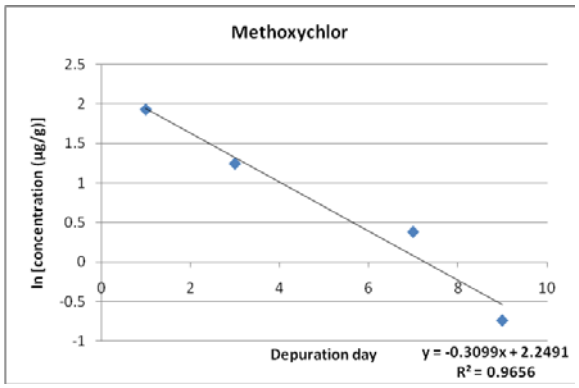

o-Terphenyl
ln [amount/fish (µg)]
Depuration day
y = -0.2601x + 5.3354
R² = 0.9972

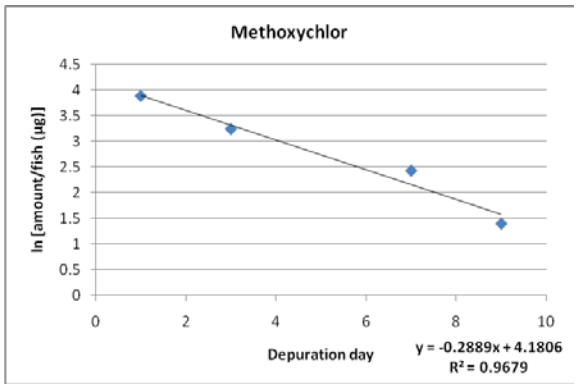

o-Terphenyl
ln [concentration (µg/g)]
Depuration day
y = -0.3505x + 2.4429
R² = 0.9827

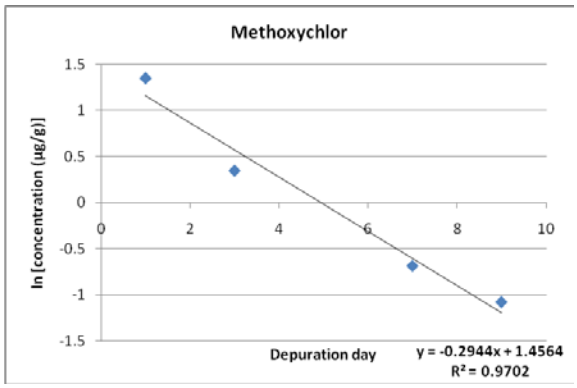

o-Terphenyl
ln [amount/fish (µg)]
Depuration day
y = -0.3055x + 4.2865
R² = 0.9665

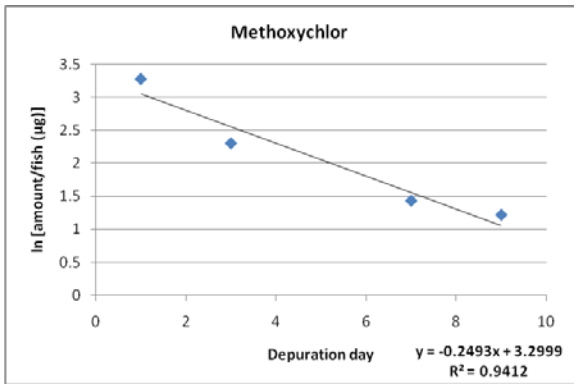

o-Terphenyl
ln [concentration (µg/g)]
Depuration day
y = -0.2969x - 0.2168
R² = 0.9944

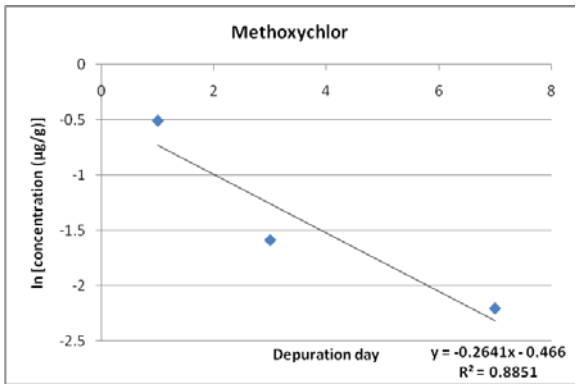

o-Terphenyl
ln [amount/fish (µg)]
Depuration day
y = -0.2478x + 1.6331
R² = 0.9913

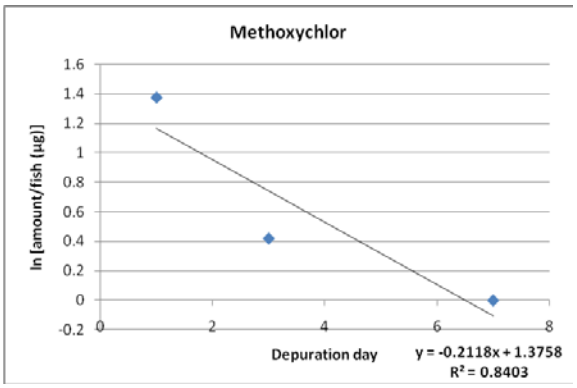

Methoxychlor
ln [concentration (µg/g)]
Depuration day
y = -0.3099x + 2.2491
R² = 0.9656


Methoxychlor
ln [amount/fish (µg)]
Depuration day
y = -0.2889x + 4.1806
R² = 0.9679


Methoxychlor
ln [concentration (µg/g)]
Depuration day
y = -0.2944x + 1.4564
R² = 0.9702

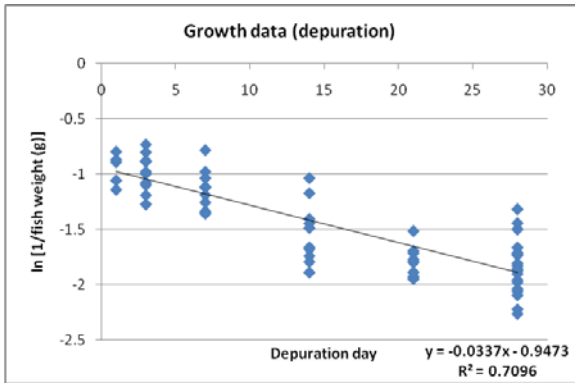

Methoxychlor
ln [amount/fish (µg)]
Depuration day
y = -0.2493x + 3.2999
R² = 0.9412


Methoxychlor
ln [concentration (µg/g)]
0
-0.5
-1
-1.5
-2
-2.5
0
2
4
6
8
Depuration day
y = -0.2641x - 0.466
R² = 0.8851

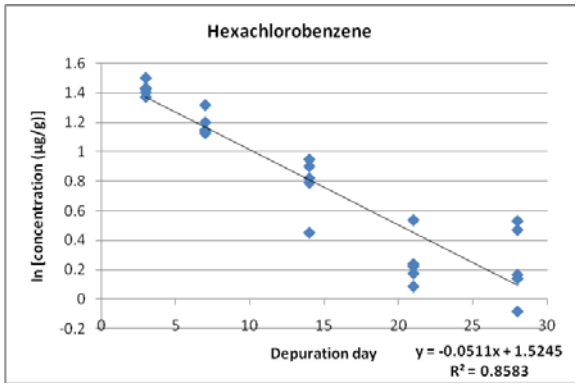

Methoxychlor
ln [amount/fish (µg)]
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
0
2
4
6
8
Depuration day
y = -0.2118x + 1.3758
R² = 0.8403

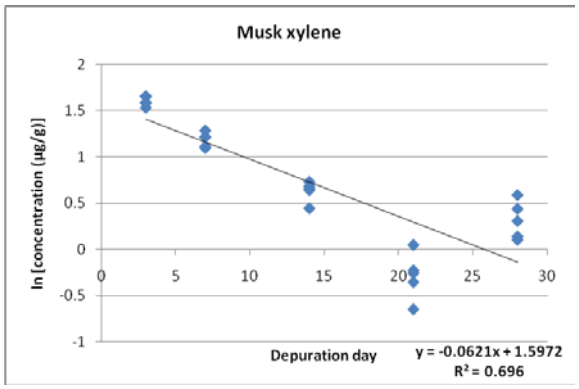
Study E

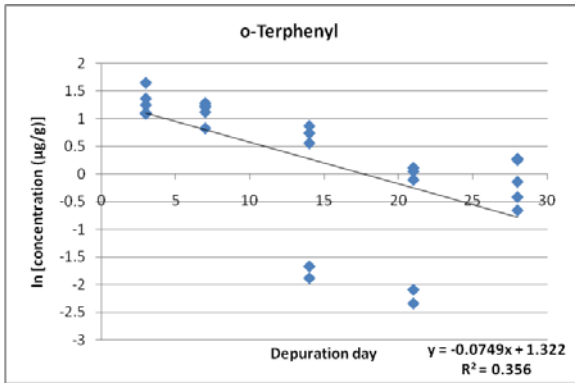
Growth data



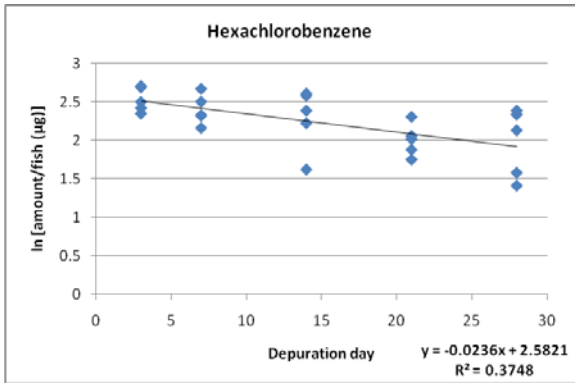
Rate constant subtraction method

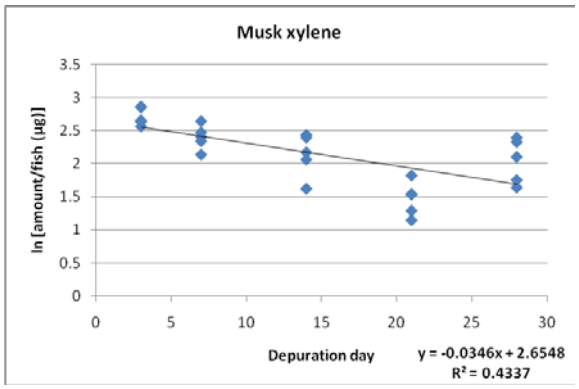


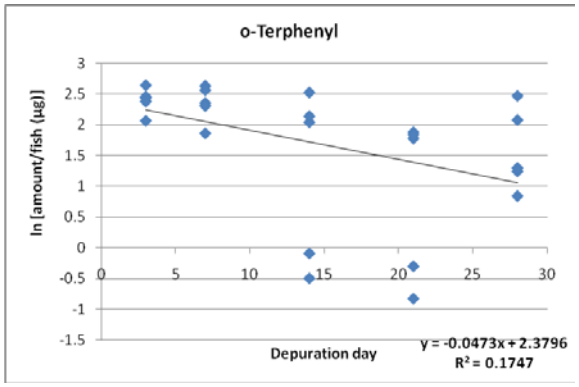


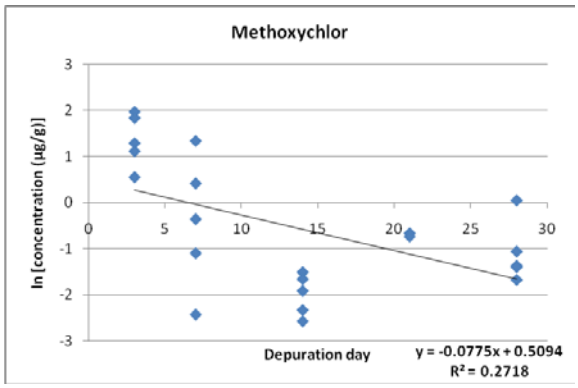


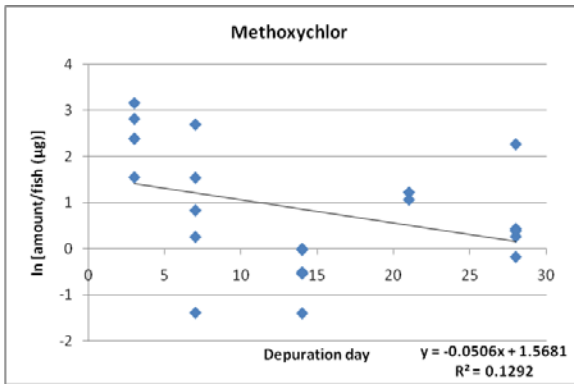
Alternative method





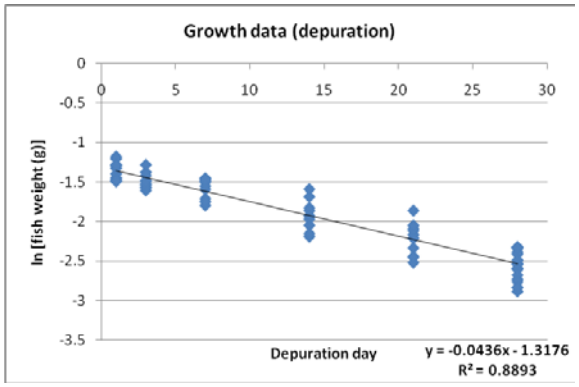



Methoxychlor
ln [concentration (µg/g)]
Depuration day
y = -0.0775x + 0.5094
R² = 0.2718

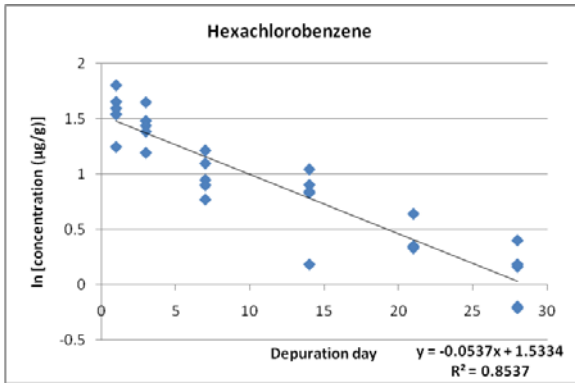

Methoxychlor
ln [amount/fish (µg)]
Depuration day
y = -0.0506x + 1.5681
R² = 0.1292

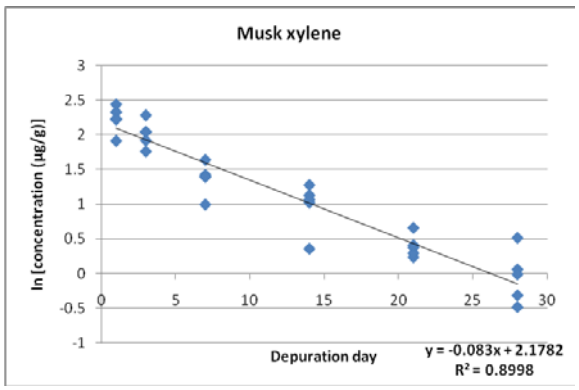
Study F

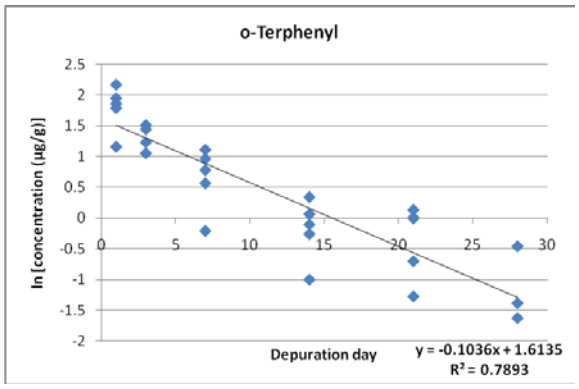
Growth data



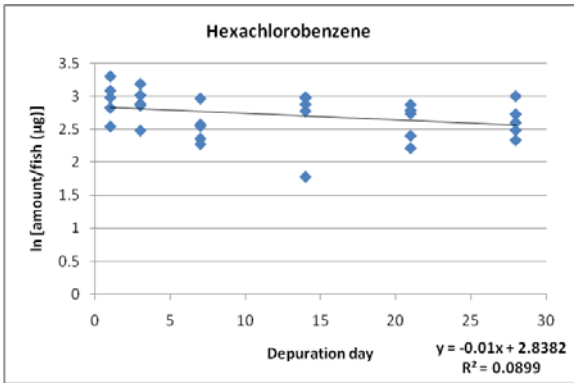
Rate constant subtraction method

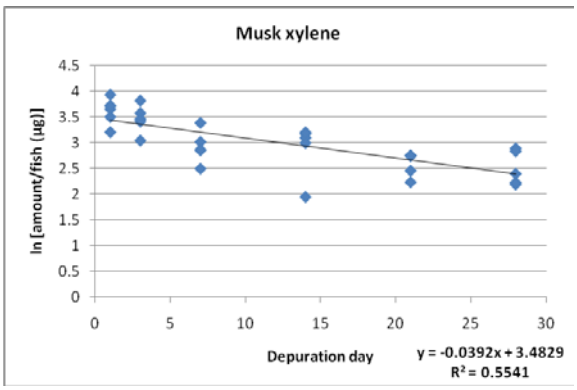


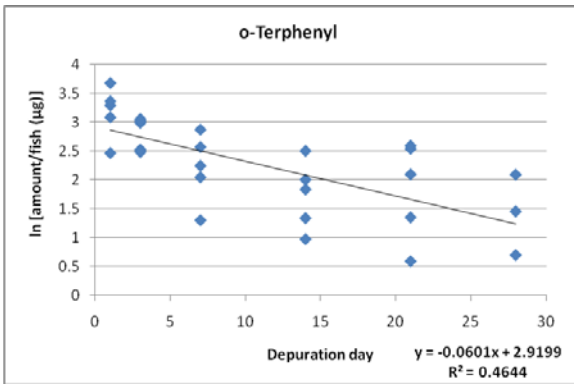


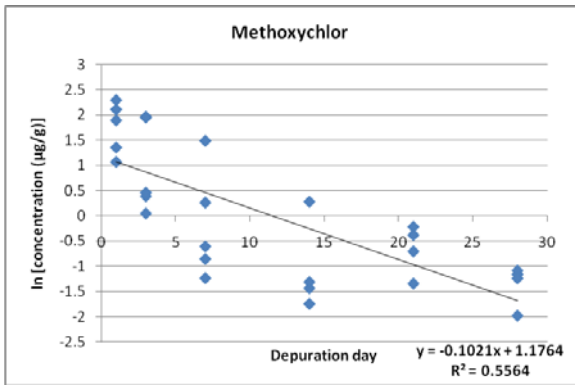


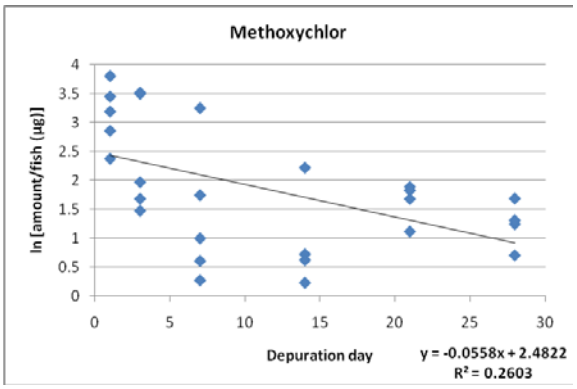
Alternative method





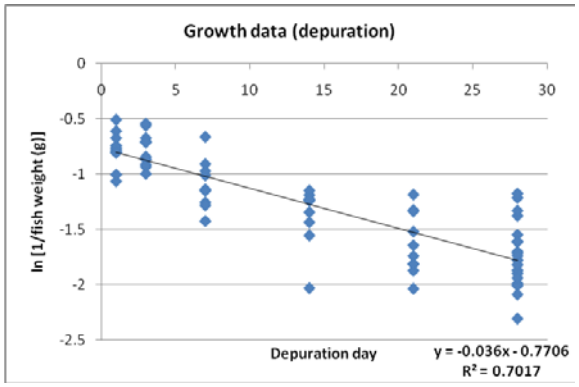



Methoxychlor
ln [concentration (µg/g)]
Depuration day
y = -0.1021x + 1.1764
R² = 0.5564

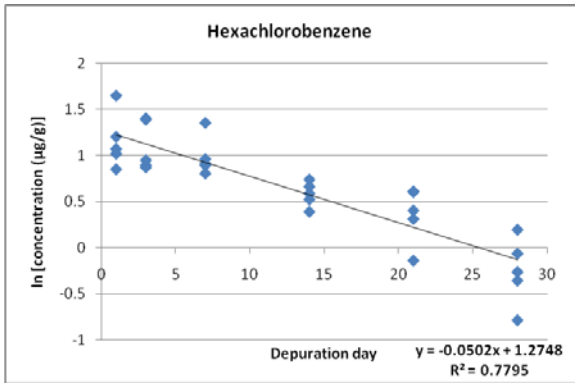

Methoxychlor
ln [amount/fish (µg)]
Depuration day
y = -0.0558x + 2.4822
R² = 0.2603

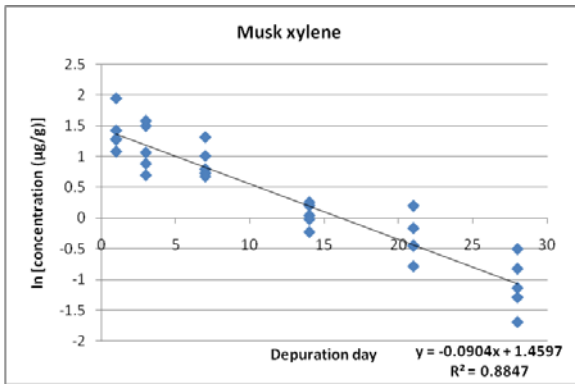
Study G

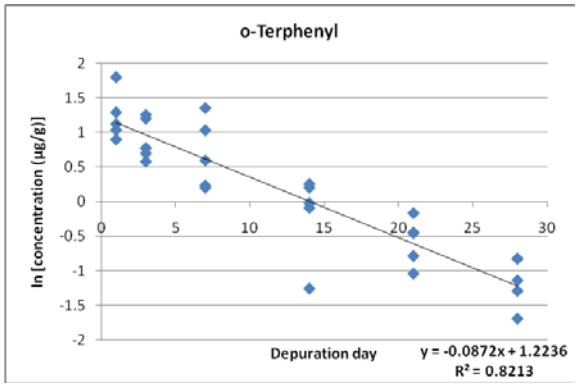
Growth data



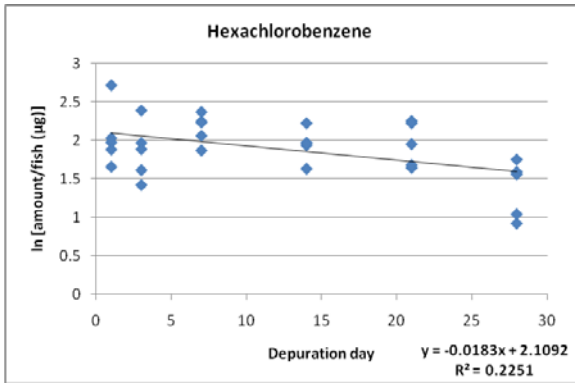
Rate constant subtraction method

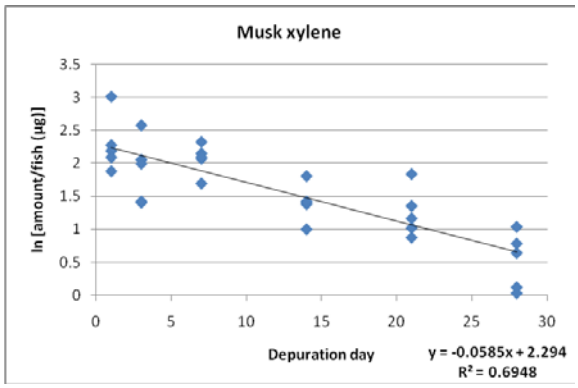


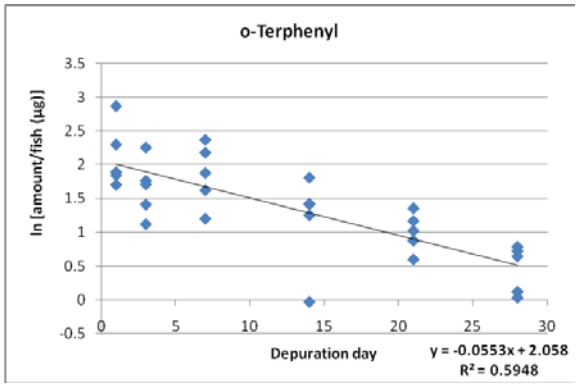


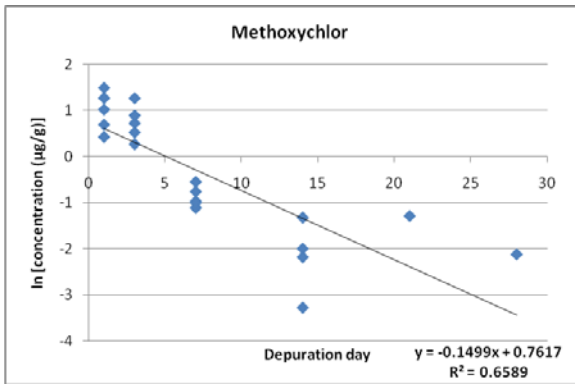


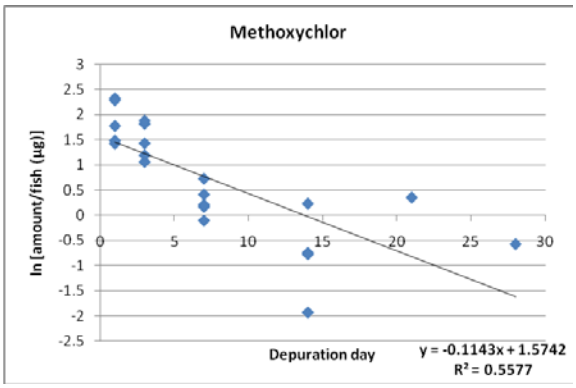
Alternative method





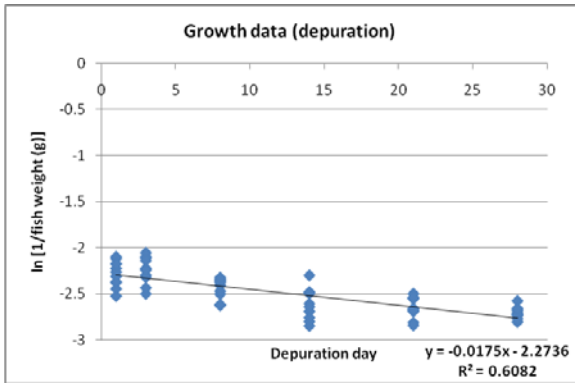



Methoxychlor
ln [concentration (µg/g)]
Depuration day
y = -0.1499x + 0.7617
R² = 0.6589

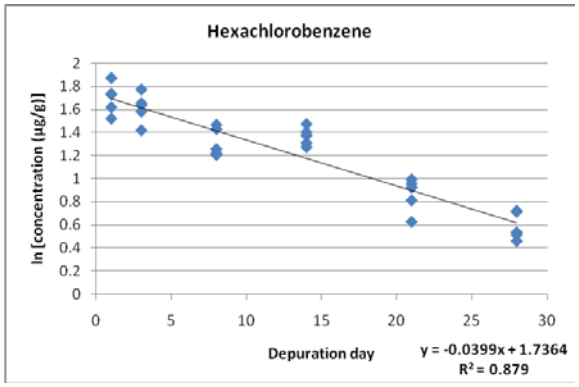

Methoxychlor
ln [amount/fish (µg)]
Depuration day
y = -0.1143x + 1.5742
R² = 0.5577

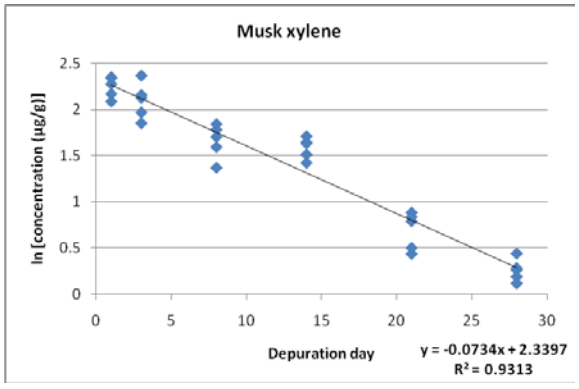
Study H

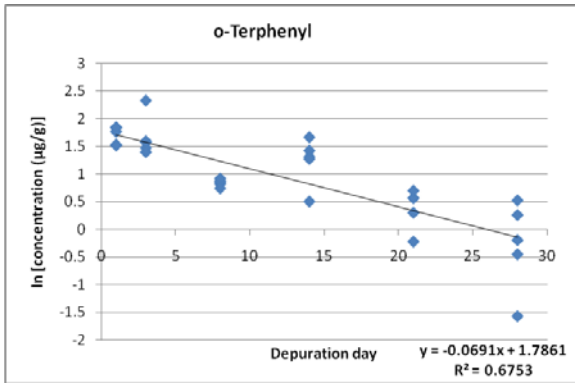
Growth data



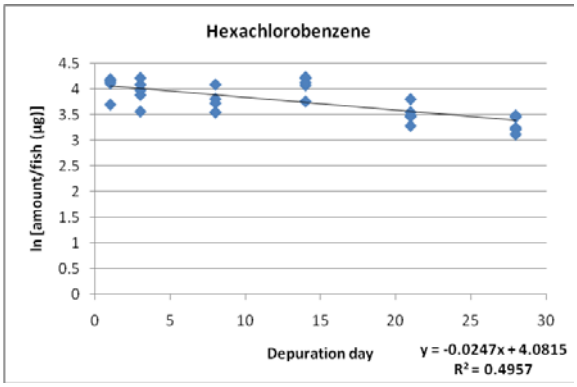
Rate constant subtraction method

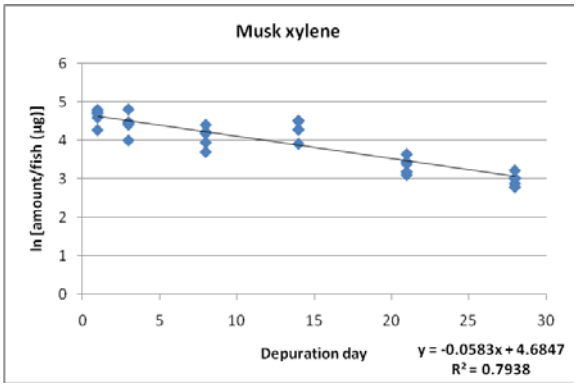


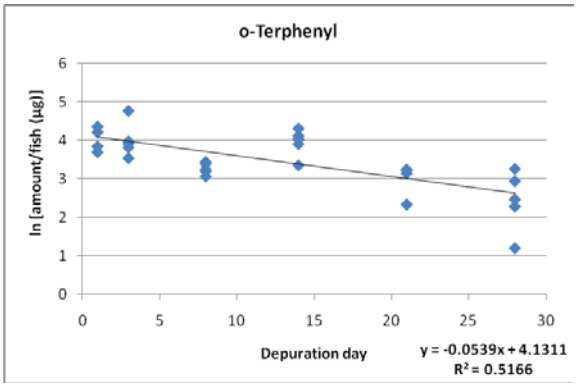


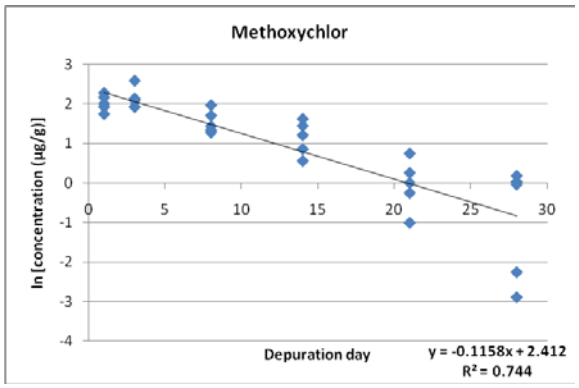


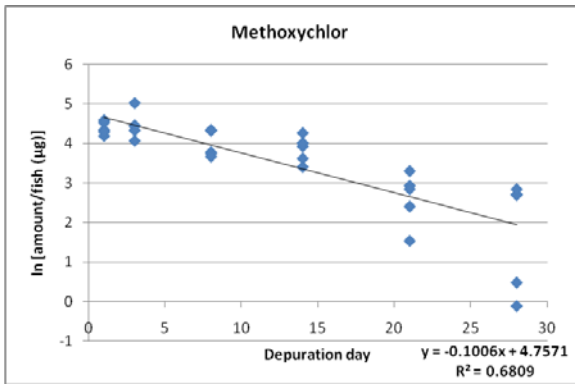
Alternative method

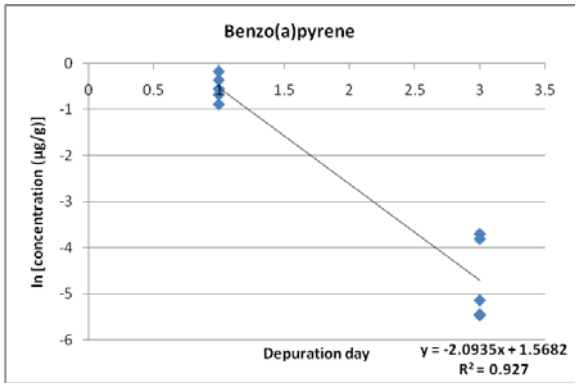


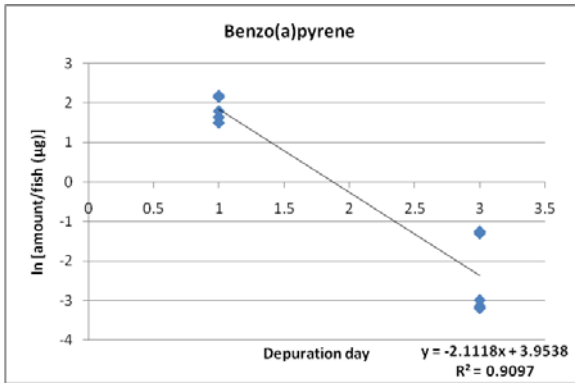





Methoxychlor
ln [concentration (µg/g)]
Depuration day
y = -0.1158x + 2.412
R² = 0.744


Methoxychlor
ln [amount/fish (µg)]
Depuration day
y = -0.1006x + 4.7571
R² = 0.6809

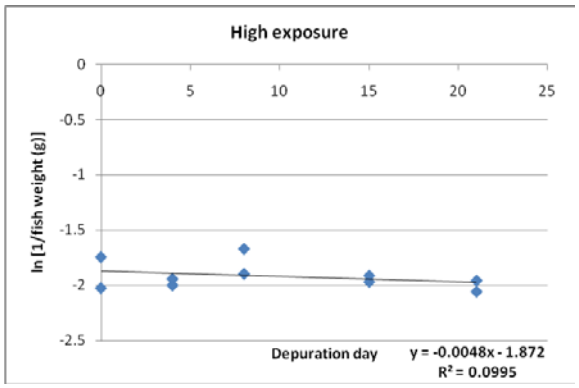

Benzo(a)pyrene
ln [concentration (µg/g)]
Depuration day
y = -2.0935x + 1.5682
R² = 0.927


Benzo(a)pyrene
ln [amount/fish (µg)]
Depuration day
y = -2.1118x + 3.9538
R² = 0.9097

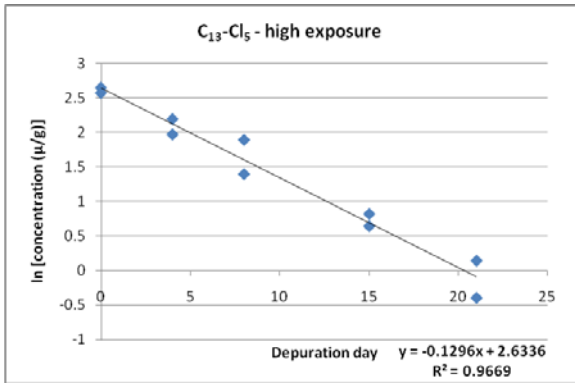
Appendix B: Depuration curves for the C_{13} chlorinated paraffins

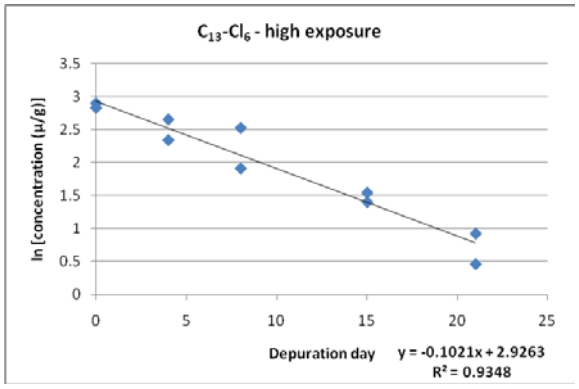
Higher exposure concentration

Growth data

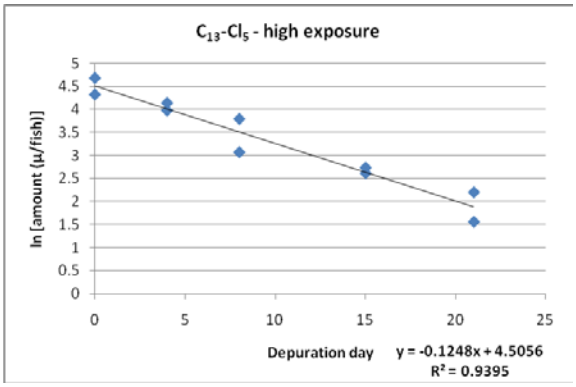


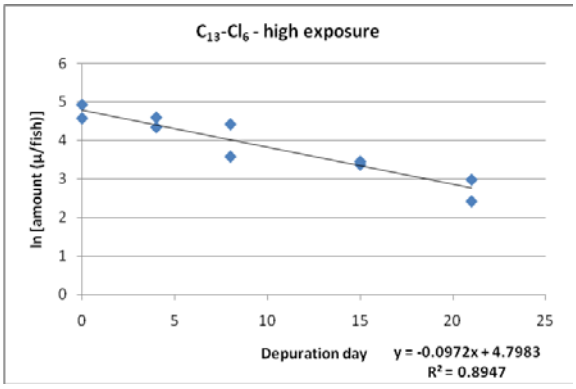
Rate constant subtraction method

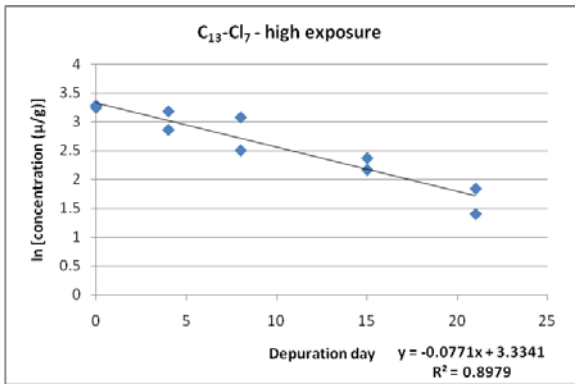


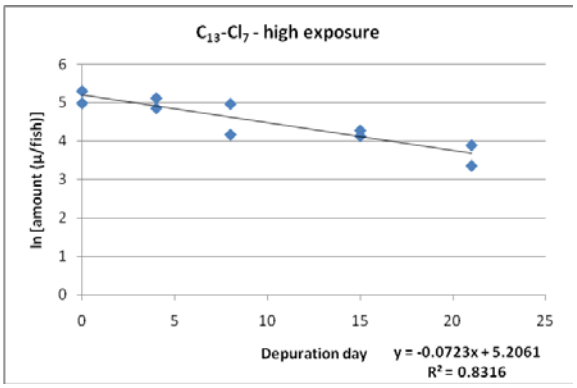


Alternative method



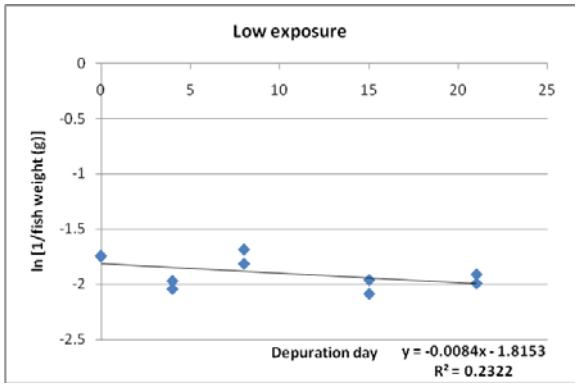



C_{13}-Cl_7 - high exposure
ln [concentration (µ/g)]
Depuration day
y = -0.0771x + 3.3341
R² = 0.8979

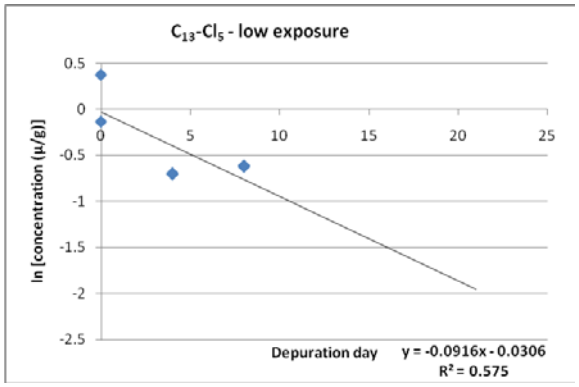

C_{13}-Cl_7 - high exposure
ln [amount (µ/fish)]
Depuration day
y = -0.0723x + 5.2061
R² = 0.8316

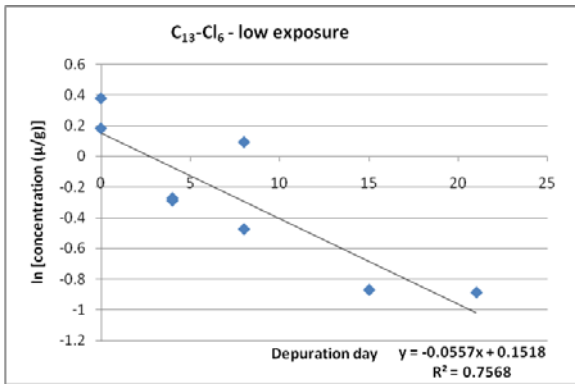
Lower exposure concentration

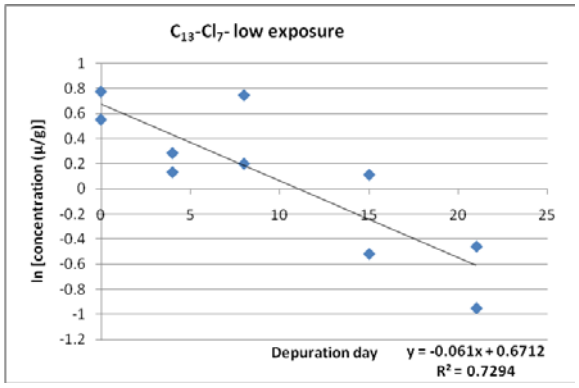
Growth data



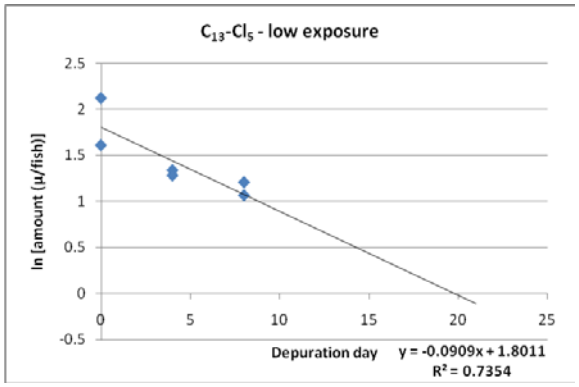
Rate constant subtraction method

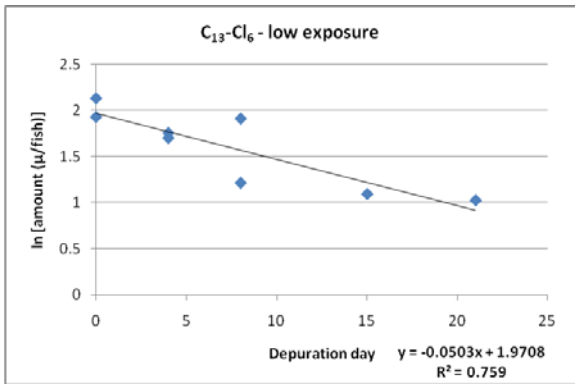


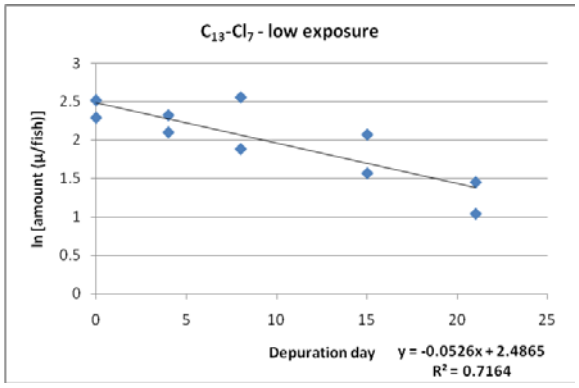




Alternative method







Appendix C: Data sets used for the analysis of k_2 values

Table C.1 Arnot data set – substance identities

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
1		C-12-2-LAS	4.71	326.50	S(=O)(=O)(O)c1ccc(C(CCCCCCCCCC)C)cc1
2		Octaethylene glycol monotridecyl ether	3.07	552.80	OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCCCCCCCCCCCC
3		Octaethylene glycol monotridecyl ether	5.11	552.80	OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCCCCCCCCCCCC
4		C-12-5-LAS	4.71	326.50	S(=O)(=O)(O)c1ccc(C(CCCCCCC)CCCC)cc1
8		NL-63A	6.90	306.35	FC(F)(Oc1ccc(cc1)C(C)(C)CC(C)(C)C)C(F)F
9		NL-63B	6.85	306.35	FC(F)(Oc1ccc(cc1)C(C)(C)C(C)(C)C)C(F)F
11		Methylisocyanothion	3.58	277.66	S=P(OC)(OC)Oc1c(C(#N))cc(Cl)cc1
17	55-38-9	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylthio)phenyl]ester phosphorothioic acid	4.17	278.32	COP(=S)(OC)Oc1ccc(SC)c(C)c1
18	55-38-9	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylthio)phenyl]ester phosphorothioic acid	4.17	278.32	COP(=S)(OC)Oc1ccc(SC)c(C)c1
19	55-38-9	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylthio)phenyl]ester phosphorothioic acid	4.17	278.32	COP(=S)(OC)Oc1ccc(SC)c(C)c1
20	55-38-9	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylthio)phenyl]ester phosphorothioic acid	4.17	278.32	COP(=S)(OC)Oc1ccc(SC)c(C)c1
29	56-55-3	Benzo[a]anthracene	5.76	228.30	c(c(c(c(c1)ccc2)c2)cc(c3ccc4)c4)(c1)c3
34	58-89-9	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	3.72	290.83	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl
35	58-89-9	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	3.72	290.83	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl
36	58-89-9	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	3.72	290.83	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl
37	58-89-9	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	3.72	290.83	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl
38	58-89-9	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	3.72	290.83	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
54	62-53-3	Benzenamine	0.90	93.13	Nc(cccc1)c1
111	80-05-7	Phenol, 4,4-(1-methylethylidene)bis-	3.32	228.29	Oc(ccc(c1)C(c(ccc(O)c2)c2)(C)C)c1
145	87-61-6	Benzene, 1,2,3-trichloro-	4.05	181.45	c(c(c(cc1)Cl)Cl)(c1)Cl
158	87-86-5	Phenol, pentachloro-	5.12	266.34	Oc(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl
159	87-86-5	Phenol, pentachloro-	5.12	266.34	Oc(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl
160	87-86-5	Phenol, pentachloro-	5.12	266.34	Oc(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl
161	87-86-5	Phenol, pentachloro-	5.12	266.34	Oc(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl
162	87-86-5	Phenol, pentachloro-	5.12	266.34	Oc(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl
163	87-86-5	Phenol, pentachloro-	5.12	266.34	Oc(c(c(c(c1Cl)Cl)Cl)Cl)c1Cl
164	88-06-2	2,4,6-Trichlorophenol	3.69	197.45	Oc(c(cc(c1)Cl)Cl)c1Cl
200	92-86-4	4,4'-dibromobiphenyl	5.72	312.01	c(ccc(c(ccc(c1)Br)c1)c2)(c2)Br
214	95-51-2	Benzenamine, 2-chloro-	1.90	127.57	Nc(c(ccc1)Cl)c1
215	95-51-2	Benzenamine, 2-chloro-	1.90	127.57	Nc(c(ccc1)Cl)c1
236	95-94-3	Benzene, 1,2,4,5-tetrachloro-	4.64	215.89	c(c(cc(c1Cl)Cl)Cl)(c1)Cl
311	104-88-1	4-Chlorobenzaldehyde	2.10	140.57	O=Cc(ccc(c1)Cl)c1
316	106-37-6	Benzene, 1,4-dibromo-	3.79	235.91	c(ccc(c1)Br)(c1)Br
321	106-46-7	Benzene, 1,4-dichloro-	3.44	147.00	c(ccc(c1)Cl)(c1)Cl
326	106-47-8	Benzenamine, 4-chloro-	1.83	127.57	Nc(ccc(c1)Cl)c1
327	106-47-8	Benzenamine, 4-chloro-	1.83	127.57	Nc(ccc(c1)Cl)c1
328	106-47-8	Benzenamine, 4-chloro-	1.83	127.57	Nc(ccc(c1)Cl)c1
338	108-42-9	Benzenamine, 3-chloro-	1.88	127.57	Nc(cccc1Cl)c1
339	108-42-9	Benzenamine, 3-chloro-	1.88	127.57	Nc(cccc1Cl)c1
381	115-86-6	Phosphoric acid, triphenyl ester	4.59	326.29	O=P(Oc(cccc1)c1)(Oc(cccc2)c2)Oc(cccc3)c3
383	115-96-8	Ethanol, 2-chloro-, phosphate (3:1)	1.44	285.49	O=P(OCCCl)(OCCCl)OCCCl
386	117-18-0	1,2,4,5-Tetrachloro-3-nitrobenzene	4.38	260.89	Clc1cc(Cl)c(Cl)c(N(=O)=O)c1Cl
394	117-81-7	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	7.73	390.57	O=C(OCC(CCCC)CC)c(c(ccc1)C(=O)OCC(CCCC)CC)c1
395	117-81-7	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	7.73	390.57	O=C(OCC(CCCC)CC)c(c(ccc1)C(=O)OCC(CCCC)CC)c1

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
396	117-81-7	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	7.73	390.57	O=C(OCC(CCCC)CC)c(c(ccc1)C(=O)OCC(CCCC)CC)c1
397	117-81-7	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	7.73	390.57	O=C(OCC(CCCC)CC)c(c(ccc1)C(=O)OCC(CCCC)CC)c1
418	118-96-7	Benzene, 2-methyl-1,3,5-trinitro-	1.60	227.13	O=N(=O)c(cc(N(=O)=O)c(c1N(=O)=O)C)c1
419	119-12-0	Phosphorothioic acid, *O*-(1,6-dihydro-6-oxo-1-phenyl-3-pyridazinyl) *O*,*O*-diethyl ester	3.20	340.34	S=P(OCC)(OCC)OC1=NN(c2ccccc2)C(=O)C=C1
441	120-82-1	Benzene, 1,2,4-trichloro-	4.02	181.45	c(ccc(c1Cl)Cl)(c1)Cl
451	121-14-2	Benzene, 1-methyl-2,4-dinitro-	1.98	182.14	N(=O)(=O)c(ccc(c1N(=O)(=O))C)c1
452	121-14-2	Benzene, 1-methyl-2,4-dinitro-	1.98	182.14	N(=O)(=O)c(ccc(c1N(=O)(=O))C)c1
456	121-75-5	Butanedioic acid, [(dimethoxyphosphinothioyl)thio]-, diethylester	2.36	330.35	CCOC(=O)CC(SP(=S)(OC)OC)C(=O)OCC
458	121-82-4	1,3,5-Triazine, hexahydro-1,3,5-trinitro- (RDX)	0.87	222.12	N(=O)(=O)N(CN(N(=O)(=O))CN1N(=O)(=O))C1
459	121-82-4	1,3,5-Triazine, hexahydro-1,3,5-trinitro- (RDX)	0.87	222.12	N(=O)(=O)N(CN(N(=O)(=O))CN1N(=O)(=O))C1
460	122-14-5	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl)ester phosphorothioic acid (Fenitrothion)	3.47	277.23	COP(=S)(OC)Oc1ccc(N(=O)=O)c(C)c1
461	122-14-5	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl)ester phosphorothioic acid (Fenitrothion)	3.47	277.23	COP(=S)(OC)Oc1ccc(N(=O)=O)c(C)c1
462	122-14-5	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl)ester phosphorothioic acid (Fenitrothion)	3.47	277.23	COP(=S)(OC)Oc1ccc(N(=O)=O)c(C)c1
463	122-14-5	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl)ester phosphorothioic acid (Fenitrothion)	3.47	277.23	COP(=S)(OC)Oc1ccc(N(=O)=O)c(C)c1
464	122-14-5	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl)ester phosphorothioic acid (Fenitrothion)	3.47	277.23	COP(=S)(OC)Oc1ccc(N(=O)=O)c(C)c1
465	122-14-5	*O*,*O*-Dimethyl *O*-(3-methyl-4-	3.47	277.23	COP(=S)(OC)Oc1ccc(N(=O)=O)c(C)c1

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
		nitrophenyl)ester phosphorothioic acid (Fenitrothion)			
466	122-14-5	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl)ester phosphorothioic acid (Fenitrothion)	3.47	277.23	COP(=S)(OC)Oc1ccc(N(=O)=O)c(C)c1
467	122-14-5	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl)ester phosphorothioic acid (Fenitrothion)	3.47	277.23	COP(=S)(OC)Oc1ccc(N(=O)=O)c(C)c1
476	122-34-9	Simazine	2.18	201.66	n(c(nc(n1)NCC)NCC)c1Cl
493	126-73-8	Phosphoric acid tributyl ester	4.00	266.32	O=P(OCCCC)(OCCCC)OCCCC
507	133-06-2	1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]-	2.80	300.59	O=C(N(SC(Cl)(Cl)Cl)C(=O)C1CC=CC2)C12
508	133-06-2	1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloromethyl)thio]-	2.80	300.59	O=C(N(SC(Cl)(Cl)Cl)C(=O)C1CC=CC2)C12
515	140-66-9	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	5.28	206.33	Oc(ccc(c1)C(CC(C)(C)C)(C)C)c1
531	226-36-8	Dibenz(a,h)acridine	5.67	279.34	c1ccc4c(c1)ccc5nc2c(ccc3ccccc23)cc45
533	298-00-0	Phosphorothioic acid, *O*,*O*-dimethyl O-(4-nitrophenyl)ester	3.04	263.21	COP(=S)(OC)Oc1ccc(cc1)N(=O)=O
539	299-84-3	Phosphorothioic acid, *O*,*O*-dimethyl O-(2,4,5-trichlorophenyl)ester	5.07	321.54	COP(=S)(OC)Oc1cc(Cl)c(Cl)cc1Cl
543	319-84-6	(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.80	290.83	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl
546	319-85-7	(1alpha,2beta,3alpha,4beta,5alpha,6beta)-1,2,3,4,5,6-Hexachlorocyclohexane	3.80	290.83	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl
547	319-86-8	(1alpha,2alpha,3alpha,4beta,5alpha,6beta)-1,2,3,4,5,6-hexachlorocyclohexane	4.14	290.83	C(C(C(C(C1Cl)Cl)Cl)Cl)(C1Cl)Cl
556	333-41-5	Phosphorothioic acid, *O*,*O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester	3.81	304.35	O(P(OCC)(Oc(nc(nc1C)C(C)C)c1)=S)CC
557	333-41-5	Phosphorothioic acid, *O*,*O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester	3.81	304.35	O(P(OCC)(Oc(nc(nc1C)C(C)C)c1)=S)CC
558	333-41-5	Phosphorothioic acid, *O*,*O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl]	3.81	304.35	O(P(OCC)(Oc(nc(nc1C)C(C)C)c1)=S)CC

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
		ester			
559	333-41-5	Phosphorothioic acid, *O*,*O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester	3.81	304.35	O(P(OCC)(Oc(nc(nc1C)C(C)C)c1)=S)CC
581	500-28-7	Phosphorothioic acid, *O*-(3-chloro-4-nitrophenyl) *O*,*O*-dimethyl ester	3.63	297.65	COP(=S)(OC)Oc1ccc(N(=O)=O)c(Cl)c1
606	556-67-2	Octamethylcyclotetrasiloxane (D4)	5.10	296.62	C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1
641	626-39-1	Benzene, 1,3,5-tribromo-	4.51	314.80	c(cc(cc1Br)Br)(c1)Br
652	634-67-3	2,3,4-Trichloroaniline	3.33	196.46	Nc1ccc(Cl)c(Cl)c1Cl
653	634-91-3	3,4,5-Trichloroaniline	3.32	196.46	Nc1cc(Cl)c(Cl)c(Cl)c1
654	634-93-5	2,4,6-Trichloroaniline	3.52	196.46	Nc(c(cc(c1)Cl)Cl)c1Cl
659	636-30-6	2,4,5-Trichloroaniline	3.45	196.46	Nc(c(cc(c1Cl)Cl)Cl)c1
673	873-63-2	3-Chlorobenzenemethanol	1.94	142.59	OCc1cc(Cl)ccc1
680	935-95-5	2,3,5,6-Tetrachlorophenol	3.88	231.89	Oc1c(Cl)c(Cl)cc(Cl)c1Cl
685	950-37-8	S-((5-Methoxy-2-oxo-1,3,4-thiadiazol-3(2H)-yl)methyl) *O*,*O*-dimethyl ester phosphorodithioic acid	2.20	302.32	S=P(OC)(OC)SCN1C(=O)SC(OC)=N1
706	1582-09-8	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	5.34	335.29	CCCN(CCC)c1c(cc(cc1N(=O)(=O))C(F)(F)F)N(=O)(=O)
707	1582-09-8	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	5.34	335.29	CCCN(CCC)c1c(cc(cc1N(=O)(=O))C(F)(F)F)N(=O)(=O)
708	1582-09-8	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	5.34	335.29	CCCN(CCC)c1c(cc(cc1N(=O)(=O))C(F)(F)F)N(=O)(=O)
709	1582-09-8	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	5.34	335.29	CCCN(CCC)c1c(cc(cc1N(=O)(=O))C(F)(F)F)N(=O)(=O)
710	1582-09-8	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	5.34	335.29	CCCN(CCC)c1c(cc(cc1N(=O)(=O))C(F)(F)F)N(=O)(=O)
711	1582-09-8	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	5.34	335.29	CCCN(CCC)c1c(cc(cc1N(=O)(=O))C(F)(F)F)N(=O)(=O)
712	1582-09-8	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(trifluoromethyl)-	5.34	335.29	CCCN(CCC)c1c(cc(cc1N(=O)(=O))C(F)(F)F)N(=O)(=O)
725	1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]dioxin	6.80	321.98	Clc3cc2Oc1cc(Cl)c(Cl)cc1Oc2cc3Cl

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
726	1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]dioxin	6.80	321.98	Clc3cc2Oc1cc(Cl)c(Cl)cc1Oc2cc3Cl
727	1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]dioxin	6.80	321.98	Clc3cc2Oc1cc(Cl)c(Cl)cc1Oc2cc3Cl
728	1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]dioxin	6.80	321.98	Clc3cc2Oc1cc(Cl)c(Cl)cc1Oc2cc3Cl
729	1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]dioxin	6.80	321.98	Clc3cc2Oc1cc(Cl)c(Cl)cc1Oc2cc3Cl
730	1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]dioxin	6.80	321.98	Clc3cc2Oc1cc(Cl)c(Cl)cc1Oc2cc3Cl
731	1746-01-6	2,3,7,8-Tetrachlorodibenzo[b,e][1,4]dioxin	6.80	321.98	Clc3cc2Oc1cc(Cl)c(Cl)cc1Oc2cc3Cl
739	1897-45-6	1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro-	3.05	265.91	N#Cc(c(c(c(c1C#N)Cl)Cl)Cl)c1Cl
746	2051-24-3	Decachlorobiphenyl	8.18	498.66	Clc1c(Cl)c(Cl)c(c(Cl)c1Cl)c2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl
747	2104-64-5	Ethyl *p*-nitrophenyl phenylphosphonothioate	4.78	323.31	CCOP(=S)(Oc1ccc(cc1)N(=O)=O)c2ccccc2
748	2104-64-5	Ethyl *p*-nitrophenyl phenylphosphonothioate	4.78	323.31	CCOP(=S)(Oc1ccc(cc1)N(=O)=O)c2ccccc2
755	2104-96-3	Bromophos	5.21	365.99	COP(=S)(OC)Oc1cc(Cl)c(Br)cc1Cl
764	2255-17-6	Dimethylphosphoric acid 3-methyl-4-nitrophenyl	1.69	261.17	O=P(OC)(OC)Oc1cc(C)c(N(=O)(=O))cc1
765	2385-85-5	Mirex	6.89	545.55	ClC2(Cl)C4(Cl)C1(Cl)C5(Cl)C(Cl)(Cl)C3(Cl)C1(Cl)C2(Cl)C3(Cl)C45Cl
767	2463-84-5	*O*-(2-Chloro-4-nitrophenyl) *O*,*O*-dimethyl ester phosphorothioic acid	3.72	297.65	COP(=S)(OC)Oc1ccc(cc1Cl)N(=O)=O
772	2597-03-7	alpha-[(Dimethoxyphosphinothioyl)thio] benzeneacetic acid, ethyl ester	3.69	320.36	CCOC(=O)C(SP(=S)(OC)OC)c1ccccc1
784	2636-26-2	*O*-(4-Cyanophenyl) *O*,*O*-dimethyl ester, phosphorothioic acid	2.71	243.22	COP(=S)(OC)Oc1ccc(C#N)cc1
788	2691-41-0	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX)	0.19	296.16	O=N(=O)N(CN(N(=O)=O)CN(N(=O)=O)CN1N(=O)=O)C1
789	2921-88-2	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	4.96	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
790	2921-88-2	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	4.96	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
791	2921-88-2	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	4.96	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
792	2921-88-2	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	4.96	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
793	2921-88-2	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	4.96	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
794	2921-88-2	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	4.96	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
795	2921-88-2	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	4.96	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
796	2921-88-2	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	4.96	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
797	2921-88-2	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	4.96	350.59	CCOP(=S)(OCC)Oc1nc(Cl)c(Cl)cc1Cl
808	3268-87-9	1,2,3,4,5,6,7,8-Octachlorodibenzo-*p*-dioxin	8.20	459.76	Clc3c(Cl)c(Cl)c2Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Oc2c3Cl
811	3761-41-9	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylsulfinyl)phenyl]ester phosphorothioic acid	1.93	294.32	COP(=S)(OC)Oc1ccc(S(C)=O)c(C)c1
812	3761-42-0	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylsulfonyl)phenylester phosphorothioic acid	2.05	310.32	S(=O)(=O)(C)c1c(C)cc(OP(=S)(OC)OC)cc1
816	3811-49-2	2-Methoxy-4H-1,3,2-benzodioxaphosphorin-2-sulfide	2.67	216.19	c1ccc2COP(=S)(OC)Oc2c1
862	13674-87-8	2-Propanol, 1,3-dichloro-, phosphate (3:1)	3.65	430.91	O=P(OC(CCl)CCl)(OC(CCl)CCl)OC(CCl)CCl
871	15862-07-4	2,4,5-Trichloro-1,1'-biphenyl	5.60	257.55	Clc1cc(Cl)c(cc1Cl)c2ccccc2
876	16606-02-3	2,4',5-Trichloro-1,1'-biphenyl	5.67	257.55	Clc1ccc(cc1)c2cc(Cl)ccc2Cl
883	18181-70-9	Phosphorothioic acid, *O*-(2,5-dichloro-4-iodophenyl) *O*,*O*-dimethyl ester	5.51	413.00	COP(=S)(OC)Oc1cc(Cl)c(I)cc1Cl
884	18708-70-8	1,3,5-Trichloro-2-nitrobenzene	3.69	226.45	O=N(=O)c(c(cc(c1)Cl)Cl)c1Cl
887	18854-01-8	Phosphorothioic acid, *O*,*O*-diethyl-*O*-(5-phenyl-3-isoxazolyl)ester	3.73	313.31	S=P(OCC)(OCC)Oc2noc(c1ccccc1)c2
888	19408-74-3	1,2,3,7,8,9-Hexachlorodibenzo-*p*-dioxin	7.30	390.87	Clc(c1c3Oc2c(c(Cl)c(c(Cl)c2)Cl)O1)c(c(Cl)c3)Cl
889	19666-30-9	3-[2,4-Dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-	4.80	345.23	CC(C)Oc1cc(c(Cl)cc1Cl)N2N=C(OC2=O)C(C)(C)C

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
		dimethylethyl)-1,3,4-oxadiazol-2(3H)-one			
919	28249-77-6	Diethylcarbamothioic acid, S-[(4-chlorophenyl)methyl]ester	3.40	257.78	CCN(CC)C(=O)SCc1ccc(Cl)cc1
929	30746-58-8	1,2,3,4-Tetrachlorodibenzo-*p*-dioxin	6.60	321.98	Clc1c(Cl)c(Cl)c2Oc3ccccc3Oc2c1Cl
932	32861-85-1	2,4-Dichloro-1-(3-methoxy-4-nitrophenoxy)benzene	4.40	314.13	c1cc(Cl)cc(Cl)c1Oc2cc(OC)c(N(=O)(=O))cc2
933	33576-92-0	*O*,*O*-Dimethyl-*O*-phenylphosphorothioate	3.00	218.21	S=P(OC)(OC)Oc1ccccc1
934	33857-26-0	2,7-Dichlorodibenzo[b,e][1,4]dioxin	5.75	253.09	Clc3ccc2Oc1cc(Cl)ccc1Oc2c3
937	35065-27-1	2,2',4,4',5,5'-Hexachloro-1,1'-biphenyl	6.92	360.88	Clc1cc(Cl)c(cc1Cl)c2cc(Cl)c(Cl)cc2Cl
938	35065-27-1	2,2',4,4',5,5'-Hexachloro-1,1'-biphenyl	6.92	360.88	Clc1cc(Cl)c(cc1Cl)c2cc(Cl)c(Cl)cc2Cl
939	35065-27-1	2,2',4,4',5,5'-Hexachloro-1,1'-biphenyl	6.92	360.88	Clc1cc(Cl)c(cc1Cl)c2cc(Cl)c(Cl)cc2Cl
940	35693-99-3	2,2',5,5'-Tetrachloro-1,1'-biphenyl	5.84	291.99	c1c(Cl)ccc(Cl)c1c2c(Cl)ccc(Cl)c2
941	35693-99-3	2,2',5,5'-Tetrachloro-1,1'-biphenyl	5.84	291.99	c1c(Cl)ccc(Cl)c1c2c(Cl)ccc(Cl)c2
942	35693-99-3	2,2',5,5'-Tetrachloro-1,1'-biphenyl	5.84	291.99	c1c(Cl)ccc(Cl)c1c2c(Cl)ccc(Cl)c2
943	35693-99-3	2,2',5,5'-Tetrachloro-1,1'-biphenyl	5.84	291.99	c1c(Cl)ccc(Cl)c1c2c(Cl)ccc(Cl)c2
945	35822-46-9	1,2,3,4,6,7,8-Heptachlorodibenzo-*p*-dioxin	7.80	425.31	Clc1c(Cl)c(Cl)c2Oc3cc(Cl)c(Cl)c(Cl)c3Oc2c1Cl
958	39001-02-0	1,2,3,4,5,6,7,8-Octachlorodibenzofuran	8.20	443.76	Clc3c(Cl)c(Cl)c1c(oc2c(Cl)c(Cl)c(Cl)c(Cl)c12)c3Cl
959	39227-28-6	1,2,3,4,7,8-Hexachlorodibenzo-*p*-dioxin	7.30	390.87	Clc1c(Cl)c(Cl)c2Oc3ccc(Cl)c(Cl)c3Oc2c1Cl
960	39227-58-2	1,2,4-Trichlorodibenzo[b,e][1,4]dioxin	6.35	287.53	Clc3cc(Cl)c2Oc1ccccc1Oc2c3Cl
961	40321-76-4	1,2,3,7,8-Pentachlorodibenzo-*p*-dioxin	6.64	356.42	ClC(C1=C2OC(C=C3Cl)=C(C=C3Cl)O1)=C(C(Cl)=C2)Cl
965	50512-35-1	Bis(1-methylethyl)ester, 1,3-dithiolan-2-ylidene propanedioic acid	2.88	290.39	CC(C)OC(=O)C(C(=O)OC(C)C)=C1SCCS1
966	50512-35-1	Bis(1-methylethyl)ester, 1,3-dithiolan-2-ylidene propanedioic acid	2.88	290.39	CC(C)OC(=O)C(C(=O)OC(C)C)=C1SCCS1
967	50512-35-1	Bis(1-methylethyl)ester, 1,3-dithiolan-2-ylidene propanedioic acid	2.88	290.39	CC(C)OC(=O)C(C(=O)OC(C)C)=C1SCCS1
968	51207-31-9	2,3,7,8-Tetrachlorodibenzofuran	6.53	305.98	Clc3cc2oc1cc(Cl)c(Cl)cc1c2cc3Cl
970	51630-58-1	Cyano(3-phenoxyphenyl)methyl ester, 4-Chloro-alpha-(1-methylethyl) benzeneacetic acid	6.20	419.91	CC(C)C(C(=O)OC(C#N)c2cccc(Oc1ccccc1)c2)c3ccc(Cl)cc3

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
971	52918-63-5	[1R-[1 alpha(S*),3 alpha]]Cyano(3-phenoxyphenyl)methyl ester 3-(2,2-dibromoethenyl)-2,2-dimethyl cyclopropane carboxylic acid	6.20	505.21	CC1(C)C(C=C(Br)Br)C1C(=O)OC(C#N)c3cccc(Oc2ccccc2)c3
975	57018-04-9	*O*-(2,6-Dichloro-4-methylphenyl) *O*,*O*-dimethyl ester, phosphorothioic acid	4.56	301.13	S=P(OC)(OC)Oc1c(Cl)cc(C)cc1Cl
982	57117-31-4	2,3,4,7,8-Pentachlorodibenzofuran	6.64	340.42	c1(Cl)cc2c3cc(Cl)c(Cl)cc3oc2c(Cl)c1Cl
984	57117-44-9	1,2,3,6,7,8-Hexachlorodibenzofuran	7.30	374.87	Clc1c(Cl)c2c3cc(Cl)c(Cl)c(Cl)c3Oc2cc1Cl
985	57653-85-7	1,2,3,6,7,8-Hexachlorodibenzo-*p*-dioxin	7.30	390.87	Clc2cc1Oc3c(Oc1c(Cl)c2Cl)cc(Cl)c(Cl)c3Cl
986	59080-33-0	2,4,6-Tribromobiphenyl	6.03	390.90	Brc2c(c(cc(c2)Br)Br)c1ccccc1
987	59080-37-4	2,2',5,5'-Tetrabromobiphenyl	6.50	469.80	Brc2c(c(ccc2)Br)c1c(cccc1Br)Br
988	59261-08-4	2,2',4,4',6,6'-Hexabromobiphenyl	7.20	627.59	Brc2c(c(cc(c2)Br)Br)c1c(cc(cc1Br)Br)Br
991	60851-34-5	2,3,4,6,7,8-Hexachlorodibenzofuran	7.30	374.87	Clc1cc2c3cc(Cl)c(Cl)c(Cl)c3Oc2c(Cl)c1Cl
992	61949-76-6	cis-Permethrin	7.43	391.30	O=C(OCC2=CC=CC(OC3=CC=CC=C3)=C2)C1C(C)(C)C1C=C(Cl)Cl
993	66332-96-5	*N*-[3-(1-Methylethoxy)phenyl]-2-(trifluoromethyl)benzamide	3.70	323.32	C(F)(F)(F)c1ccccc1C(=O)Nc2cccc(OC(C)C)c2
994	67375-30-8	[1 alpha(S*), 3 alpha]-(+-)-3-(2,2-dichloroethenyl)-2,2-dimethylcyclopropane carboxylic acid cyano (3-phenoxyphenyl)methyl ester	6.38	416.31	ClC(Cl)=CC1C(C)(C)C1C(=O)OC(C#N)c2cccc(Oc3ccccc3)c2
995	67562-39-4	1,2,3,4,6,7,8-Heptachlorodibenzofuran	7.40	409.31	c1(Cl)c(Cl)c2c3cc(Cl)c(Cl)c(Cl)c3oc2c(Cl)c1Cl
998	84852-15-3	Phenol, 4-nonyl-, branched,	5.92	220.36	Oc1ccc(cc1)CCCCCCC(C)C

Notes: [1] Reference number from the original data set.

Table C.2 Arnot data set – bioconcentration data

Ref No. [1]	Substance	Common name	Scientific name	BCF (l/kg)	k_2 (day^{-1})	Depuration half-life (days)	Fish lipid content [2] (kg/kg)	Reference [3]
1	C-12-2-LAS	Fathead minnow	*Pimephales promelas*	144	0.7	1.0	0.050	Tolls and Sijm (1999)
2	Octaethylene glycol monotridecyl ether	Fathead minnow	*Pimephales promelas*	32	10.1	0.1	0.033	Tolls and Sijm (1999)
3	Octaethylene glycol monotridecyl ether	Fathead minnow	*Pimephales promelas*	32	10.1	0.1	0.033	Tolls and Sijm (1999)
4	C-12-5-LAS	Fathead minnow	*Pimephales promelas*	10	1.2	0.6	0.050	Tolls (1998)
8	NL-63A	Common carp	*Cyprinus carpio*	8,400	0.18	3.9	0.038	Yakata et al. (2003)
9	NL-63B	Common carp	*Cyprinus carpio*	5,080	0.16	4.3	0.038	Yakata et al. (2003)
11	Methyl isocyanothion	Guppy	*Poecilia reticulata*	216	1.18	0.6	0.088	De Bruijn and Hermens (1991)
17	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylthio)phenyl]ester phosphorothioic acid	Guppy	*Poecilia reticulata*	1,461	0.6	1.2	0.088	De Bruijn and Hermens (1991)
18	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylthio)phenyl]ester phosphorothioic acid	Medaka	*Oryzias latipes*	154	4.8	0.1	0.048	Tsuda et al. (1996)
19	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylthio)phenyl]ester phosphorothioic acid	Common carp	*Cyprinus carpio*	26	8.16	0.1	0.048	Tsuda et al. (1993a)
20	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylthio)phenyl]ester phosphorothioic acid	Medaka	*Oryzias latipes*	100	3.36	0.2	0.048	Tsuda et al. (1995)
29	Benzo[a]anthracene	Fathead minnow	*Pimephales promelas*	260	1.53	0.5	0.048	de Maagd et al. (1998)
34	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	Zebrafish	*Brachydanio rerio*	850	1.32	0.5	0.066	Butte et al. (1991)
35	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	Bluegill sunfish	*Lepomis macrochirus*	297	0.56	1.2	0.022	La Rocca et al. (1991)

Ref No. [1]	Substance	Common name	Scientific name	BCF (l/kg)	k_2 (day^{-1})	Depuration half-life (days)	Fish lipid content [2] (kg/kg)	Reference [3]
36	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	Rainbow trout	*Oncorhynchus mykiss*	360	0.72	1.0	0.028	La Rocca et al. (1991)
37	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	Zebrafish	*Brachydanio rerio*	560	0.92	0.8	0.042	La Rocca et al. (1991)
38	Cyclohexane, 1,2,3,4,5,6-hexachloro-, (1a,2a,3B,4a,5a,6B)-	Guppy	*Poecilia reticulata*	730	0.36	1.9	0.056	La Rocca et al. (1991)
54	Benzenamine	Medaka	*Oryzias latipes*	2	154	0.004	0.048	Bradbury et al. (1993)
111	Phenol, 4,4 -(1-methylethylidene)bis-	Zebrafish	*Brachydanio rerio*	6	15.1	0.05	0.048	Lindholst et al. (2003)
145	Benzene, 1,2,3-trichloro-	Guppy	*Poecilia reticulata*	794	0.43	1.6	0.137	de Wolf et al. (1993)
158	Phenol, pentachloro-	Rainbow trout	*Oncorhynchus mykiss*	200	0.6	1.2	0.070	McKim et al. (1986)
159	Phenol, pentachloro-	Rainbow trout	*Oncorhynchus mykiss*	460	0.26	2.6	0.070	McKim et al. (1986)
160	Phenol, pentachloro-	Flagfish	*Jordanella floridae*	216	1.03	0.7	0.133	Smith et al. (1990)
161	Phenol, pentachloro-	Rainbow trout	*Oncorhynchus mykiss*	219	1.56	0.4	0.048	Stehly and Hayton (1989)
162	Phenol, pentachloro-	Goldfish	*Carassius auratus*	129	3.94	0.2	0.048	Stehly and Hayton (1990)
163	Phenol, pentachloro-	Goldfish	*Carassius auratus*	607	1.56	0.4	0.048	Stehly and Hayton (1990)
164	2,4,6-Trichlorophenol	Flagfish	*Jordanella floridae*	88	4.78	0.1	0.124	Smith et al. (1990)
200	4,4'-Dibromo biphenyl	Guppy	*Poecilia reticulata*	17,495	0.12	5.6	0.065	Gobas et al. (1989)
214	Benzenamine, 2-chloro-	Common carp	*Cyprinus carpio*	2	4.56	0.2	0.048	Tsuda et al. (1993b)
215	Benzenamine, 2-chloro-	Common carp	*Cyprinus carpio*	4	4.56	0.2	0.048	Tsuda et al. (1993b)
236	Benzene, 1,2,4,5-tetrachloro-	Flagfish	*Jordanella floridae*	4,050	0.4	1.7	0.085	Smith et al. (1990)
311	4-Chlorobenzaldehyde	Medaka	*Oryzias latipes*	2	2.64	0.3	0.048	Tsuda et al. (1997a)
316	Benzene, 1,4-dibromo-	Guppy	*Poecilia reticulata*	91	1.41	0.5	0.065	Gobas et al. (1989)
321	Benzene, 1,4-dichloro-	Flagfish	*Jordanella floridae*	296	0.98	0.7	0.085	Smith et al. (1990)
326	Benzenamine, 4-chloro-	Medaka	*Oryzias latipes*	7	99	0.0	0.048	Bradbury et al. (1993)

Ref No. [1]	Substance	Common name	Scientific name	BCF (l/kg)	k_2 (day^{-1})	Depuration half-life (days)	Fish lipid content [2] (kg/kg)	Reference [3]
327	Benzenamine, 4-chloro-	Common carp	*Cyprinus carpio*	1	3.84	0.2	0.048	Tsuda et al. (1993b)
328	Benzenamine, 4-chloro-	Common carp	*Cyprinus carpio*	2	3.84	0.2	0.048	Tsuda et al. (1993b)
338	Benzenamine, 3-chloro-	Common carp	*Cyprinus carpio*	1	5.04	0.1	0.048	Tsuda et al. (1993b)
339	Benzenamine, 3-chloro-	Common carp	*Cyprinus carpio*	2	5.04	0.1	0.048	Tsuda et al. (1993b)
381	Phosphoric acid, triphenyl ester	Medaka	*Oryzias latipes*	191	13.9	0.1	0.048	Sasaki et al. (1982)
383	Ethanol, 2-chloro-, phosphate (3:1)	Medaka	*Oryzias latipes*	1	23.8	0.0	0.048	Sasaki et al. (1982)
386	1,2,4,5-Tetrachloro-3-nitrobenzene	Rainbow trout	*Oncorhynchus mykiss*	1,362	0.28	2.5	0.084	Niimi et al. (1989)
394	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	Fathead minnow	*Pimephales promelas*	588	0.049	14.2	0.048	Mayer (1976)
395	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	Fathead minnow	*Pimephales promelas*	620	0.11	6.2	0.048	Mayer (1976)
396	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	Fathead minnow	*Pimephales promelas*	930	0.059	11.8	0.048	Mayer (1976)
397	1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	Fathead minnow	*Pimephales promelas*	1,000	0.11	6.2	0.048	Mayer (1976)
418	Benzene, 2-methyl-1,3,5-trinitro-	Sheepshead minnow	*Cyprinodon variegatus*	10	24.5	0.0	0.048	Lotufo and Lydy (2005)
419	Phosphorothioic acid, *O*-(1,6-dihydro-6-oxo-1-phenyl-3-pyridazinyl) *O*,*O*-diethyl ester	Common carp	*Cyprinus carpio*	5	10.3	0.1	0.048	Tsuda et al. (1993a)
441	Benzene, 1,2,4-trichloro-	Flagfish	*Jordanella floridae*	2,026	0.57	1.2	0.114	Smith et al. (1990)
451	Benzene, 1-methyl-2,4-dinitro-	Common carp	*Cyprinus carpio*	4	11.9	0.1	0.094	Lang et al. (1997)
452	Benzene, 1-methyl-2,4-dinitro-	Common carp	*Cyprinus carpio*	9	1.35	0.5	0.094	Lang et al. (1997)
456	Butanedioic acid, [(dimethoxyphosphinothioyl)thio] -, diethylester	Medaka	*Oryzias latipes*	11	6.48	0.1	0.048	Tsuda et al. (1997b)
458	1,3,5-Triazine, hexahydro-1,3,5-trinitro- (RDX)	Channel catfish	*Ictalurus punctatus*	2	15.3	0.0	0.048	Belden et al. (2005)
459	1,3,5-Triazine, hexahydro-1,3,5-trinitro- (RDX)	Sheepshead minnow	*Cyprinodon variegatus*	2	2.11	0.3	0.048	Lotufo and Lydy (2005)

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460	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl) ester phosphorothioic acid (Fenitrothion)	Guppy	*Poecilia reticulata*	202	1.13	0.6	0.088	De Bruijn and Hermens (1991)
461	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl) ester phosphorothioic acid (Fenitrothion)	Striped mullet	*Mugil cephalus*	30	2.67	0.3	0.027	Takimoto et al. (1987)
462	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl) ester phosphorothioic acid (Fenitrothion)	Striped mullet	*Mugil cephalus*	179	1.93	0.4	0.031	Takimoto et al. (1987)
463	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl) ester phosphorothioic acid (Fenitrothion)	Medaka	*Oryzias latipes*	235	2.89	0.2	0.049	Takimoto et al. (1987)
464	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl) ester phosphorothioic acid (Fenitrothion)	Medaka	*Oryzias latipes*	303	2.77	0.3	0.048	Takimoto et al. (1987)
465	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl) ester phosphorothioic acid (Fenitrothion)	Medaka	*Oryzias latipes*	339	2.67	0.3	0.082	Takimoto et al. (1987)
466	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl) ester phosphorothioic acid (Fenitrothion)	Medaka	*Oryzias latipes*	102	2.64	0.3	0.048	Tsuda et al. (1997b)
467	*O*,*O*-Dimethyl *O*-(3-methyl-4-nitrophenyl) ester phosphorothioic acid (Fenitrothion)	Medaka	*Oryzias latipes*	48	4.08	0.2	0.048	Tsuda et al. (1995)
476	Simazine	Willow shiner	*Gnathopogon caerulescens*	4	18.5	0.0	0.048	Tsuda et al. (1992)
493	Phosphoric acid tributyl ester	Medaka	*Oryzias latipes*	30	13.3	0.1	0.048	Sasaki et al. (1982)

Ref No. [1]	Substance	Common name	Scientific name	BCF (l/kg)	k_2 (day^{-1})	Depuration half-life (days)	Fish lipid content [2] (kg/kg)	Reference [3]
507	1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloro methyl)thio]-	Common carp	*Cyprinus carpio*	96	0.24	2.9	0.048	Tsuda et al. (1992)
508	1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-2-[(trichloro methyl)thio]-	Willow shiner	*Gnathopogon coerulescens*	362	0.48	1.4	0.048	Tsuda et al. (1992)
515	Phenol, 4-(1,1,3,3-tetramethyl butyl)-	Medaka	*Oryzias latipes*	261	2.16	0.3	0.022	Tsuda et al. (2001)
531	Dibenz(a,h) acridine	Fathead minnow	*Pimephales promelas*	107	3.36	0.2	0.048	Southworth et al. (1980)
533	Phosphorothioic acid, *O*,*O*-dimethyl *O*-(4-nitrophenyl) ester	Guppy	*Poecilia reticulata*	84	2.38	0.3	0.088	De Bruijn and Hermens (1991)
539	Phosphorothioic acid, *O*,*O*-dimethyl *O*-(2,4,5-trichlorophenyl)ester	Guppy	*Poecilia reticulata*	3,841	0.38	1.8	0.088	De Bruijn and Hermens (1991)
543	(1alpha,2alpha,3beta,4alpha,5 beta,6beta) 1,2,3,4,5,6-Hexachloro cyclohexane	Zebrafish	*Brachydanio rerio*	1,100	1.09	0.6	0.066	Butte et al. (1991)
546	(1alpha,2beta, 3alpha,4beta, 5alpha,6beta)-1,2,3,4,5,6-Hexachloro-cyclohexane	Zebrafish	*Brachydanio rerio*	1,460	0.67	1.0	0.066	Butte et al. (1991)
547	(1alpha,2alpha,3alpha,4beta, 5alpha,6 beta)-1,2,3,4,5,6-hexachlorocyclohexane	Zebrafish	*Brachydanio rerio*	1,770	0.80	0.9	0.066	Butte et al. (1991)
556	Phosphorothioic acid, *O*,*O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester	Guppy	*Poecilia reticulata*	59	1.92	0.4	0.048	Keizer et al. (1993)
557	Phosphorothioic acid, *O*,*O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester	Guppy	*Poecilia reticulata*	188	0.72	1.0	0.048	Keizer et al. (1993)
558	Phosphorothioic acid, *O*,*O*-diethyl *O*-[6-methyl-2-(1-methylethyl)-4-pyrimidinyl] ester	Medaka	*Oryzias latipes*	48	2.88	0.2	0.048	Tsuda et al. (1997b)
559	Phosphorothioic acid, *O*,*O*-diethyl *O*-[6-methyl-2-(1-	Medaka	*Oryzias latipes*	25	5.04	0.1	0.048	Tsuda et al. (1995)

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	methylethyl)-4-pyrimidinyl] ester							
581	Phosphorothioic acid, *O*-(3-Chloro-4-nitrophenyl) *O*,*O*-dimethyl ester	Guppy	*Poecilia reticulata*	36	6.98	0.1	0.088	De Bruijn and Hermens (1991)
606	Octamethyl cyclotetra siloxane (D4)	Fathead minnow	*Pimephales promelas*	12,169	0.18	3.8	0.064	Fackler et al. (1995)
641	Benzene, 1,3,5-tribromo-	Guppy	*Poecilia reticulata*	1,700	0.42	1.7	0.065	Gobas et al. (1989)
652	2,3,4-Trichloroaniline	Guppy	*Poecilia reticulata*	100	4.8	0.1	0.137	de Wolf et al. (1993)
653	3,4,5-Trichloroaniline	Guppy	*Poecilia reticulata*	229	3.12	0.2	0.137	de Wolf et al. (1993)
654	2,4,6-Trichloroaniline	Guppy	*Poecilia reticulata*	214	0.70	1.0	0.137	de Wolf et al. (1993)
659	2,4,5-Trichloroaniline	Guppy	*Poecilia reticulata*	214	3.84	0.2	0.137	de Wolf et al. (1993)
673	3-Chloro benzene methanol	Medaka	*Oryzias latipes*	19	2.16	0.3	0.048	Tsuda et al. (1997a)
680	2,3,5,6-Tetra chlorophenol	Flagfish	*Jordanella floridae*	142	1.71	0.4	0.098	Smith et al. (1990)
685	S-((5-Methoxy-2-oxo-1,3,4-thiadiazol-3(2H)-yl)methyl) *O*,*O*-dimethyl ester phosphoro dithioic acid	Common carp	*Cyprinus carpio*	3	13.0	0.1	0.048	Tsuda et al. (1993a)
706	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(tri fluoromethyl)-	Rainbow trout	*Oncorhynchus mykiss*	1,920	1.07	0.6	0.048	Schultz and Hayton (1994)
707	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(tri fluoromethyl)-	Rainbow trout	*Oncorhynchus mykiss*	2,050	0.46	1.5	0.074	Schultz and Hayton (1994)
708	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(tri fluoromethyl)-	Rainbow trout	*Oncorhynchus mykiss*	2,280	0.12	6.0	0.076	Schultz and Hayton (1994)
709	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(tri fluoromethyl)-	Bluegill sunfish	*Lepomis macrochirus*	1,819	0.23	3.0	0.070	Schultz and Hayton (1999)
710	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(tri fluoromethyl)-	Channel catfish	*Ictalurus punctatus*	2,548	0.17	4.1	0.040	Schultz and Hayton (1999)
711	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(tri fluoromethyl)-	Channel catfish	*Ictalurus punctatus*	3,880	0.22	3.2	0.070	Schultz and Hayton (1999)
712	Benzenamine, 2,6-dinitro-*N*,*N*-dipropyl-4-(tri fluoromethyl)-	Fathead minnow	*Pimephales promelas*	3,261	0.23	3.0	0.048	Spacie and Hamelink (1979)
725	2,3,7,8-Tetrachlorodibenzo	Common carp	*Cyprinus carpio*	49,000	0.014	48.0	0.096	Cook et al. (1991)

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	[b,e][1,4] dioxin							
726	2,3,7,8-Tetrachlorodibenzo [b,e][1,4]dioxin	Common carp	*Cyprinus carpio*	64,000	0.012	58.0	0.085	Cook et al. (1991)
727	2,3,7,8-Tetrachlorodibenzo [b,e][1,4]dioxin	Common carp	*Cyprinus carpio*	89,000	0.0083	84.0	0.055	Cook et al. (1991)
728	2,3,7,8-Tetrachlorodibenzo [b,e][1,4]dioxin	Fathead minnow	*Pimephales promelas*	97,000	0.013	52.0	0.190	Cook et al. (1991)
729	2,3,7,8-Tetrachlorodibenzo [b,e][1,4]dioxin	Fathead minnow	*Pimephales promelas*	159,000	0.012	59.0	0.190	Cook et al. (1991)
730	2,3,7,8-Tetrachlorodibenzo [b,e][1,4]dioxin	Guppy	*Poecilia reticulata*	16,857	0.049	14.1	0.097	Loonen et al. (1994)
731	2,3,7,8-Tetrachlorodibenzo [b,e][1,4]dioxin	Rainbow trout	*Oncorhynchus mykiss*	39,000	0.047	14.7	0.048	Mehrle et al. (1988)
739	1,3-Benzene dicarbonitrile, 2,4,5,6-tetrachloro-	Willow shiner	*Gnathopogon caerulescens*	18	0.96	0.7	0.048	Tsuda et al. (1992)
746	Decachloro biphenyl	Guppy	*Poecilia reticulata*	17,445	0.0050	138.3	0.065	Gobas et al. (1989)
747	Ethyl *p*-nitro phenyl phenyl phosphono thioate	Medaka	*Oryzias latipes*	1,119	0.48	1.4	0.048	Tsuda et al. (1997b)
748	Ethyl *p*-nitro phenyl phenyl phosphono thioate	Common carp	*Cyprinus carpio*	65	4.32	0.2	0.048	Tsuda et al. (1993a)
755	Bromophos	Guppy	*Poecilia reticulata*	3,931	0.33	2.1	0.088	De Bruijn and Hermens (1991)
764	Dimethylphosphoric acid 3-methyl-4-nitrophenyl	Medaka	*Oryzias latipes*	3	7.2	0.1	0.048	Tsuda et al. (1997b)
765	Mirex	Guppy	*Poecilia reticulata*	20,555	0.0046	151.6	0.065	Gobas et al. (1989)
767	*O*-(2-Chloro-4-nitrophenyl) *O*,*O*-dimethyl ester phosphorothioic acid	Guppy	*Poecilia reticulata*	78	2.54	0.3	0.088	De Bruijn and Hermens (1991)
772	alpha-[(Dimethoxyphosphinothioyl) thio]benzene acetic acid, ethyl ester	Common carp	*Cyprinus carpio*	28	12.5	0.1	0.048	Tsuda et al. (1993a)
784	*O*-(4-Cyano phenyl) *O*,*O*-	Guppy	*Poecilia reticulata*	37	4.2	0.2	0.088	De Bruijn and

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	dimethyl ester, phosphorothioic acid							Hermens (1991)
788	Octahydro-1,3,5,7-tetra nitro-1,3,5,7-tetrazocine (HMX)	Sheepshead minnow	*Cyprinodon variegatus*	1	2.95	0.2	0.048	Lotufo and Lydy (2005)
789	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	Guppy	*Poecilia reticulata*	600	0.51	1.4	0.090	Deneer (1993)
790	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	Guppy	*Poecilia reticulata*	875	0.4	1.7	0.090	Deneer (1993)
791	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	Guppy	*Poecilia reticulata*	1,523	0.46	1.5	0.090	Deneer (1993)
792	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	Guppy	*Poecilia reticulata*	1,563	0.49	1.4	0.090	Deneer (1993)
793	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	Guppy	*Poecilia reticulata*	3,150	0.3	2.3	0.090	Deneer (1993)
794	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	Guppy	*Poecilia reticulata*	3,363	0.25	2.8	0.090	Deneer (1993)
795	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	Threespine stickleback	*Gasterosteus aculeatus*	1,133	1.23	0.6	0.053	Deneer (1994)
796	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	Common carp	*Cyprinus carpio*	451	0.48	1.4	0.048	Tsuda et al. (1992)
797	Phosphorothioic acid, *O*,*O*-diethyl *O*-(3,5,6-trichloro-2-pyridinyl) ester	Guppy	*Poecilia reticulata*	1,650	0.49	1.4	0.048	Welling and de Vries (1992)
808	1,2,3,4,5,6,7,8-Octachlorodibenzo-*p*-dioxin	Guppy	*Poecilia reticulata*	1,529,000	0.12	5.8	0.097	Loonen et al. (1994)
811	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylsulfinyl)phenyl]ester	Medaka	*Oryzias latipes*	1	5.76	0.1	0.048	Tsuda et al. (1996)

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	phosphorothioic acid							
812	*O*,*O*-Dimethyl *O*-[3-methyl-4-(methylsulfonyl)phenylester phosphorothioic acid	Medaka	*Oryzias latipes*	3	3.84	0.2	0.048	Tsuda et al. (1996)
816	2-Methoxy-4H-1,3,2-benzodi oxaphosphorin-2-sulfide	Common carp	*Cyprinus carpio*	7	13.0	0.1	0.048	Tsuda et al. (1993a)
862	2-Propanol, 1,3-dichloro-, phosphate (3:1)	Medaka	*Oryzias latipes*	70	10.1	0.1	0.048	Sasaki et al. (1982)
871	2,4,5-Trichloro-1,1'-biphenyl	Guppy	*Poecilia reticulata*	6,066	0.063	11.0	0.065	Gobas et al. (1989)
876	2,4',5-Trichloro-1,1'-biphenyl	Guppy	*Poecilia reticulata*	14,127	0.063	11.0	0.075	Gobas and Schrap (1990)
883	Phosphorothioic acid, *O*-(2,5-dichloro-4-iodophenyl) *O*,*O*-dimethyl ester	Guppy	*Poecilia reticulata*	4,212	0.36	1.9	0.088	De Bruijn and Hermens (1991)
884	1,3,5-Trichloro-2-nitrobenzene	Rainbow trout	*Oncorhynchus mykiss*	760	0.28	2.5	0.084	Niimi et al. (1989)
887	Phosphorothioic acid, *O*,*O*-diethyl-*O*-(5-phenyl-3-isoxazolyl)ester	Common carp	*Cyprinus carpio*	405	0.72	1.0	0.048	Tsuda et al. (1992)
888	1,2,3,7,8,9-Hexachlorodibenzo-p-dioxin	Guppy	*Poecilia reticulata*	8,256	0.074	9.4	0.097	Loonen et al. (1994)
889	3-[2,4-Dichloro-5-(1-methyl ethoxy)phenyl]-5-(1,1-dimethyl ethyl)-1,3,4-oxadiazol-2(3H)-one	Willow shiner	*Gnathopogon coerulescens*	1,208	0.3	2.3	0.048	Tsuda et al. (1990)
919	Diethylcarbamothioic acid, S-[(4-chloro phenyl)methyl] ester	Medaka	*Oryzias latipes*	295	4.56	0.2	0.048	Tsuda et al. (1997a)
929	1,2,3,4-Tetrachlorodibenzo-*p*-dioxin	Guppy	*Poecilia reticulata*	3,812	1.2	0.6	0.075	Gobas and Schrap (1990)
932	2,4-Dichloro-1-(3-methoxy-4-nitrophenoxy) benzene	Willow shiner	*Gnathopogon coerulescens*	3,877	0.21	3.3	0.048	Tsuda et al. (1990)
933	*O*,*O*-Dimethyl-*O*-phenyl phosphoro thioate	Guppy	*Poecilia reticulata*	78	1.54	0.5	0.088	De Bruijn and Hermens (1991)
934	2,7-Dichloro dibenzo[b,e] [1,4]dioxin	Guppy	*Poecilia reticulata*	362	1.5	0.5	0.075	Gobas and Schrap (1990)

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937	2,2',4,4',5,5'-Hexachloro-1,1'-biphenyl	Guppy	*Poecilia reticulata*	270,000	0.002	346.6	0.048	Opperhuizen and Schrap (1987)
938	2,2',4,4',5,5'-Hexachloro-1,1'-biphenyl	Guppy	*Poecilia reticulata*	420,000	0.002	346.6	0.048	Opperhuizen and Schrap (1987)
939	2,2',4,4',5,5'-Hexachloro-1,1'-biphenyl	Guppy	*Poecilia reticulata*	440,000	0.002	346.6	0.048	Opperhuizen and Schrap (1987)
940	2,2',5,5'-Tetrachloro-1,1'-biphenyl	Guppy	*Poecilia reticulata*	68,063	0.016	42.7	0.065	Gobas et al. (1989)
941	2,2',5,5'-Tetrachloro-1,1'-biphenyl	Guppy	*Poecilia reticulata*	39,565	0.023	30.1	0.048	Opperhuizen and Schrap (1987)
942	2,2',5,5'-Tetrachloro-1,1'-biphenyl	Guppy	*Poecilia reticulata*	40,952	0.021	33.0	0.048	Opperhuizen and Schrap (1987)
943	2,2',5,5'-Tetrachloro-1,1'-biphenyl	Guppy	*Poecilia reticulata*	43,478	0.023	30.1	0.048	Opperhuizen and Schrap (1987)
945	1,2,3,4,6,7,8-Heptachlorodibenzo-p-dioxin	Guppy	*Poecilia reticulata*	4,643	0.081	8.6	0.097	Loonen et al. (1994)
958	1,2,3,4,5,6,7,8-Octachlorodibenzofuran	Guppy	*Poecilia reticulata*	771	0.17	4.0	0.097	Loonen et al. (1994)
959	1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	Guppy	*Poecilia reticulata*	9,926	0.065	10.7	0.097	Loonen et al. (1994)
960	1,2,4-Trichlorodibenzo[b,e][1,4]dioxin	Guppy	*Poecilia reticulata*	660	0.91	0.8	0.075	Gobas and Schrap (1990)
961	1,2,3,7,8-Pentachlorodibenzo-p-dioxin	Guppy	*Poecilia reticulata*	18,062	0.03	23.1	0.097	Loonen et al. (1994)
965	Bis(1-methyl ethyl)ester, 1,3-dithiolan-2-ylidene propanedioic acid	Medaka	*Oryzias latipes*	37	7.68	0.1	0.048	Tsuda et al. (1997c)
966	Bis(1-methyl ethyl)ester, 1,3-dithiolan-2-ylidene propanedioic acid	Medaka	*Oryzias latipes*	43	7.68	0.1	0.048	Tsuda et al. (1997c)
967	Bis(1-methyl ethyl)ester, 1,3-dithiolan-2-ylidene propanedioic acid	Common carp	*Cyprinus carpio*	27	4.56	0.2	0.048	Tsuda et al. (1992)
968	2,3,7,8-Tetrachlorodibenzo furan	Guppy	*Poecilia reticulata*	1,502	0.29	2.4	0.097	Loonen et al. (1994)

Ref No. [1]	Substance	Common name	Scientific name	BCF (l/kg)	k_2 (day^{-1})	Depuration half-life (days)	Fish lipid content [2] (kg/kg)	Reference [3]
970	Cyano(3-phenoxyphenyl)methyl ester, 4-chloro-alpha-(1-methylethyl) benzeneacetic acid	Rainbow trout	*Oncorhynchus mykiss*	702	0.22	3.1	0.080	Muir et al. (1994)
971	[1R-[1 alpha(S*),3 alpha]]Cyano(3-phenoxyphenyl)methyl ester 3-(2,2-dibromo ethenyl)-2,2-dimethyl cyclopropane carboxylic acid	Rainbow trout	*Oncorhynchus mykiss*	321	0.33	2.1	0.080	Muir et al. (1994)
975	*O*-(2,6-Dichloro-4-methylphenyl) *O*,*O*-dimethyl ester, Phosphorothioic acid	Common carp	*Cyprinus carpio*	222	0.96	0.7	0.048	Tsuda et al. (1992)
982	2,3,4,7,8-Pentachloro dibenzofuran	Guppy	*Poecilia reticulata*	13,390	0.044	15.8	0.097	Loonen et al. (1994)
984	1,2,3,6,7,8-Hexachloro dibenzofuran	Guppy	*Poecilia reticulata*	8,645	0.078	8.9	0.097	Loonen et al. (1994)
985	1,2,3,6,7,8-Hexachloro dibenzo-p-dioxin	Guppy	*Poecilia reticulata*	8,448	0.05	13.9	0.097	Loonen et al. (1994)
986	2,4,6-tri bromobiphenyl	Guppy	*Poecilia reticulata*	7,463	0.15	4.7	0.065	Gobas et al. (1989)
987	2,2',5,5'-tetra bromobiphenyl	Guppy	*Poecilia reticulata*	93,954	0.0098	70.9	0.065	Gobas et al. (1989)
988	2,2',4,4',6,6'-hexa bromobiphenyl	Guppy	*Poecilia reticulata*	46,017	0.0071	97.9	0.065	Gobas et al. (1989)
991	2,3,4,6,7,8-Hexachloro dibenzofuran	Guppy	*Poecilia reticulata*	9,479	0.10	6.7	0.097	Loonen et al. (1994)
992	*cis*-Permethrin	Rainbow trout	*Oncorhynchus mykiss*	448	0.45	1.5	0.080	Muir et al. (1994)
993	*N*-[3-(1-Methyl ethoxy)phenyl]-2-(trifluoro methyl) benzamide	Common carp	*Cyprinus carpio*	20	2.88	0.2	0.048	Tsuda et al. (1992)
994	[1 alpha(S*), 3 alpha]-(+-)-3-(2,2-Dichloro ethenyl)-2,2-dimethylcyclo propane carboxylic acid cyano (3-phenoxyphenyl)methyl ester	Rainbow trout	*Oncorhynchus mykiss*	278	0.22	3.2	0.080	Muir et al. (1994)
995	1,2,3,4,6,7,8-Heptachloro dibenzofuran	Guppy	*Poecilia reticulata*	2,798	0.13	5.5	0.097	Loonen et al. (1994)

Ref No. [1]	Substance	Common name	Scientific name	BCF (l/kg)	k_2 (day^{-1})	Depuration half-life (days)	Fish lipid content [2] (kg/kg)	Reference [3]
998	Phenol, 4-nonyl-, branched,	Medaka	*Oryzias latipes*	167	1.68	0.4	0.022	Tsuda et al. (2001)

Notes: [1]Reference number from the original data set.

[2]The lipid contents were either reported in the original paper or estimated by Arnot (it was not clear from the data set provided which is an estimated value and which is a measured value).

[3]References for the bioconcentration data are as follows.

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Table C.3 UBA set – substance identities

Ref No. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
UBA 3	Confidential	Confidential	5.10	Confidential	Confidential
UBA 10	Confidential	Confidential	3.20	Confidential	Confidential
UBA 10	Confidential	Confidential	3.20	Confidential	Confidential
UBA 11	Confidential	Confidential	3.80	Confidential	Confidential
UBA 11	Confidential	Confidential	3.80	Confidential	Confidential
UBA 13	Confidential	Confidential	3.40	Confidential	Confidential
UBA 13	Confidential	Confidential	3.40	Confidential	Confidential
UBA 14	Confidential	Confidential	3.40	Confidential	Confidential
UBA 14	Confidential	Confidential	3.40	Confidential	Confidential
UBA 3	Confidential	Confidential	5.10	Confidential	Confidential
UBA 4	Confidential	Confidential	2.90	Confidential	Confidential
UBA 4	Confidential	Confidential	2.90	Confidential	Confidential
UBA 5	Confidential	Confidential	4.90	Confidential	Confidential
UBA 5	Confidential	Confidential	4.90	Confidential	Confidential
UBA 6	Confidential	Confidential	2.86	Confidential	Confidential
UBA 6	Confidential	Confidential	2.86	Confidential	Confidential
UBA 9	Confidential	Confidential	2.59	Confidential	Confidential
UBA 9	Confidential	Confidential	2.59	Confidential	Confidential

Notes: [1]Reference number from the original data set.

Table C.4 UBA data set – bioconcentration data

Ref No. [1]	Substance	Common name	Scientific name	Experimental data				Reference [2]
				BCF (l kg^{-1})	k_2 (day^{-1})	Depuration half-life (days)	Fish lipid content (kg/kg)	
UBA 3	Confidential	Zebrafish	*Brachydanio rerio*	2,904	0.17	4.0	0.123	UBA
UBA 10	Confidential	Fathead minnow	*Pimephales promelas*	35	1.88	0.4	0.110	UBA
UBA 10	Confidential	Fathead minnow	*Pimephales promelas*	48	0.43	1.6	0.110	UBA
UBA 11	Confidential	Bluegill sunfish	*Lepomis macrochirus*	124	0.31	2.3	0.061	UBA
UBA 11	Confidential	Bluegill sunfish	*Lepomis macrochirus*	128	0.21	3.4	0.061	UBA
UBA 13	Confidential	Rainbow trout	*Oncorhynchus mykiss*	70	0.52	1.3	no data	UBA
UBA 13	Confidential	Rainbow trout	*Oncorhynchus mykiss*	59	0.13	5.5	no data	UBA
UBA 14	Confidential	Rainbow trout	*Oncorhynchus mykiss*	63	0.12	5.5	0.032	UBA
UBA 14	Confidential	Rainbow trout	*Oncorhynchus mykiss*	65	0.12	5.8	0.032	UBA
UBA 3	Confidential	Zebrafish	*Brachydanio rerio*	2,900	0.17	4.1	0.123	UBA
UBA 4	Confidential	Bluegill sunfish	*Lepomis macrochirus*	117	0.10	7.1	0.129	UBA
UBA 4	Confidential	Bluegill sunfish	*Lepomis macrochirus*	8	0.08	9.0	0.130	UBA
UBA 5	Confidential	Rainbow trout	*Oncorhynchus mykiss*	1,540	0.27	2.6	0.049	UBA
UBA 5	Confidential	Rainbow trout	*Oncorhynchus mykiss*	1,367	0.26	2.7	0.049	UBA
UBA 6	Confidential	Bluegill sunfish	*Lepomis macrochirus*	57	0.10	6.8	0.063	UBA
UBA 6	Confidential	Bluegill sunfish	*Lepomis macrochirus*	44	0.12	5.8	0.063	UBA
UBA 9	Confidential	Zebrafish	*Brachydanio rerio*	145	8.80	0.1	0.049	UBA
UBA 9	Confidential	Zebrafish	*Brachydanio rerio*	62	7.85	0.1	0.049	UBA

Notes: [1]Reference number from the original data set.

[2]All data provided by UBA. The test reports are confidential.

Table C.5 Gold standard data set – substance identities

Ref no. [1]	CAS No	Name	Log Kow	Molecular weight	Smiles
GS32	120-82-1	1,2,4-Trichlorobenzene	4.02	181.45	c(ccc(c1Cl)Cl)(c1)Cl
GS45	118-74-1	Hexachlorobenzene	5.73	284.78	c(c(c(c(c1Cl)Cl)Cl)Cl)(c1Cl)Cl
GS44	615-54-3	1,2,4-Tribromobenzene	4.66	314.80	c(ccc(c1Br)Br)(c1)Br
GS43	634-90-2	1,2,3,5-Tetrachlorobenzene	4.56	215.89	c(cc(c(c1Cl)Cl)Cl)(c1)Cl
GS42	87-61-6	1,2,3-Trichlorobenzene	4.05	181.45	c(c(c(cc1)Cl)Cl)(c1)Cl
GS41	106-37-6	1,4-Dibromobenzene	3.79	235.91	c(ccc(c1)Br)(c1)Br
GS40	106-46-7	1,4-Dichlorobenzene	3.44	147.00	c(ccc(c1)Cl)(c1)Cl
GS7	2027-17-0	2-Isopropylnaphthalene	4.63	170.26	c(c(ccc1C(C)C)ccc2)(c2)c1
GS8	2027-17-0	2-Isopropylnaphthalene	4.63	170.26	c(c(ccc1C(C)C)ccc2)(c2)c1
GS5	575-41-7	1,3-Dimethylnaphthalene	4.42	156.23	Cc2cc(C)c1ccccc1c2
GS3	91-57-6	2-Methylnaphthalene	3.86	142.20	c(c(ccc1C)ccc2)(c2)c1
GS4	91-57-6	2-Methylnaphthalene	3.86	142.20	c(c(ccc1C)ccc2)(c2)c1
GS6	575-41-7	1,3-Dimethylnaphthalene	4.42	156.23	Cc2cc(C)c1ccccc1c2
GS9	85-01-8	Phenanthrene	4.46	178.24	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3
GS1	91-20-3	Naphthalene	3.3	128.18	c(c(ccc1)ccc2)(c1)c2
GS2	91-20-3	Naphthalene	3.3	128.18	c(c(ccc1)ccc2)(c1)c2
GS13	3674-75-7	9-Ethylphenanthrene	5.38	206.29	c(ccc1c(ccc2)c3c2)cc1cc3CC
GS10	85-01-8	Phenanthrene	4.46	178.24	c(c(c(c(c1)ccc2)c2)ccc3)(c1)c3
GS11	883-20-5	9-Methylphenanthrene	4.89	192.26	c(ccc1c(ccc2)c3c2)cc1cc3C
GS12	883-20-5	9-Methylphenanthrene	4.89	192.26	c(ccc1c(ccc2)c3c2)cc1cc3C
GS14	3674-75-7	9-Ethylphenanthrene	5.38	206.29	c(ccc1c(ccc2)c3c2)cc1cc3CC
GS16	129-00-0	Pyrene	4.88	202.26	c(c(c(cc1)ccc2)c2cc3)(c1ccc4)c34
GS15	129-00-0	Pyrene	4.88	202.26	c(c(c(cc1)ccc2)c2cc3)(c1ccc4)c34

Notes: [1]Reference number from the original data set

Table C.6 Gold standard data set – bioconcentration data

Ref no. [1]	Substance	Common name	Scientific name	Experimental data				Reference[2]
				BCF (l kg^{-1})	k_2 (day^{-1})	Depuration half-life (days)	Fish lipid content (kg/kg)	
GS32	1,2,4-Trichlorobenzene	Guppy	*Poecilia reticulata*	1,139	0.49	1.4	not determined	van Eck et al. (1997)
GS45	Hexachlorobenzene	Mosquito fish	*Gambusia affinis*	3,730	0.49	1.4	0.031	Chaisuksant et al. (1997)
GS44	1,2,4-Tribromobenzene	Mosquito fish	*Gambusia affinis*	1,800	0.58	1.2	0.031	Chaisuksant et al. (1997)
GS43	1,2,3,5-Tetrachlorobenzene	Mosquito fish	*Gambusia affinis*	1,320	0.48	1.4	0.031	Chaisuksant et al. (1997)
GS42	1,2,3-Trichlorobenzene	Mosquito fish	*Gambusia affinis*	430	1.1	0.6	0.031	Chaisuksant et al. (1997)
GS41	1,4-Dibromobenzene	Mosquito fish	*Gambusia affinis*	220	1.32	0.5	0.031	Chaisuksant et al. (1997)
GS40	1,4-Dichlorobenzene	Mosquito fish	*Gambusia affinis*	78	1.44	0.5	0.031	Chaisuksant et al. (1997)
GS7	2-Isopropylnaphthalene	Sheepshead minnow	*Cyprinodon variegatus*	12,405	0.09	7.7	0.097	Jonsson et al. (2004)
GS8	2-Isopropylnaphthalene	Sheepshead minnow	*Cyprinodon variegatus*	13,420	0.16	4.3	0.097	Jonsson et al. (2004)
GS5	1,3-Dimethylnaphthalene	Sheepshead minnow	*Cyprinodon variegatus*	4,761	0.35	2.0	0.097	Jonsson et al. (2004)
GS3	2-Methylnaphthalene	Sheepshead minnow	*Cyprinodon variegatus*	2,921	0.62	1.1	0.097	Jonsson et al. (2004)
GS4	2-Methylnaphthalene	Sheepshead minnow	*Cyprinodon variegatus*	2,852	0.6	1.2	0.097	Jonsson et al. (2004)
GS6	1,3-Dimethylnaphthalene	Sheepshead minnow	*Cyprinodon variegatus*	3,426	0.47	1.5	0.097	Jonsson et al. (2004)
GS9	Phenanthrene	Sheepshead minnow	*Cyprinodon variegatus*	1,623	0.8	0.9	0.097	Jonsson et al. (2004)
GS1	Naphthalene	Sheepshead minnow	*Cyprinodon variegatus*	714	1.45	0.5	0.097	Jonsson et al. (2004)

Ref no. [1]	Substance	Common name	Scientific name	Experimental data				Reference[2]
				BCF (l kg^{-1})	k_2 (day^{-1})	Depuration half-life (days)	Fish lipid content (kg/kg)	
GS2	Naphthalene	Sheepshead minnow	*Cyprinodon variegatus*	692	1.27	0.5	0.097	Jonsson et al. (2004)
GS13	9-Ethylphenanthrene	Sheepshead minnow	*Cyprinodon variegatus*	875	0.56	1.2	0.097	Jonsson et al. (2004)
GS10	Phenanthrene	Sheepshead minnow	*Cyprinodon variegatus*	700	0.84	0.8	0.097	Jonsson et al. (2004)
GS11	9-Methylphenanthrene	Sheepshead minnow	*Cyprinodon variegatus*	595	0.72	1.0	0.097	Jonsson et al. (2004)
GS12	9-Methylphenanthrene	Sheepshead minnow	*Cyprinodon variegatus*	224	0.8	0.9	0.097	Jonsson et al. (2004)
GS14	9-Ethylphenanthrene	Sheepshead minnow	*Cyprinodon variegatus*	298	0.61	1.1	0.097	Jonsson et al. (2004)
GS16	Pyrene	Sheepshead minnow	*Cyprinodon variegatus*	50	0.89	0.8	0.097	Jonsson et al. (2004)
GS15	Pyrene	Sheepshead minnow	*Cyprinodon variegatus*	53	1.19	0.6	0.097	Jonsson et al. (2004)

Notes: [1]Reference number from the original data set.

[2]References for the bioconcentration data are as follows:

Chaisuksant Y, Yu, Q. and Connell, D.W., 1997. Bioconcentration of bromo- and chlorobenzenes by fish (*Gambusia affinis*). *Water Research*, 31, 61-68.

Jonsson, G., Bechmann, R.K., Bamber, S.D. and Baussant, T, 2004. Bioconcentration, biotransformation, and elimination of polycyclic aromatic hydrocarbons in sheepshead minnows (*Cyprinodon variegatus*) exposed to contaminated seawater. *Environmental Toxicology and Chemistry*, 23, 1538-1548.

Van Eck, J.M.C., Koelmans, A.A. and Deneer, J.W., 1997. Uptake and elimination of 1,2,4-trichlorobenzene in the guppy (*Poecilia reticulata*) at sublethal and lethal aqueous concentrations. *Chemosphere*, 34, 2259-2270.

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