Development and Application of Models of Chemical Fate in Canada

Practical Methods for Estimating Environmental Biodegradation Rates

Report to Environment Canada

CEMN Report No. 200503

Prepared by:

Jon Arnot, Todd Gouin, Don Mackay

Practical Methods for Estimating Environmental Biodegradation Rates

Jon Arnot
Todd Gouin
Don Mackay

Canadian Environmental Modelling Network

March 31, 2005

Executive Summary

Extensive research has been conducted towards understanding and estimating biodegradation processes, yet for the vast majority of chemicals in commerce environmentally relevant biodegradation half-life values remain uncertain and difficult to access or estimate. The uncertainty in these rates is partially attributable to the observed natural variability resulting from different environmental conditions such as temperature, bioavailability and the genetic competence of microbial communities that may or may not be present. It is important to maximize the accuracy of chemical biodegradation rate data in the environment to minimize uncertainty associated with hazard and risk assessments. In this report a practical method for estimating biodegradation rates is described. It utilizes the inherent knowledge of the BIOWIN suite of biodegradation models. The models are calibrated to empirical aerobic environmental half-life data from 40 selected "training set" chemicals. The outcome of this calibration is compared to 115 "evaluation set" chemicals of environmental aerobic biodegradation. The calibrated BIOWIN estimation method is further compared with empirical half-life data and illustrative estimates from another biodegradation model (CATABOL). This evaluation reveals that the average absolute error is 116 and 2537 for the proposed method and CATABOL, respectively. The root mean square error is 279 and 5119 for the proposed method and CATABOL, respectively. This evaluation is not intended to be a direct model comparison since the revised BIOWIN predictions are a result of calibration to a subset of the evaluation set, whereas CATABOL is not. The potential application of the modified BIOWIN estimation method to a large number of chemical substances is investigated. A companion and more speculative method suggested in this report incorporates a "slide rule" approach for assessing all available empirical and estimated data for the biotransformation rate of a chemical.

Table of Contents

Introduction

Chemicals in the environment are subject to processes such as transport (e.g., advection in a river), multimedia partitioning (e.g., air-water) and reaction (e.g., photolysis, hydrolysis and biodegradation). Chemical and biological reactions, or transformations, are the only mechanisms that alter and ultimately remove a chemical from the global environment. Biodegradation is the transformation of a chemical as a result of a living organism. All organisms including microorganisms, plants, insects and animals perform enzymatic chemical transformations. Generally, higher order organisms transform chemicals so that they can be more readily eliminated, whereas simpler organisms such as bacteria and fungi are responsible for most of the extensive biodegradation in the environment. Primary biodegradation changes the identity of the parent chemical as a first step to more extensive mineralisation, whereas ultimate biodegradation results in the complete mineralisation of the chemical to water, carbon dioxide and inorganic compounds [1]. Biodegradation is arguably one of the most important processes influencing the amount and persistence of chemical in the environment [2] but unfortunately the rates of these processes are poorly understood.

Multimedia models are used to provide quantitative understandings of the environmental fate of chemicals and to assess potential risks to ecosystems and humans. Accurate media specific half-lives are essential for the reliable assessment of chemicals. Assuming first order kinetics the half-life $t_{1/2}$ can be derived from a rate constant k as 0.693 / k. Fairly reliable methods are available for estimating the chemical half-life due to abiotic processes (e.g., [3]) but environmentally relevant biodegradation half-life information remains a major source of uncertainty [4]. Hazard assessment requires persistence data, which are dependent on the half-lives. Emissions and persistence control the mass and concentration of a chemical in the environment and hence the ultimate exposure and potential risk of a chemical. There is a need to improve existing methods of estimating environmental primary biodegradation half-lives to provide greater confidence in chemical assessments.

The objective of this report is to describe and evaluate pragmatic methods for estimating environmentally relevant aerobic primary biodegradation half-lives as required for multimedia fate models. Two relatively simple and robust methods are described and evaluated. In the first method the inherent knowledge from four BIOWIN models is "calibrated" to empirical field-based half-life data. The ensuing predictions are then evaluated with empirical data and an example of other estimation methods (i.e., CATABOL). The potential for applying this method to a large number of chemicals, i.e., 10,600 organic chemicals, is investigated. The second, and more speculative, companion method describes a "slide-rule" approach that can be used to combine biotransformation information from all estimation sources and thus assess a substance's inherent susceptibility to degradation in a more pictorial manner.

Sources of biodegradation data

Current sources of empirical biodegradation information include laboratory tests, field data, environmental handbooks and other databases. Standardized laboratory tests are

used to obtain empirical estimates of a chemical's biodegradation potential. These include a suite of guideline tests recommended by the Organization for Economic Cooperation and Development (OECD). These tests are considered as standards for estimating the "ready" or "nonready" biodegradability of a substance. The protocols are not designed to provide an estimated rate for primary chemical transformation and the conditions employed are not relevant to environmental conditions. Extrapolation methods from laboratory tests have been suggested but these have been met with mixed reviews [5, 6]. Field studies (e.g., grab samples, river die-away) have been conducted for a few chemicals but such data are non-existent for most chemicals. Environmental handbooks (e.g, [7, 8]) provide collections of empirical data and can also provide guidelines for overall media specific half-lives. These sources provide compiled data and expert judgment, however they are generally limited in the scope of information they can offer for the vast number of chemicals used in commerce. Qualitative information is available for many biodegradation pathways most notably the University of Minnesota Biocatalysis/Biodegradation Database [2] and a Biodegradability Evaluation and Simulation System (BESS). Two other major sources of empirical information are the Syracuse Research Corporation's BIODEG database, which contains over 5,800 records of experimental results on biodegradation studies for approximately 800 chemicals and the Japanese Ministry of International Trade and Industry (MITI) database. Most of these data are derived from laboratory studies. These databases have been used in model development but these models are not considered to be directly applicable for estimating environmentally relevant biodegradation rates for a large number of chemicals.

A variety of models has been developed to predict biodegradation. These include structure-biodegradability relationships (SBRs) and quantitative structure-biodegradability relationships (QSBRs). SBRs provide qualitative endpoints such as passing or failing a ready biodegradation test while QSBRs provide an estimation of rate or half-life. Examples of such models include BESS, BIOWIN, CATABOL, TOPKAT, and Multicase. Howard [1] and Jaworska et al [9] provide reviews for many of the different estimation methods currently available. These models are continually being refined and improved.

The Biodegradation Probability Program (BIOWIN) estimates the probability for the rapid biodegradation of an organic chemical in the presence of mixed populations of environmental microorganisms [10-14]. BIOWIN was developed by the Syracuse Research Corporation (SRC) and the US EPA as part of the EPIWIN/EPISUITE™ model package and is freely available from the US EPA website [15]. BIOWIN includes six different models including: (1) linear probability BIODEG, (2) nonlinear probability BIODEG, (3) expert survey ultimate biodegradation model (USM), (4) expert survey primary biodegradation model (PSM), (5) Japanese MITI linear, and (6) Japanese MITI nonlinear. These are generally referred to as BIOWIN1_6. Estimates are based on fragment constants and molecular weight and require only a chemical structure. These models have been developed and tested for a range of chemical substances for assessing the biodegradation potential of chemicals by regulatory agencies.

The BIOWIN models have been developed to screen and classify chemical biodegradability (i.e., ready and nonready). The expert survey models (BIOWIN3_4) provide estimates for the time required to achieve primary and ultimate aerobic biodegradation in water. Boethling et al have provided recommendations for converting this

information to environmental half-lives, however they suggest that these estimates not be used as inputs for multimedia modelling assessments [16]. The BIOWIN models include significant inherent information on the relative biodegradability of chemicals derived from different sources (i.e., SRC and MITI empirical data sets and expert judgment). If this knowledge could be adapted to empirical and estimated field based measures of primary biodegradation half-lives then perhaps the utility of the BIOWIN models could be extended.

Methods

Environmental aerobic biodegradation half-life estimation

In an attempt to develop a pragmatic method of selecting biodegradation half-lives for regulatory assessment purposes, a total of 40 chemicals were selected as a "training set" for the calibration of BIOWIN models 1, 3, 4, 5 (i.e., linear BIODEG, USM, PSM and linear MITI) to reliable assessments of aerobic biodegradation environmental half-lives. The 40 chemicals were selected based on the availability of reliable measurements (i.e., sample size). Chemical and structural diversity were included to the greatest extent possible. Data were compiled from handbooks [7, 8], the Syracuse Research Corporation BIODEG database and the primary literature. Primary research sources were obtained and the data evaluated for quality. The selected empirical data were largely aqueous aerobic half-lives although some values were estimated from soil based studies (i.e., [7]). These half-life values for soil were included if it was observed that they were in the range of aqueous data. Only those half-lives interpreted as being primary biodegradation rates were considered. Table 1 provides a list of the 40 chemical "training set" and summary statistics of the empirical environmental half-lives. Figure 1 illustrates the log normal distribution of half-lives considered for the calibration. Appendix 1 includes further information on the physical-chemical properties and illustrates the range of chemical structures included in this compilation.

Raw numerical output from each of the four BIOWIN models was generated for the 40 chemicals. The raw output for each model was then calibrated by linear regression to the corresponding arithmetic means from the empirical biodegradation half-lives. The arithmetic mean was selected as a metric for calibration rather than the geometric mean because there are generally few observations for each chemical with many exhibiting a wide range in half-lives. Given the uncertainty in measurement and the variability associated with environmental half-lives it was decided to calibrate to a higher average to provide a modest degree of conservatism.

If a value for biodegradation was reported as the %BOD (Biochemical Oxygen Demand) or as the percentage of chemical degraded then this information was converted to a half-life estimate. Assuming first order decay from an initial quantity C_0 to C in time t gives:

$$C = C_0 \exp(-kt) \tag{1}$$

where k is a rate constant. The percent loss or BOD is then

$$BOD = 100 \bullet \left(\frac{(C_0 - C)}{C_0} \right) = 100 \bullet (1 - \exp(-kt)) \tag{2}$$

From which k can be calculated as

$$k = \left(\frac{-1}{t} \right) \ln \left(\frac{(100 - \% BOD)}{100} \right) \tag{3}$$

The half-life $t_{1/2}$ is then $0.693 / k$ or

$$t_{1/2} = -0.693t / \ln \left(\frac{(100 - \% BOD)}{100} \right) \tag{4}$$

This approach assumes first order decay and it does not allow for an initiation period during which the microbial community becomes activated or acclimated.

The regressions for each model (see Table 2 and Figure 2) were then used to calculate estimations of biodegradation half-lives from numerical model output for each chemical. For example, for benzene (CAS# 71-43-2) the numerical output from the primary survey model is 3.39, which is calculated to a $\log_{10}$ biodegradation estimate of 1.56 days or a value of 36 days. The estimated half-life values obtained from each of the four models was combined and compared in a series of model evaluations.

Environmental biodegradation half-life estimation evaluation

The extrapolation of environmental biodegradation half-lives from BIOWIN model output was evaluated in three different ways. First, the averaged estimates of the four models were compared to an "evaluation set" of 115 chemicals for which empirical data were available. This included the 40 chemicals used in the "training set" regressions. A list of the additional 75 chemicals including summary statistics is provided in the Appendix. Second, the models were compared as a total group (i.e., averaged values for all four models) as well as in "round robin" combinations to determine if a particular combination could produce more reliable results. Third, the extrapolated BIOWIN estimated half-lives and CATABOL estimated half-life values were compared to empirical data. CATABOL provides estimates of %BOD for a 28-day period. These values were converted to half-life estimates using equation 4.

General assessment of BIOWIN model output

The four selected BIOWIN models were run in "batch mode" for approximately 10,600 diverse organic chemicals on Canada's Domestic Substances List (DSL). The DSL includes a large number of chemical classes and encompasses a wide range of physical chemical properties. The raw numerical output from the four models was evaluated.

Statistical analyses

Statistical analyses were conducted using Microsoft EXCEL™ and JMPIN™ (SAS institute).

Results and Discussion

Environmental aerobic biodegradation half-life estimation

  The series of plots in Figure 2 illustrates the calibration of BIOWIN model output to 40 selected "training set" chemicals. The empirical half-lives are the arithmetic mean for each chemical and are plotted on a logarithmic scale. These calibrations indicate a good correlation between the empirical data and the model predictions. For these 40 chemicals the relationship is strongest for the survey models followed by the linear BIODEG model and the linear MITI model. Table 2 summarizes the resulting equations and statistics for each regression. Restrictions were applied to low values of model output. For example, if PSM output was less than 2 the chemical was considered to have a maximum half-life of 3650 days (10 years). Likewise, a USM output less than 0.85 corresponds to a maximum half-life of 2190 days (6 years), linear BIODEG output less than -0.95 corresponds to 3300 days (~9 years) and linear MITI output less than -0.7 corresponds to 3650 days (10 years). The purpose of this calibration is to provide a means to estimate "real world" biodegradation half-lives for application in multimedia fate models. The aim is not provide accurate biodegradation rates for extremely recalcitrant chemicals. For the purposes of multimedia fate modelling there is a point at which low biodegradation rates become relatively less important in comparison to other processes such as advective losses.

  These equations provide an estimate of aerobic environmental half-life (i.e., y) from the output of each BIOWIN model (i.e., x). The regression equations provide the $\log_{10}$ biodegradation environmental half-lives. The estimated environmental biodegradation half-lives were averaged in an effort to obtain "balance" between model errors. The models could be used to produce either an arithmetic mean or a geometric mean. The coefficient of variation could be used to identify the relative agreement or disagreement between the four models. Professional judgment could also be used to remove a particular model prediction that does not follow a pattern identified by the other models (i.e., an extreme value).

Estimation method evaluation

  The estimated environmental half-lives were evaluated in comparison to empirical data and to other model estimates. Figure 3 illustrates the log-normal distribution of empirical half-life values from the "evaluation set" of 115 chemicals. This indicates that a wide range of empirical half-life information was included for the evaluation. Figure 4 compares aerobic biodegradation half-lives using the arithmetic mean from half-life estimates from all four models with empirical data for 115 chemicals. Using this approach 98% and 77% of the 115 chemicals are predicted within a factor of 10 and a factor of 3 of the empirical data, respectively. Those values that lie outside a factor of 10 are all conservative model predictions. For screening level assessments conservative errors are preferable.

An effort was made to compare the different possible model calibration combinations that may result in significantly better relationships with the empirical data against which they are tested. For example, the calibration of the linear MITI model appears to be the weakest of the 4 models. Table 3 provides results from the "round robin". It appears that averaging the information from all four models provides the most reliable predictions.

Figure 5 compares estimated environmental biodegradation half-lives derived in this study (n = 116) with half-lives estimated using CATABOL (n = 112) and geometric means of available empirical data (n = 116). The empirical data include the upper and lower 95% confidence limits. The CASRN and chemical names reported in Figure 5 are tabulated in the Appendix. It is observed that the revised BIOWIN estimated values are within the 95% confidence limits of the empirical values for all but 17 of the chemicals. Modified BIOWIN estimated values are not always in agreement with the CATABOL predictions. In general the CATABOL predicted half-life values are greater than those estimated by this method, particularly for more "persistent" chemicals. CATABOL half-life predictions are also usually greater than empirical data.

There are 112 chemicals for which estimated values are available for both CATABOL and BIOWIN and for which reliable empirical data are available. Comparisons of both estimation methods to empirical data reveals that average absolute errors (AAE) and root mean square errors (RMSE) are 116 d and 279 d for the proposed method and 2537 d and 5119 d for CATABOL, respectively. It is important to realize that this evaluation is not intended to be a direct model performance comparison since the revised BIOWIN predictions are a result of calibration to a subset of the evaluation data set the derived CATABOL predictions are not a result of calibration to a subset of the evaluation data set. CATABOL (v5.0763) estimates were provided by Environment Canada and are included only as a general comparison in the absence of other available biodegradation predictions for the "evaluation" data set.

It is concluded that the preferred method is to run all four models (BIOWIN 1, 3, 4, and 5) and average extrapolated environmental estimates as the biodegradation rate in water. It is also useful to run CATABOL for comparison purposes.

General assessment of BIOWIN model output

Figure 6 compares numerical model output from BIODEG (B1), USM (B3) and MITI (B5) against PSM (B4) for 10,600 DSL chemicals. This evaluation shows that the slopes of the regressions are near unity for the BIODEG and MITI models against PSM. The slope is greater than one when comparing USM to PSM. This is encouraging in that the scoring for the ultimate biodegradation model is lower than the scoring for the primary model for the same chemical. Likewise, these two models also show the greatest agreement with the highest correlation coefficients. This analysis suggests that for a large number and diverse set of chemicals that the models are generally in strong qualitative agreement and in good quantitative agreement with one another. This agreement varies between models. There are obvious cases in which the models do not agree well and these chemicals could

be investigated to have a better understanding as to why these differences exist and how such differences can be corrected or minimized. More importantly, addressing these differences may identify aspects of the models that could be improved.

Residuals from the model correlations tend to increase for predictions of "more persistent" chemicals, i.e., longer half-lives. One explanation for this is that the survey models are "more accurate" for relatively more biodegradable chemicals compared to less biodegradable chemicals as a result of their design. For example, the survey asked experts to assign a value of 5, 4, 3, 2, or 1 corresponding to general time categories of either primary or ultimate aerobic biodegradation in the environment. These categories are "hours", "days", "weeks", "months" or "longer". Provided with this scale for classification an expert would likely interpret "hours" as less than or equal to approximately 1 day, whereas months would perhaps have been interpreted as 60 to 365 days. It is difficult to quantify the "longer" category. Clearly, the associated errors and uncertainties in assigning a number to these qualitative descriptors will increase with increasing temporal scale. This is unfortunate because a major regulatory effort is to identify, evaluate and possibly regulate persistent chemicals in the environment. Although this expert knowledge is difficult to obtain and is subjective, a more quantitatively explicit survey in the future could result in reduced uncertainty for developing environmental half-life models for both primary and ultimate biodegradation.

Figure 7 illustrates the distributions of model output from the four BIOWIN models for 10,600 substances. This evaluation provides a reasonable assessment for the range of possible model outputs that can be expected for organic chemicals. These distributions suggest that the "extreme" model predictions are generally observed for "more persistent" chemicals. Figure 8 indicates that extreme model output is largely associated with increasing molecular weight. This can be interpreted as a "residual effect" of the contribution method for larger chemicals. It may also reflect the lower solubility in water and hence availability of these substances. This has also been observed for physical-chemical property estimations when applying EPIWIN and other contribution models to high molecular weight chemicals. This preliminary analysis identifies extreme BIOWIN model outputs and suggests careful analysis of the results for chemicals with molecular weight greater than approximately 500. This information also suggests that there are possible limiting values for each model that should be restricted.

A speculation on methods of improving the selection of biodegradation data

The objective of this section is to speculate on methods that may be developed in the future and to display empirical and estimate biodegradation rate data leading to an optimal selection of half-lives for various environmental compartments.

First it is useful to set an ultimate target in terms of accuracy for these estimates. Rather than give actual numerical estimates of half-lives, e.g., 100 hours, it is probably more honest to assign a chemical to a "bin" or half-life range of say 50 to 200 hours. The "width" of these bins can be varied according to the perceived accuracy. Mackay et al [8] have suggested that these bins could be "semi-decade" wide, i.e., factor of approximately 3

from low to high end. For abiotic reactions such as atmospheric oxidation and hydrolysis this is certainly achievable, but it is currently optimistic for biodegradation kinetics.

The semi-decade or factor of 3 level of discrimination is a compromise between conveying an exaggerated impression of accuracy (as would be implied by a factor of 2 range) and a rather pessimistic use of factor of 10 ranges. In many cases the rates are known with error limits of factor of 2 or 3. Half-life data can be obtained from field tests, STP treatability, QSARs and expert judgment. Obviously the results from each source will differ, for example the following is a hypothetical list.

Source	Half-life (hours)
Metabolism in rat	20
Sewage treatment plant (STP)	40
BOD test	100
Water test (e.g., river die away)	300
Soil test	600
Sediment test or expert judgment	1000
QSAR1	200
QSAR2	500
QSAR3	120

These different quantities represent different "currencies" but they all refer to biodegradation phenomena, albeit in different environments at different conditions and probably with different microbial systems. If a large database can be compiled it may be possible to develop relationships between, for example, typical STP half-lives and water or soil half-lives. A difficulty is that x, y correlations can only be done on two quantities at a time. It would be useful if a correlation or multiple regression approach could be devised in which all the data are treated simultaneously. It is suggested that this can be done using a "slide rule" approach in which the logarithmic half-life scales are displaced by an amount corresponding to the slope of the x, y plot on a logarithmic basis. The slope is essentially a factor.

It is useful to review briefly the principle of the slide rule. Regrettably, slide rules, which were once standard equipment for the engineer, are now virtually obsolete. Two logarithmic scales can be slid past each other or displaced to a desired extent. To multiply 2 by 3 the point 1.0 on the mobile slide is set at 2.0 on the stationary scale and the answer (6.0) is read off on the slide opposite 3.0 on the slide, Effectively log 2 is added to log 3 to give log 6.

In this case each biodegradation data source is an individual slide rule marked in classes as shown in Figure 9. The relative data source to data source adjustment is obtained by correlation of log half-life versus log half-life (t) forcing a parameter correlation of the type

$$\log t_1 = A + \log t_2 \tag{5}$$

This is equivalent to

$$t_1 = 10^A t_2 \tag{6}$$

An even simpler correlation is to force A to adopt one of several positive or negative values such as 0.5, 1.0, 2.0, -0.5, -1.5 etc. where n is a positive or negative integer. This essentially relates the half-life ranges to each other rather than the numerical values. The factors 10^A then adopt values such as 3.1, 10, 31, 0.31, and 0.1 i.e., $10^{0.5n}$ where n in these examples is 1, 2, 3, -1, and -2.

Figure 9 gives a fictitious result for a "persistent" and a "non-persistent" substance in which the correlations have been fairly successful and take the form of displacement by the specified number of ranges. It is not expected that it will be possible to align all the ranges for all substances but the diagram has the potential to convey an impression of persistence, to assess the consistency between data inputs (or more strictly test if they fit the correlation implied by the specified displacement) and in the absence of any experimental data they enable QSAR data to be used to estimate the ranges in which other half-lives are likely to lie. Using ranges avoids conveying an impression of excessive accuracy. The user is at liberty to select single numerical half-lives from the range, but that selection is clearly the responsibility of the user.

In order to construct the slide rule a quantity of reliable biodegradation data should be gathered and correlations sought between the various sources. Pairs of sources are compared and mean factors relating the half-lives are established. For example, soil half-life is 3 times the water half-life value on average. Some of these factors are subject to varying accuracy. From the matrix of pairs of factors a single set is established and used to set the slide rules. If the factors apply to a specific chemical, the classes will be aligned horizontally, but it is expected that there will be deviations. If the method has validity the data should lied generally on a horizontal band, the location of which indicates the biodegradability. This has the advantage that the output is pictorial rather than numerical and the results may be more readily understood.

Inherent in this approach is the assumption that the biodegradation process is fundamentally second order in nature, specifically first order with respect to the chemical and first order with respect to the microbial community that prevails in that compartment.

It is recommended that this approach be explored by applying it to a set of biodegradation data for chemicals in a variety of media. The usefulness of the method can only be evaluated in the light of experience.

Conclusions

From this analysis it is suggested that for DSL chemicals the most reliable and robust approach is to

(1) Gather all available empirical data for the substance of interest in all relevant media.
(2) Run the four BIOWIN models (1, 3, 4, and 5) and the CATABOL model, average the BIOWIN half-lives and check that the results are generally consistent with the CATABOL results.
(3) The empirical and model data are then combined using expert judgment to suggest a range of half-lives which may be applicable to that substance.
(4) Apply factors to relate water, soil, and sediment half-lives and possibly STP half-lives. This can be done directly or using the slide rule pictorial approach.

It is recommended that the feasibility and usefulness of the slide rule approach be evaluated in a companion study.

Table 1. A list and statistical summary of empirical aerobic environmental half-lives for 40 chemicals selected as a "training set" to calibrate the BIOWIN models.

| CAS | Chemical Name | n | Empirical $t_{1/2}$ (d) | | | log |
			Arithmetic mean	STDEV	CV	Mean
71-43-2	Benzene	8	40	46	1.15	1.60
84-66-2	Diethylphthalate (DEP)	7	11	20	1.86	1.03
87-86-5	Pentachlorophenol	7	146	183	1.25	2.16
93-76-5	2,4,5-trichlorophenoxyacetic acid	7	25	18	0.73	1.40
108-95-2	Phenol	6	5	4	0.83	0.70
1912-24-9	Atrazine	7	96	71	0.74	1.98
85-68-7	Butyl benzyl phthalate (BBP)	6	4	4	0.85	0.64
100-41-4	Ethylbenzene	6	14	13	0.92	1.15
106-44-5	*p*-cresol	5	1	1	0.95	0.10
58-89-9	γ-HCH (lindane)	5	392	299	0.76	2.59
63-25-2	Carbaryl	5	14	12	0.86	1.14
76-44-8	Heptachlor	5	824	1074	1.30	2.92
91-20-3	Naphthalene	5	40	17	0.42	1.60
91-22-5	Quinoline	4	14	18	1.30	1.14
95-95-4	2,4,5-trichlorophenol	4	366	360	0.98	2.56
116-06-3	Aldicarb	5	131	165	1.26	2.12
118-74-1	Hexachlorobenzene	5	1245	850	0.68	3.10
122-34-9	Simazine	5	81	52	0.64	1.91
131-11-3	Dimethylphthalate (DMP)	5	3	3	1.04	0.40
1563-66-2	Carbofuran	5	40	26	0.65	1.60
1746-01-6	2,3,7,8-TCDD	5	648	247	0.38	2.81
1918-00-9	Dicamba	5	69	66	0.96	1.84

| CAS | Chemical Name | n | Empirical $t_{1/2}$ (d) | | | log |
			Arithmetic mean	STDEV	CV	Mean
50-32-8	Benzo[a]pyrene	4	284	201	0.71	2.45
56-55-3	Benz[a]anthracene	4	301	261	0.87	2.48
72-43-5	Methoxychlor	4	191	147	0.77	2.28
75-01-4	Chloroethene (vinyl chloride)	4	76	75	0.98	1.88
108-60-1	Bis(2-chloroisopropyl)ether	4	66	80	1.21	1.82
108-88-3	Toluene	4	18	16	0.89	1.26
120-82-1	1,2,4-trichlorobenzene	4	61	79	1.30	1.79
121-14-2	2,4-dinitrotoluene	2	104	107	1.03	2.02
206-44-0	Fluoranthene	4	306	132	0.43	2.49
7085-19-0	Mecoprop	4	25	24	1.00	1.39
64-17-5	Ethanol	3	5	4	0.72	0.73
65-85-0	Benzoic acid	3	2	2	0.80	0.39
91-94-1	3,3'-dichlorobenzidine	3	93	78	0.83	1.97
98-86-2	Acetophenone	2	6	2	0.40	0.80
106-42-3	*p*-xylene (Benzene, 1,4-dimethyl-)	3	19	11	0.57	1.29
107-21-1	Ethylene glycol	3	8	5	0.66	0.92
108-67-8	1,3,5-trimethylbenzene	3	9	8	0.87	0.97
120-80-9	Catechol	2	4	4	1.06	0.60

Table 2. General equations used to derive estimates of aerobic environmental biodegradation half-lives from BIOWIN model output. These do not include suggested "restrictions" for the low numerical output of chemicals that are modeled to be very persistent.

BIOWIN Model	Regression Equation	r^2
B1 - linear BIODEG	$y = -1.32x + 2.24$	0.72
B3 - USM	$y = -1.07x + 4.20$	0.77
B4 - PSM	$y = -1.46x + 6.51$	0.78
B5 - linear MITI	$y = -1.86x + 2.23$	0.58

Table 3. A "round robin" comparison of different BIOWIN model scenarios to 110 empirical half-lives.

BIOWIN Model Combination	r^2	slope	factor ± 10	factor ± 5	factor ± 3	factor ± 2
1,3,4,5	0.56	0.71	97	93	78	58
1,3,4	0.57	0.75	97	89	77	55
1,3,5	0.54	0.68	97	95	77	55
1,4,5	0.54	0.69	98	92	76	56
1,3	0.57	0.73	97	92	82	56
1,4	0.56	0.75	97	88	75	55
1,5	0.51	0.64	98	93	73	52
3,4	0.56	0.76	98	88	76	54
3,5	0.5	0.66	96	94	71	54
4,5	0.52	0.69	98	92	70	52

Figure 1. The distribution of log transformed empirical biodegradation half-lives for 40 chemicals used as a "training set" to calibrate the BIOWIN models.

Distributions

log half-life (d)

Normal(1.6005,0.76554)

Fitted Normal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	Mu	1.600500	1.355667	1.845333
Dispersion	Sigma	0.765543	0.627103	0.982984

Goodness-of-Fit Test

Shapiro-Wilk W Test

W	Prob<W
0.974044	0.5944
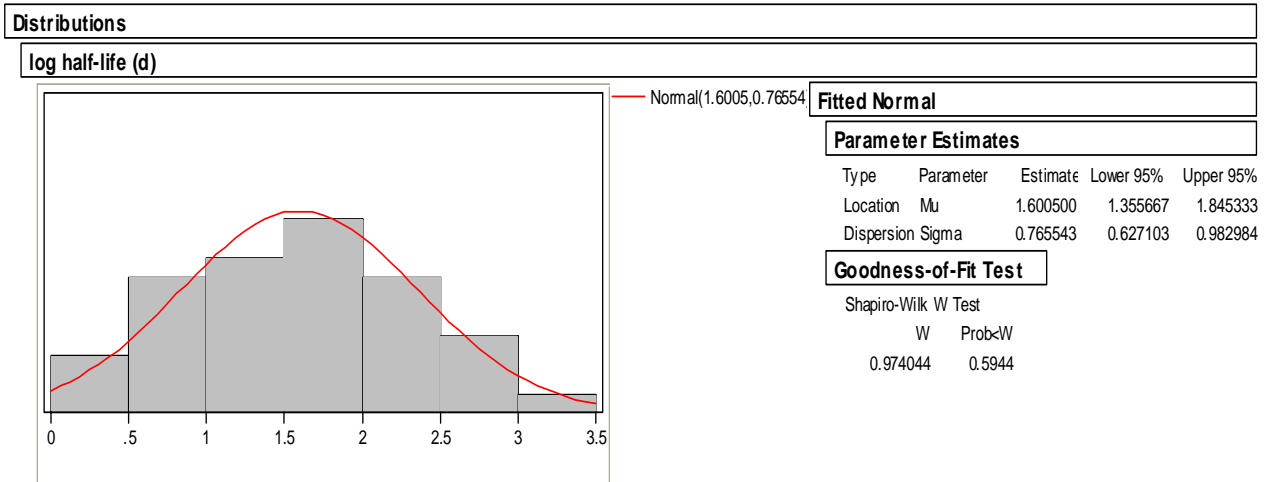
Figure 2. Log-linear regressions of BIOWIN model output to empirical aerobic half-life data and equations used to extrapolate "environmentally relevant" aerobic half-life data.

BIOWIN - BIODEG (B1)

$y = -1.32x + 2.24$
$r^2 = 0.72$

x-axis: Raw model output
y-axis: log empirical aerobic half-life (d)

BIOWIN - Ultimate Survey Model (USM-B3)

$y = -1.07x + 4.12$
$r^2 = 0.77$

x-axis: Raw model output
y-axis: log empirical aerobic half-life (d)

Figure 2. Continued

BIOWIN - Primary Survey Model (PSM-B4)

$y = -1.46x + 6.51$
$r^2 = 0.78$

BIOWIN - MITI (B5)

$y = -1.86x + 2.23$
$r^2 = 0.58$
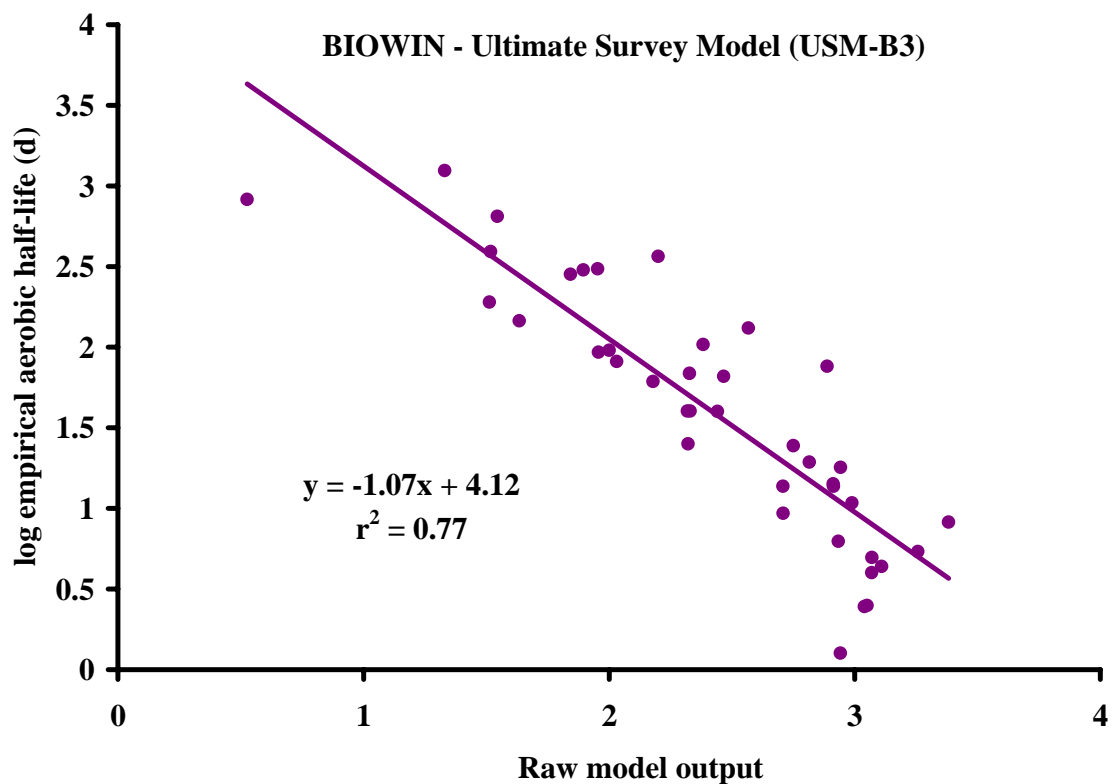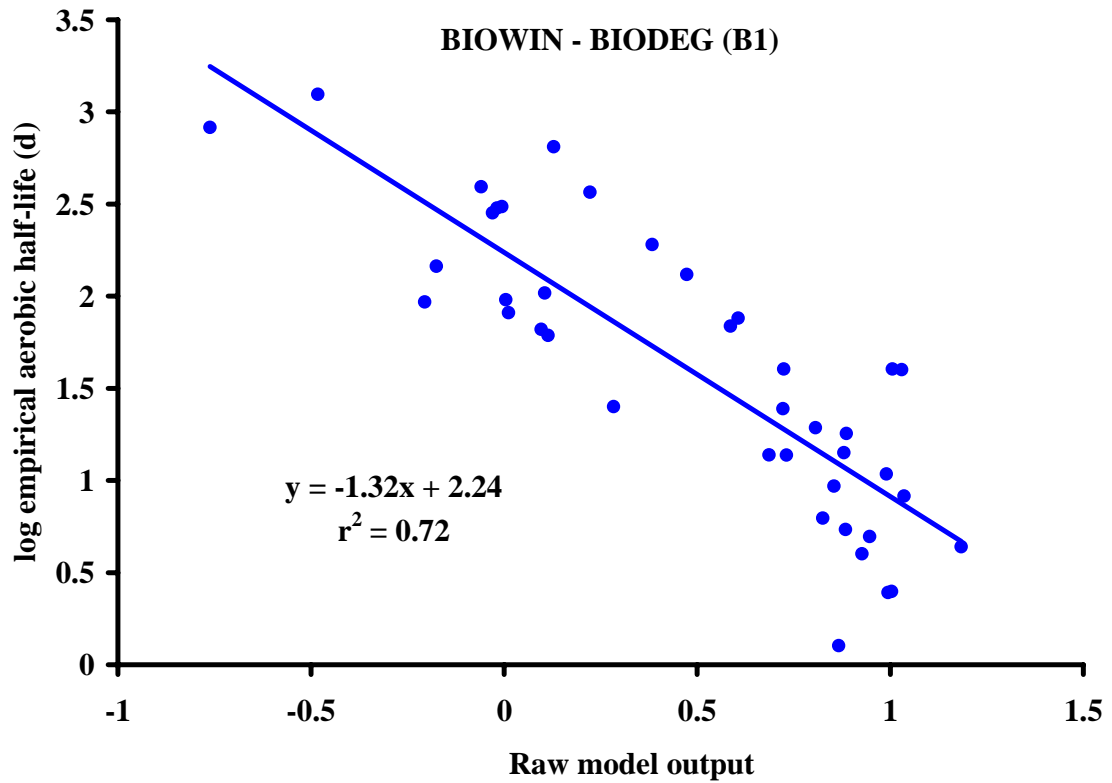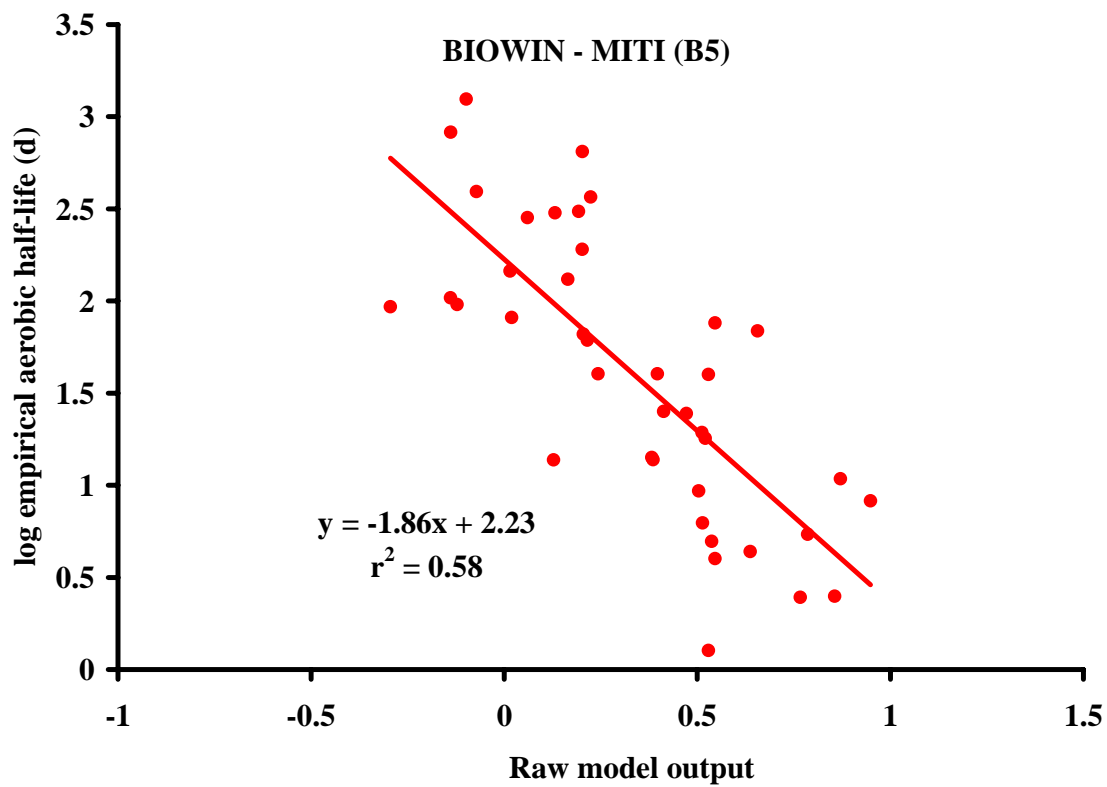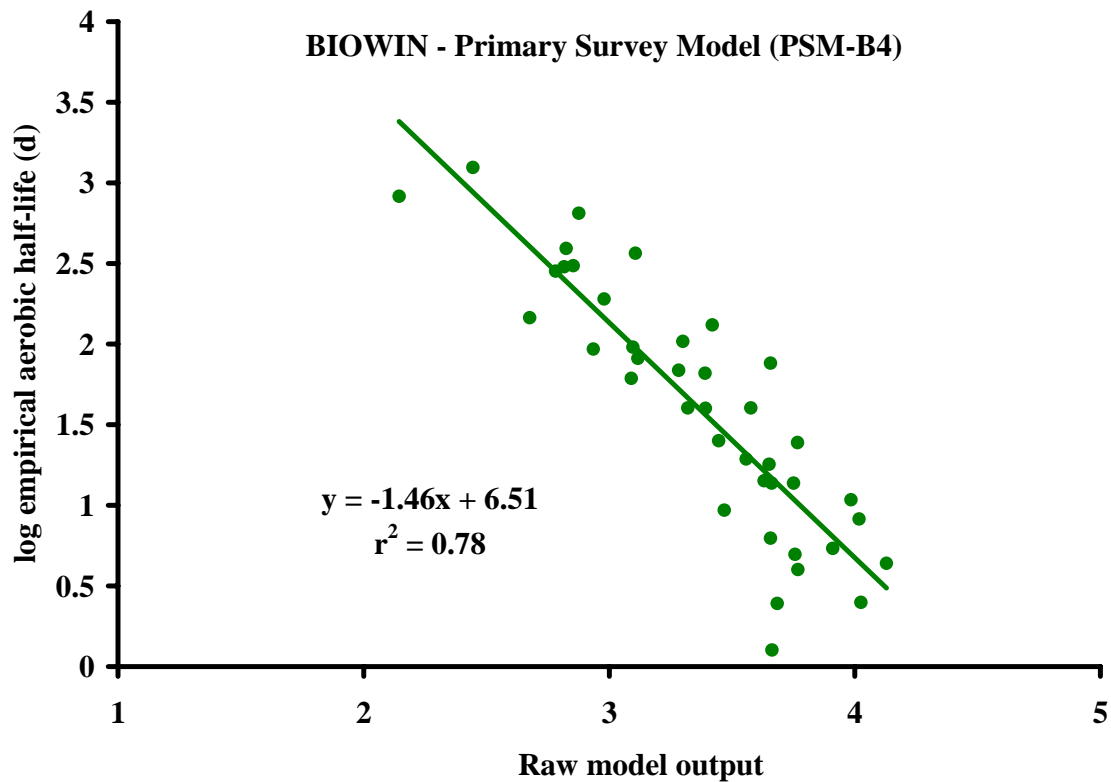
Figure 3. The distribution of log empirical half-lives used in the "evaluation set" to assess the proposed BIOWIN extrapolation method.

Distributions

Empirical Half-life (d)

Normal(1.67183,0.66177)

Fitted Normal

Parameter Estimates

Type	Parameter	Estimate	Lower 95%	Upper 95%
Location	Mu	1.671826	1.549579	1.794073
Dispersion	Sigma	0.661767	0.585887	0.760406

Goodness-of-Fit Test

Shapiro-Wilk W Test

W	Prob<W
0.979552	0.4618
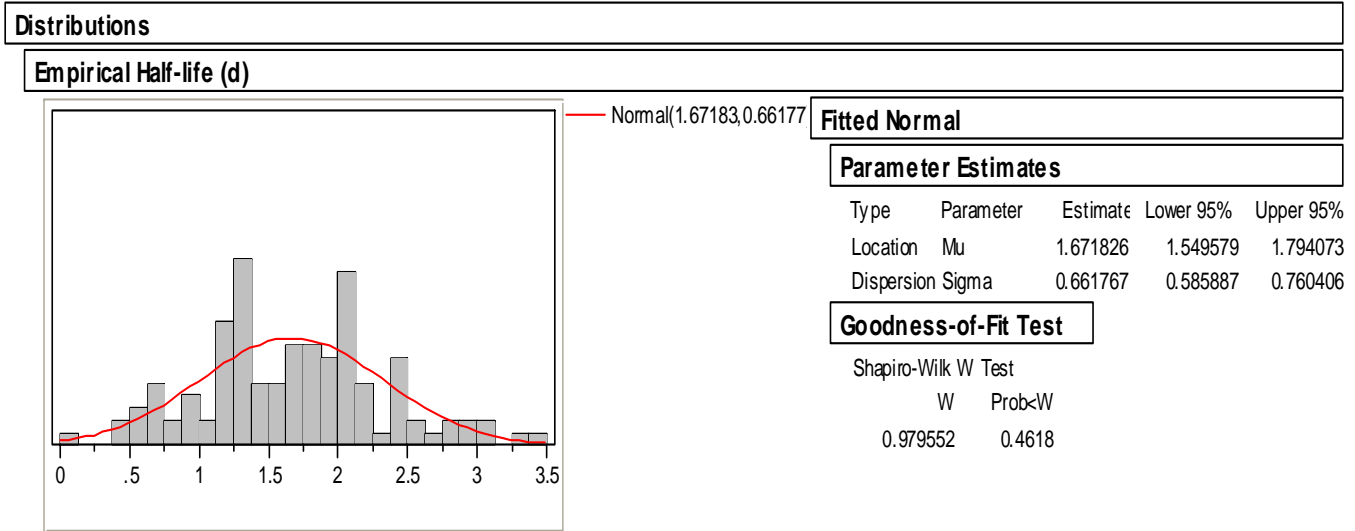
Figure 4. A comparison of estimated half-lives using the average calibrated output from the four BIOWIN models and empirical aerobic biodegradation half-lives. The black line represents a 1:1 ratio and the gray lines represent ± factors of 3 and 10.

$y = 0.73x + 0.49$

$r^2 = 0.57$

(x-axis: log aerobic empirical half-life (d); y-axis: log aerobic average BIOWIN half-life (d))
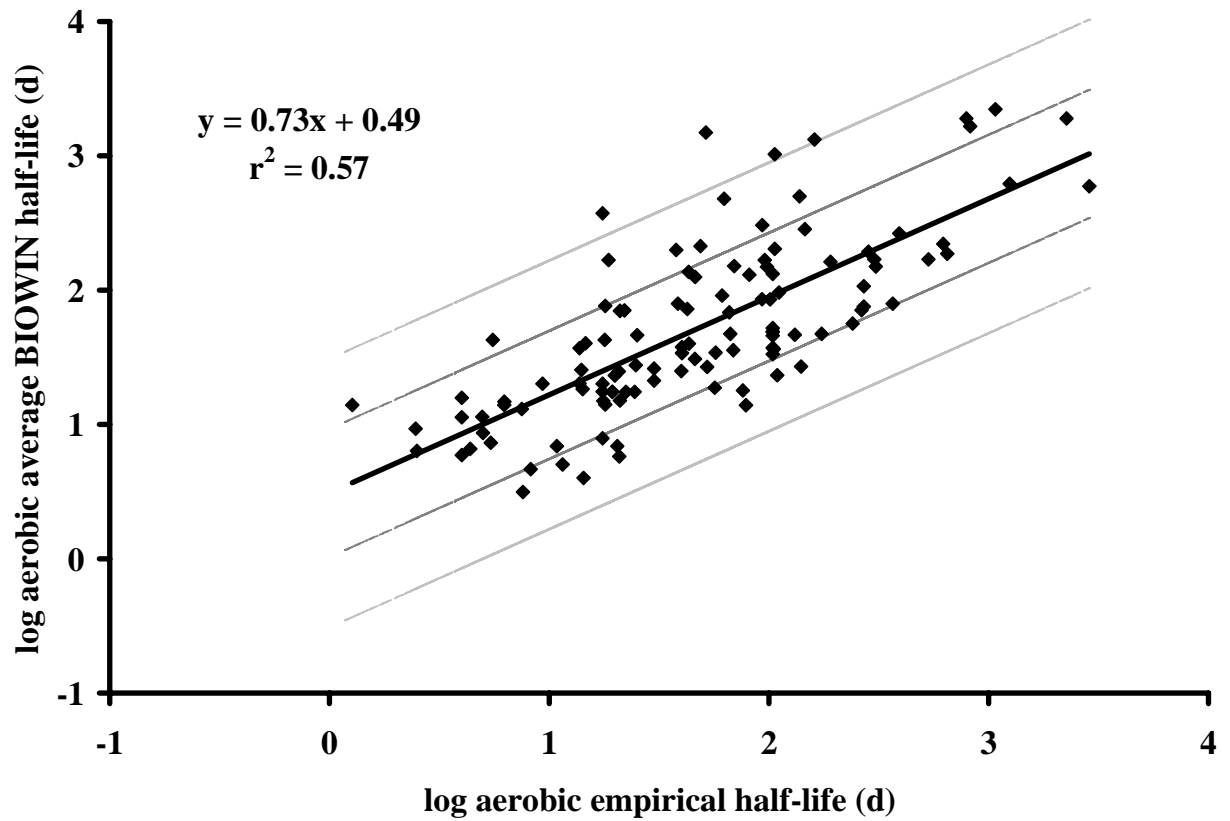
Figure 5. Estimated biodegradation half-lives from the modified BIOWIN models, CATABOL and available empirical data. (error bars represent the 95% CL)
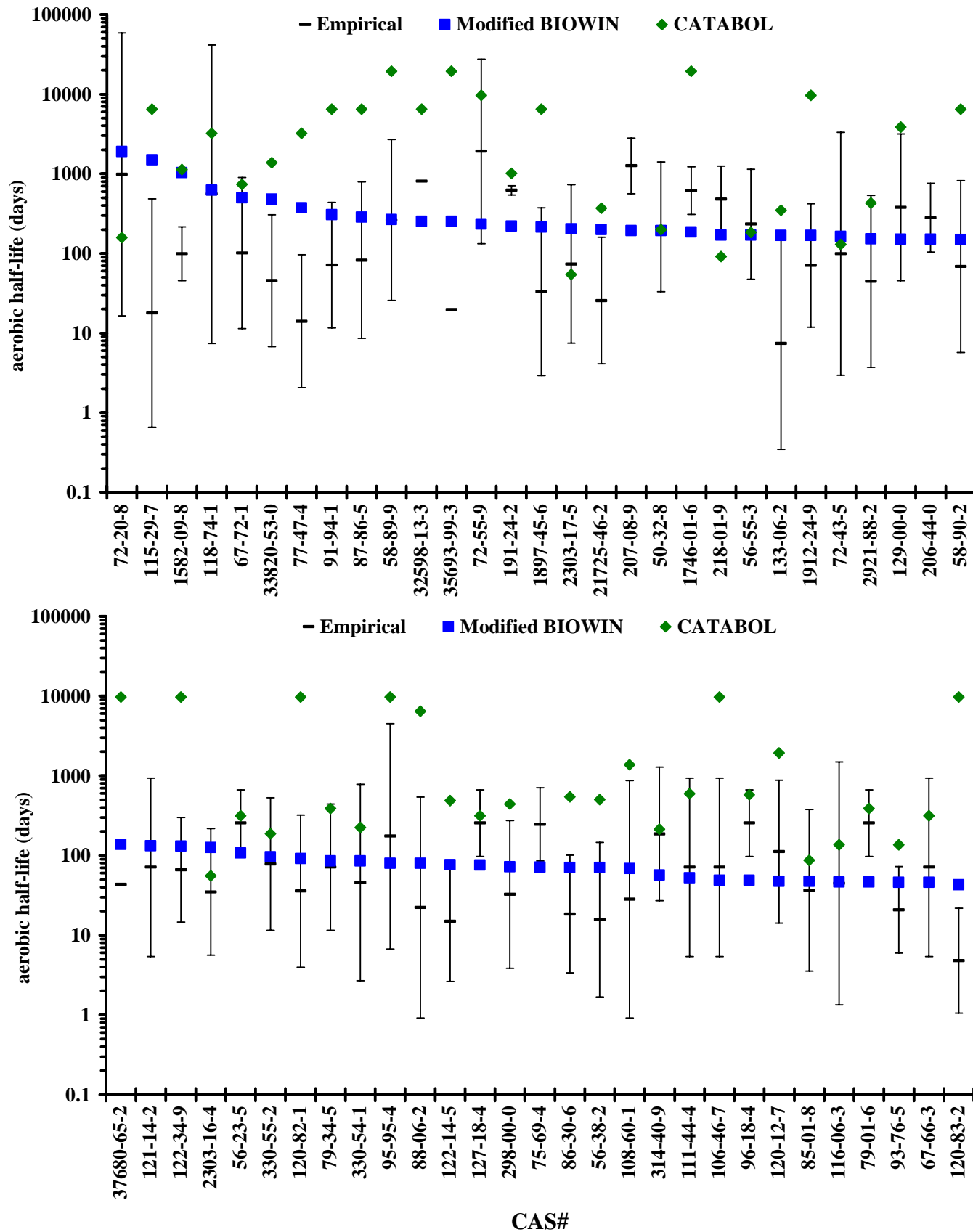
Figure 5. Continued
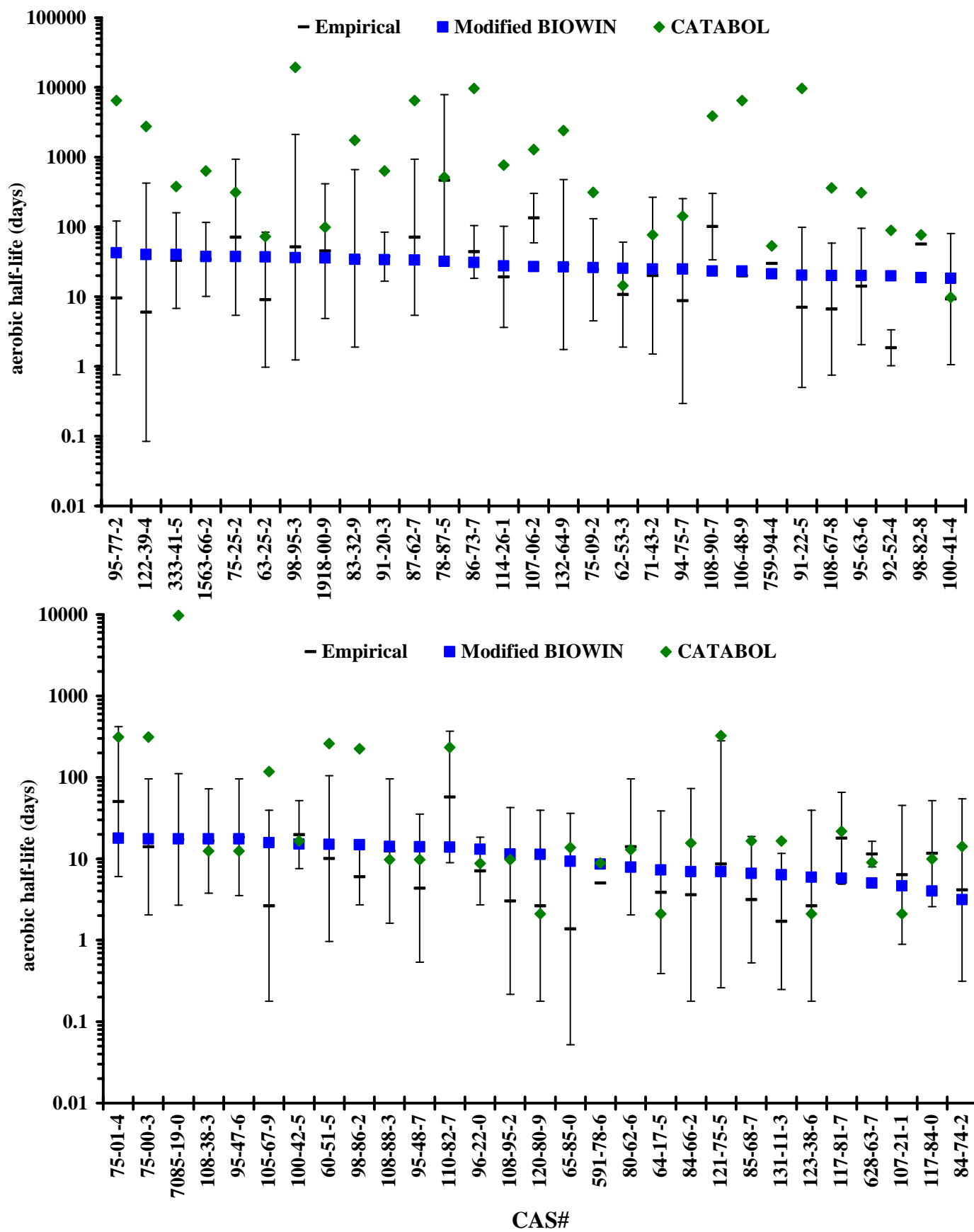
Figure 6. Numerical output comparisons of BIOWIN models for 10,600 diverse chemicals.

$y = 0.8847x - 2.5519$
$r^2 = 0.6448$

(y-axis: BIODEG (B1) numerical output; x-axis: PSM (B4) numerical output)

$y = 0.9977x - 3.2602$
$r^2 = 0.6777$

(y-axis: MITI (B5) numerical output; x-axis: PSM (B4) numerical output)
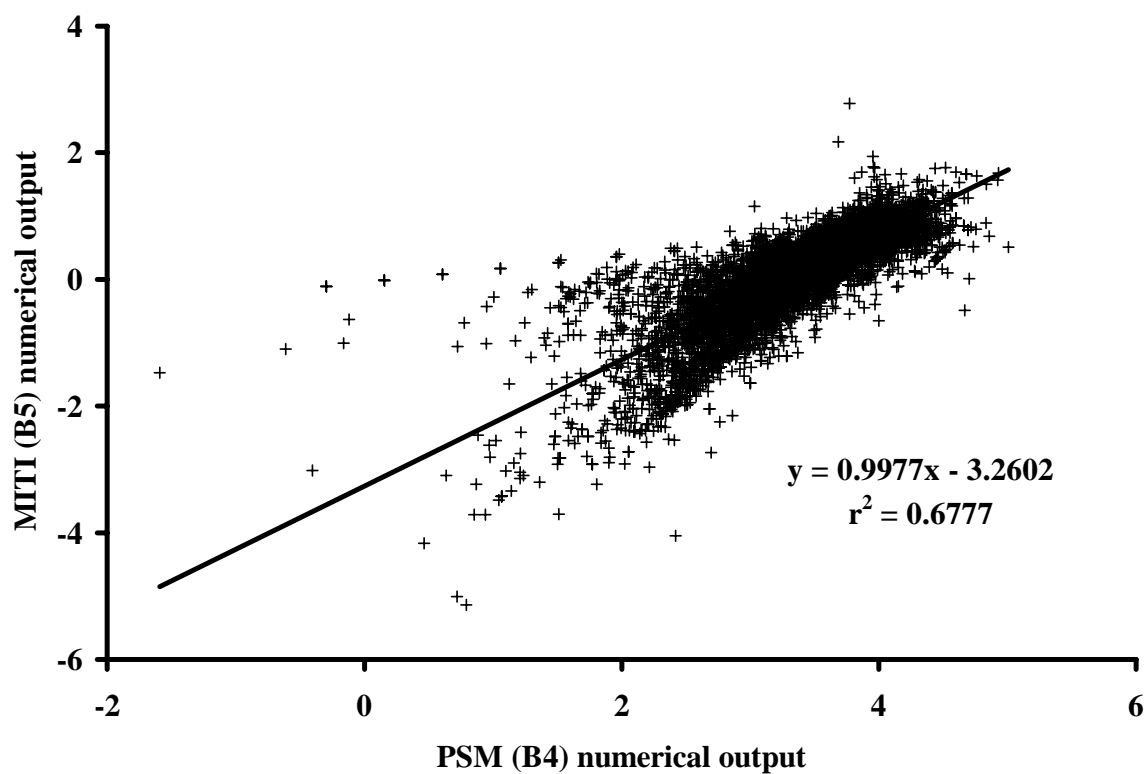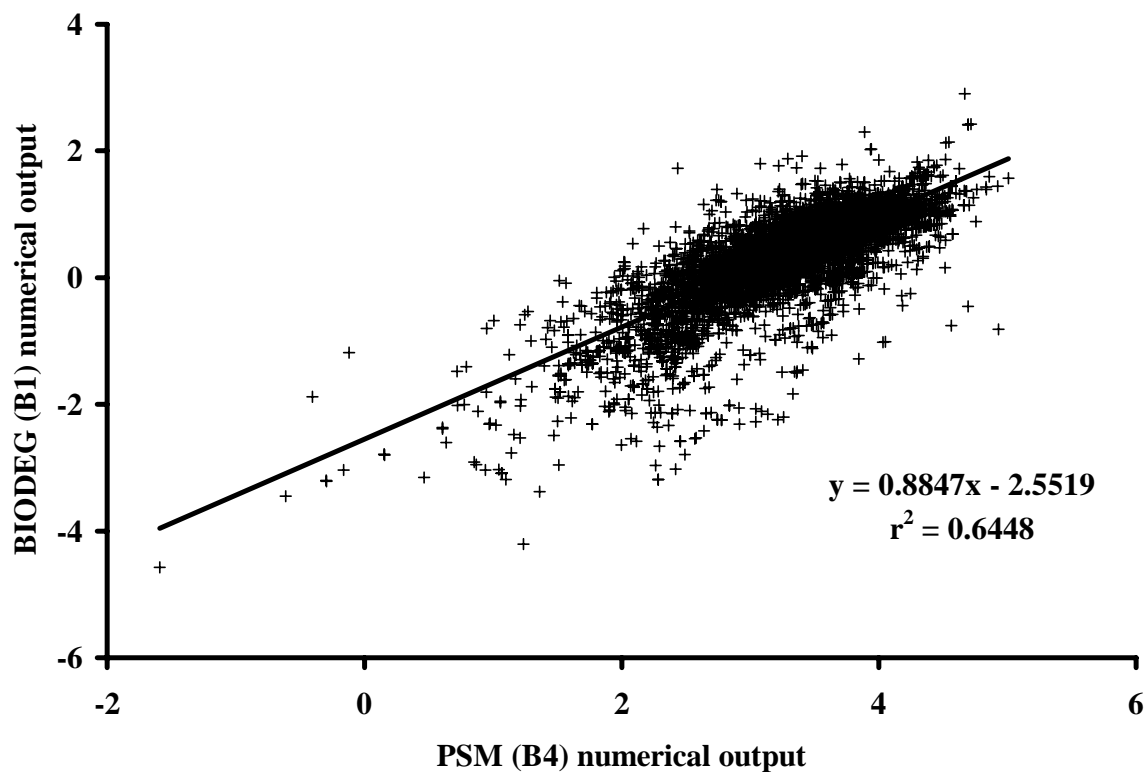
Figure 6. Continued

y = 1.3472x - 2.2034
$r^2 = 0.8828$
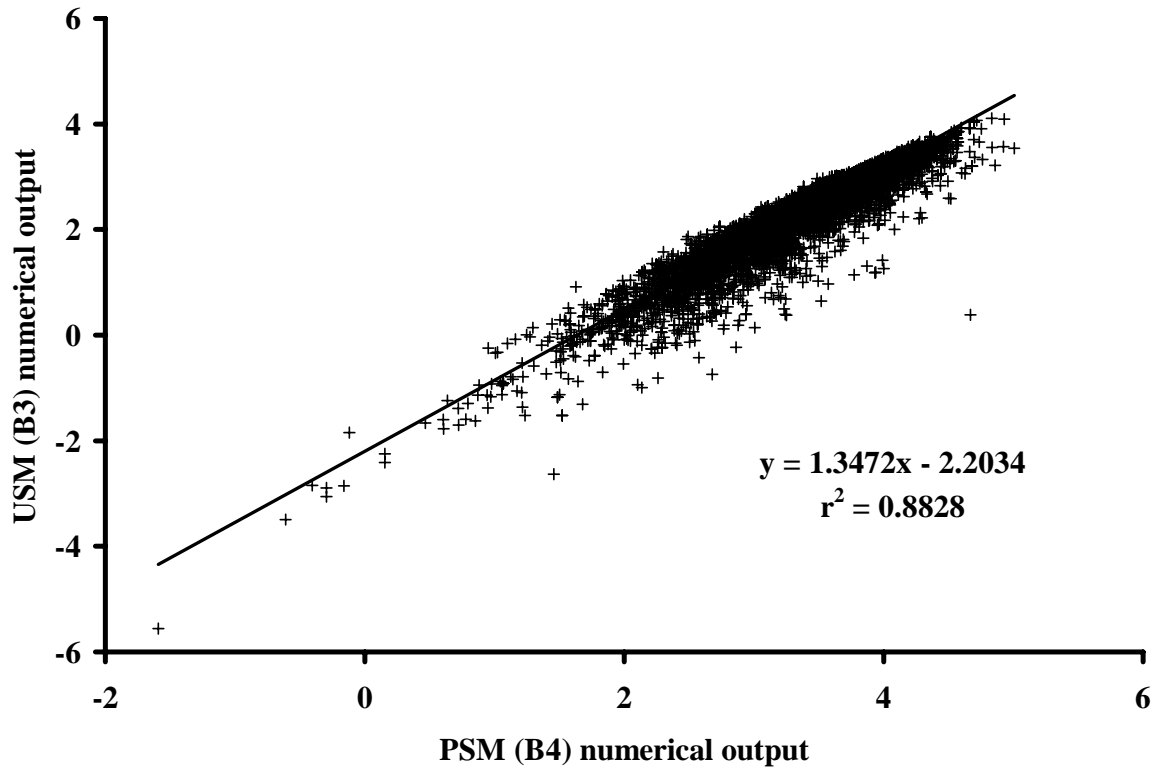
Figure 7. Distributions of BIOWN 1, 3, 4, 5 output for organic chemicals on the DSL.

Distributions

linear BIODEG (B1) 2

Quantiles			Moments	
100.0%	maximum	2.9040	Mean	0.5122272
99.5%		1.5727	Std Dev	0.5994340
97.5%		1.2157	Std Err Mean	0.0058129
90.0%		1.0266	upper 95% Mean	0.5236218
75.0%	quartile	0.8753	lower 95% Mean	0.5008326
50.0%	median	0.6751	N	10634
25.0%	quartile	0.2901		
10.0%		-0.1759		
2.5%		-1.1484		
0.5%		-2.2458		
0.0%	minimum	-4.5759		

USM (B3)

Quantiles			Moments	
100.0%	maximum	4.1039	Mean	2.462558
99.5%		3.6563	Std Dev	0.780079
97.5%		3.4171	Std Err Mean	0.007565
90.0%		3.1803	upper 95% Mean	2.477386
75.0%	quartile	2.9515	lower 95% Mean	2.447729
50.0%	median	2.6979	N	10634
25.0%	quartile	2.1693		
10.0%		1.3605		
2.5%		0.4281		
0.5%		-0.6817		
0.0%	minimum	-5.5569		

PSM (B4)

Quantiles			Moments	
100.0%	maximum	5.0064	Mean	3.463470
99.5%		4.5174	Std Dev	0.544061
97.5%		4.2802	Std Err Mean	0.005276
90.0%		4.0366	upper 95% Mean	3.473812
75.0%	quartile	3.8064	lower 95% Mean	3.453128
50.0%	median	3.5720	N	10634
25.0%	quartile	3.2273		
10.0%		2.7182		
2.5%		2.1403		
0.5%		1.4594		
0.0%	minimum	-1.5915		

linear MITI (B5)

Quantiles			Moments	
100.0%	maximum	2.7776	Mean	0.1952189
99.5%		1.3315	Std Dev	0.6593569
97.5%		1.0289	Std Err Mean	0.0063940
90.0%		0.8061	upper 95% Mean	0.2077526
75.0%	quartile	0.6111	lower 95% Mean	0.1826852
50.0%	median	0.3678	N	10634
25.0%	quartile	-0.0526		
10.0%		-0.6612		
2.5%		-1.6203		
0.5%		-2.4769		
0.0%	minimum	-5.1378		

Figure 8. A plot of the residuals of BIOWIN model output against molecular weight.

Bivariate Fit of linear BIODEG (B1) By MW
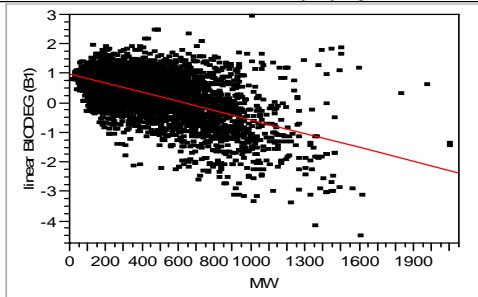
Linear Fit

Linear Fit

linear BIODEG (B1) = 1.00557 - 0.0015658 MW

Summary of Fit

RSquare	0.342648
RSquare Adj	0.342586
Root Mean Square Error	0.486028
Mean of Response	0.512227
Observations (or Sum Wgts)	10634
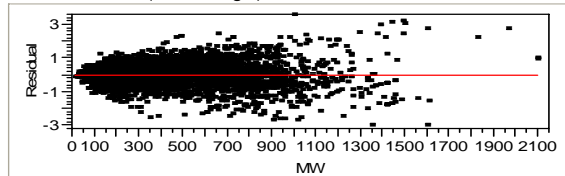
Bivariate Fit of USM (B3) By MW
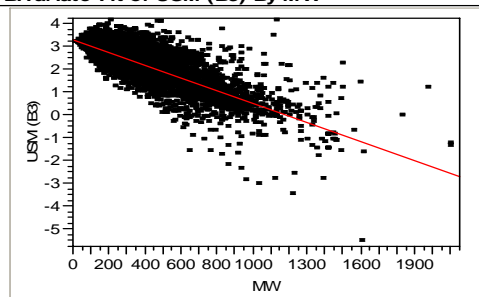
Linear Fit

Linear Fit

USM (B3) = 3.3435193 - 0.0027961 MW

Summary of Fit

RSquare	0.645164
RSquare Adj	0.645131
Root Mean Square Error	0.4647
Mean of Response	2.462558
Observations (or Sum Wgts)	10634
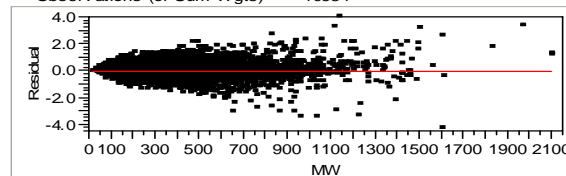
Bivariate Fit of linear MITI (B5) By MW
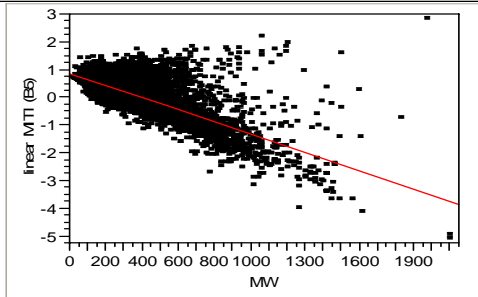
Linear Fit

Linear Fit

linear MITI (B5) = 0.8889479 - 0.0022019 MW

Summary of Fit

RSquare	0.559979
RSquare Adj	0.559937
Root Mean Square Error	0.437399
Mean of Response	0.195219
Observations (or Sum Wgts)	10634
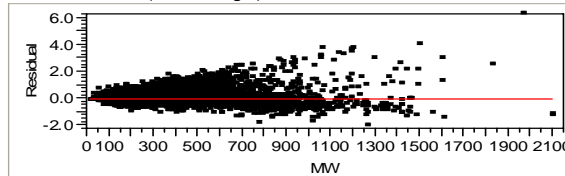
Bivariate Fit of PSM (B4) By MW
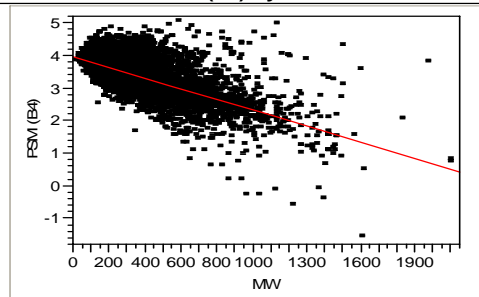
Linear Fit

Linear Fit

PSM (B4) = 3.9801803 - 0.00164 MW

Summary of Fit

RSquare	0.45628
RSquare Adj	0.456229
Root Mean Square Error	0.401195
Mean of Response	3.46347
Observations (or Sum Wgts)	10634
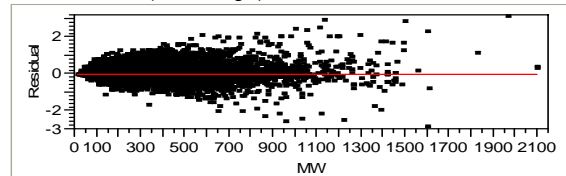
Figure 9. An example of the "slide rule" approach for half-life estimation from different sources.
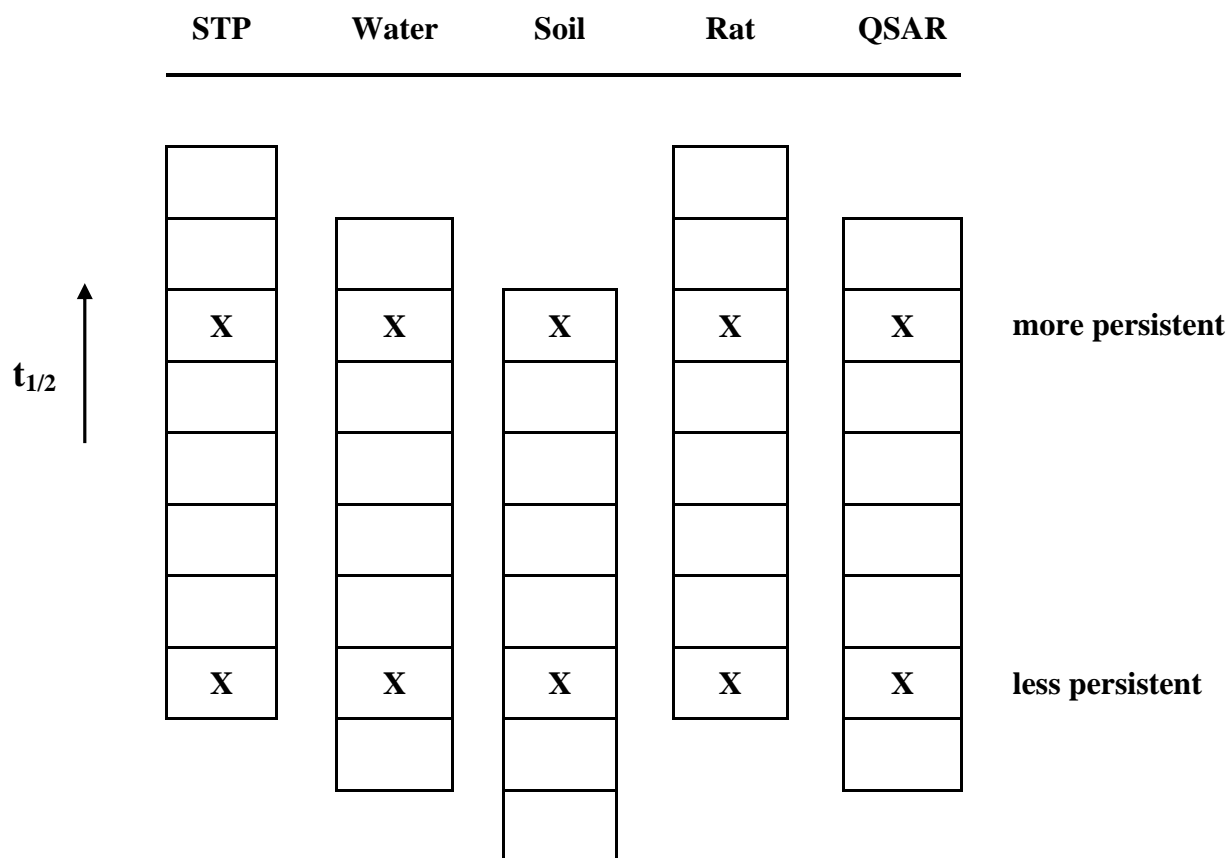
References

1. Howard, P. H., *Biodegradation.*, in *Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences.*, R. S. Boethling and D. Mackay., Editors. 2000, CRC Press: Boca Raton, FL.

2. Wackett, L. P.; Ellis, L. B. M. Predicting biodegradation. *Environmental Microbiology* **1999**, 1, 119-124.

3. Boethling, R. S.; Mackay, D., *Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences.*, R. S. Boethling and D. Mackay., Editors. 2000, CRC Press: Boca Raton, FL.

4. Fenner, K.; Scheringer, M.; Hungerbühler, K. Prediction of overall persistence and long-range transport potential with multimedia fate models: Robustness and sensitivity of results. *Environmental Pollution* **2004**, 128, 189-204.

5. Struijs, J.; van den Berg, R. Standardized biodegradability tests: Extrapolation to aerobic environments. *Water Research* **1995**, 29, 225-262.

6. Federle, T. W.; Gasior, S.; Nuck, B. A. Extrapolating mineralization rates from the ready CO_2 screening test to activated sludge, river water, and soil. *Environmental Toxicology and Chemistry* **1997**, 16, 127-134.

7. Howard, P. H.; Boethling, R. S.; Jarvis, W. F.; Meylan, W. M.; Michalenko, E. M., *Handbook of Environmental Degradation Rates*. 1991, Chelsea, MI: Lewis Publishers.

8. Mackay, D.; Shiu, W. Y.; Ma, K. C., *Physical-Chemical Properties and Environmental Fate Handbook.* 2000: CRC Press.

9. Jaworska, J. S.; Boethling, R. S.; Howard, P. H. Recent developments in broadly applicable structure-biodegradability relationships. *Environmental Toxicology and Chemistry* **2003**, 22, 1710-1723.

10. Boethling, R. S.; Sabljic, A. Screening-level model for aerobic biodegradability based on a survey of expert knowledge. *Environmental Science and Technology* **1989**, 23, 672-679.

11. Howard, P. H.; Boethling, R. S.; Stiteler, W. M.; Meylan, W. M.; Hueber, A. E.; Beauman, J. A.; Larosche, M. E. Predictive model for aerobic biodegradability developed from a file of evaluated biodegradation data. *Environmental Toxicology and Chemistry* **1992**, 11, 593-603.

12. Boethling, R. S.; Howard, P. H.; Meylan, W.; Stiteler, W.; Beaumann, J.; N., T. Group contribution method for predicting probability and rate of aerobic biodegradation. *Environmental Science and Technology* **1994**, 28, 459-65.

13. Tunkel, J.; Howard, P. H.; Boethling, R. S.; Stiteler, W.; Loonen, H. Predicting Ready Biodegradability in the Japanese Ministry of International Trade and Industry Test. *Environmental Toxicology and Chemistry* **2000**, 19, 2478-2485.

14.   Boethling, R. S.; Lynch, D. G.; Thom, G. C. Predicting Ready Biodegradability of Premanufacture Notice Chemicals. *Environmental Toxicology and Chemistry* **2003**, 22, 837-844.

15.   U.S. EPA, *EPI (Estimation Programs Interface) Suite*. 2004, U. S. EPA Office of Pollution Prevention Toxics and Syracuse Research Corporation.

16.   Environment Canada, *Guidance Manual for the Categorization of Organic and Inorganic Substances on Canada's Domestic Substances List.* 2003, Existing Substances Branch: Ottawa, ON.

Appendix

Table A-1. A list and statistical summary of empirical aerobic environmental half-lives for 75 chemicals included in the estimation method evaluation.

CAS	Chemical name	n	Empirical $t_{1/2}$ (d) Arithmetic mean	STDEV	CV	log Mean
84-74-2	Dibutylphthalate (DBP)	9	8	8	1.00	0.88
117-81-7	Di-(2-ethylhexyl)-phthalate (DEHP)	9	21	10	0.47	1.32
1582-09-8	Trifluralin	7	106	43	0.41	2.03
60-57-1	Dieldrin	6	792	491	0.62	2.90
95-48-7	*o*-cresol	5	6	5	0.74	0.79
330-55-2	Linuron	6	111	87	0.78	2.05
12789-03-6	Chlordane	6	1072	1328	1.24	3.03
60-51-5	Dimethoate	5	18	22	1.24	1.25
62-53-3	Aniline	4	14	11	0.76	1.15
75-09-2	Dichloromethane/methylenechloride	4	30	18	0.60	1.48
309-00-2	Aldrin	5	161	245	1.52	2.21
1897-45-6	Chlorothalonil	5	49	33	0.68	1.69
2921-88-2	Chloropyrifos	5	69	53	0.76	1.84
21725-46-2	Cyanazine (Bladex)	5	38	41	1.08	1.58
67-72-1	Hexachloroethane	3	138	96	0.70	2.14
85-01-8	Phenanthrene	4	67	89	1.34	1.82
94-75-7	2-(2,4-dichlorophenoxy)acetic acid	4	21	27	1.30	1.32
95-77-2	3,4-dichlorophenol	4	18	23	1.29	1.25
110-82-7	Cyclohexane	3	79	78	0.99	1.90
114-26-1	Propoxur	4	25	19	0.77	1.39
120-12-7	Anthracene	4	174	195	1.12	2.24
121-75-5	Malathion	4	20	23	1.14	1.31
133-06-2	Captan	4	19	28	1.49	1.27
218-01-9	Chrysene	4	532	312	0.59	2.73
330-54-1	Diuron	4	101	147	1.45	2.01
333-41-5	Diazinon	4	43	40	0.93	1.64

CAS	Chemical name	n	Empirical $t_{1/2}$ (d) Arithmetic mean	STDEV	CV	log Mean
2303-16-4	Diallate	4	46	35	0.75	1.66
2303-17-5	Triallate	4	106	79	0.74	2.03
33820-53-0	Isopropalin	4	63	49	0.79	1.80
95-47-6	*o*-xylene (Benzene, 1,2-dimethyl-)	3	22	13	0.60	1.35
95-63-6	1,2,4-trimethylbenzene	2	18	15	0.85	1.24
108-38-3	*m*-xylene (Benzene, 1,3-dimethyl-)	3	19	11	0.57	1.29
117-84-0	DNOP	3	14	12	0.83	1.16
132-64-9	Dibenzofuran	3	52	61	1.17	1.72
314-40-9	Bromacil	3	240	159	0.66	2.38
123-38-6	Propanal	2	4	4	1.06	0.60
75-00-3	Chloroethane	2	18	15	0.85	1.24
100-42-5	Styrene	2	21	10	0.47	1.32
591-78-6	2-hexanone	1	5	0	0.00	0.70
106-48-9	4-chlorophenol	2	20	0	0.01	1.30
628-63-7	Pentyl acetate	2	12	2	0.18	1.06
96-22-0	3-pentanone	2	8	4	0.47	0.88
759-94-4	EPTC	2	30	0	0.00	1.48
80-62-6	Methyl methacrylate	2	18	15	0.85	1.24
86-73-7	Fluorene	2	46	20	0.43	1.66
98-82-8	Isopropylbenzene (Cumene)	1	57	N/A	N/A	1.75
105-67-9	2,4-dimethylphenol	2	4	4	1.06	0.60
83-32-9	Acenapthene	2	57	63	1.11	1.76
122-39-4	Diphenylamine	2	15	19	1.29	1.17
120-83-2	2,4-dichlorophenol	2	6	4	0.70	0.74
298-00-0	Parathion-methyl	2	43	39	0.92	1.63
88-06-2	2,4,6-trichlorophenol	2	39	45	1.16	1.59
111-44-4	Bis(2-chloroethyl)ether	2	104	107	1.03	2.02
58-90-2	2,3,4,6-tetrachlorophenol	2	98	99	1.01	1.99
107-06-2	1,2-dichloroethane	2	140	57	0.40	2.15

CAS	Chemical name	n	Empirical $t_{1/2}$ (d) Arithmetic mean	STDEV	CV	log Mean
56-23-5	Carbon tetrachloride (CCl4)	2	270	127	0.47	2.43
50-29-3	p,p'-DDT	5	2872	2326	0.81	3.46
75-25-2	Tribromomethane	2	104	107	1.03	2.02
95-50-1	1,2-dichlorobenzene	2	104	107	1.03	2.02
115-29-7	Endosulfan	5	52	84	1.62	1.71
79-34-5	1,1,2,2-tetrachloroethane	3	93	78	0.84	1.97
191-24-2	Benzo[ghi]perylene	2	620	42	0.07	2.79
72-20-8	Endrin	2	2262	2882	1.27	3.35
106-46-7	1,4-dichlorobenzene	2	104	107	1.03	2.02
86-30-6	Diphenyl nitrosamine	2	22	17	0.77	1.34
67-66-3	Trrichloromethane/chloroform (CHCl3)	2	104	107	1.03	2.02
56-38-2	Parathion	2	21	20	0.94	1.32
98-95-3	Nitrobenzene	2	105	130	1.23	2.02
87-62-7	2,6-xylidine	2	104	107	1.03	2.02
122-14-5	Fenitrothion	2	18	14	0.79	1.26
108-90-7	Chlorobenzene	2	109	58	0.53	2.04
37680-65-2	PCB18	2	43	0	0.00	1.63
75-69-4	Trichlorofluoromethane	2	264	136	0.51	2.42
127-18-4	Tetrachloroethylene	2	270	127	0.47	2.43
77-47-4	1,3-cyclopentadiene, 1,2,3,4,5,5-hexachloro-	2	18	15	0.85	1.24

Table A-2. List of chemicals used in Figure 5 for the comparison of estimated aerobic biodegradation half-lives using the modified BIOWIN method and CATABOL and empirical data.
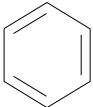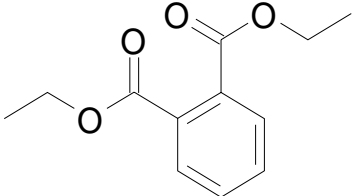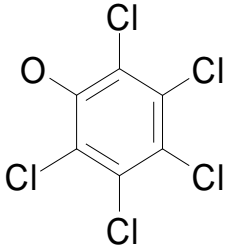
CAS	Chemical name
72-20-8	Endrin
115-29-7	Endosulfan
1582-09-8	Trifluralin
118-74-1	Hexachlorobenzene
67-72-1	Hexachloroethane
33820-53-0	Isopropalin
77-47-4	1,3-Cyclopentadiene, 1,2,3,4,5,5-hexachloro-
91-94-1	3,3-dichlorobenzidine
87-86-5	Pentachlorophenol
58-89-9	γ-HCH (lindane)
32598-13-3	PCB-77
35693-99-3	PCB-52
72-55-9	DDE
191-24-2	Benzo[ghi]perylene
1897-45-6	Chlorothalonil
2303-17-5	Triallate
21725-46-2	Cyanazine (Bladex)
207-08-9	Benzo[k]fluoranthene
50-32-8	Benzo[a]pyrene
1746-01-6	2,3,7,8-TCDD
218-01-9	Chrysene
56-55-3	Benz[a]anthracene
133-06-2	Captan
1912-24-9	Atrazine
72-43-5	Methoxychlor
2921-88-2	Chloropyrifos
129-00-0	Pyrene
206-44-0	Fluoranthene
58-90-2	2,3,4,6-TECP

CAS	Chemical name
37680-65-2	PCB-18
121-14-2	2,4-dinitrotoluene
122-34-9	Simazine
2303-16-4	Diallate
56-23-5	Carbon tetrachloride
330-55-2	Linuron
120-82-1	1,2,4-trichlorobenzene
79-34-5	1,1,2,2-tetrachloroethane
330-54-1	Diuron
95-95-4	2,4,5-trichlorophenol
88-06-2	2,4,6-trichlorophenol
122-14-5	Fenitrothion
127-18-4	Tetrachloroethylene
298-00-0	Parathion-methyl
75-69-4	Trichlorofluoromethane
86-30-6	Diphenyl nitrosamine
56-38-2	Parathion
108-60-1	Bis(2-chloroisopropyl)ether
314-40-9	Bromacil
111-44-4	Bis(2-chloroethyl)ether
106-46-7	1,4-dichlorobenzene
96-18-4	1,2,3-trichloropropane
120-12-7	Anthracene
85-01-8	Phenanthrene
116-06-3	Aldicarb
79-01-6	Trichloroethylene
93-76-5	2,4,5-trichlorophenoxyacetic acid
67-66-3	Trrichloromethane/chloroform
120-83-2	2,4-dichlorophenol
95-77-2	3,4-dichlorophenol
122-39-4	Diphenylamine
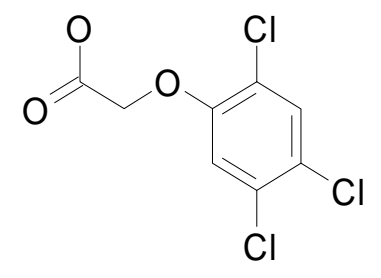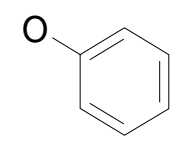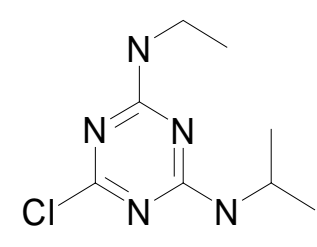
CAS	Chemical name
333-41-5	Diazinon
1563-66-2	Carbofuran
75-25-2	Tribromomethane
63-25-2	Carbaryl
98-95-3	Nitrobenzene
1918-00-9	Dicamba
83-32-9	Acenapthene
91-20-3	Naphthalene
87-62-7	2,6-xylidine
78-87-5	1,2-dichloropropane
86-73-7	Fluorene
114-26-1	Propoxur
107-06-2	1,2-dichloroethane
132-64-9	Dibenzofuran
75-09-2	Dichloromethane/methylenechloride
62-53-3	Aniline
71-43-2	Benzene
94-75-7	2-(2,4-dichlorophenoxy)acetic acid
108-90-7	Chlorobenzene
106-48-9	4-chlorophenol
759-94-4	EPTC
91-22-5	Quinoline
108-67-8	1,3,5-trimethylbenzene
95-63-6	1,2,4-trimethylbenzene
92-52-4	Biphenyl
98-82-8	Isopropylbenzene (Cumene)
100-41-4	Ethylbenzene
75-01-4	Chloroethene (Vinyl chloride)
75-00-3	Chloroethane
7085-19-0	Mecoprop
108-38-3	*m*-xylene
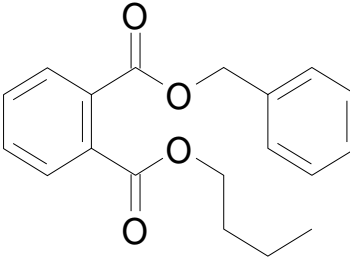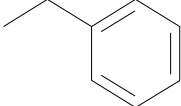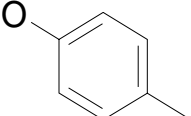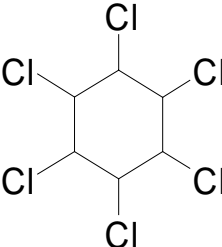
CAS	Chemical name
95-47-6	*o*-xylene
105-67-9	2,4-dimethylphenol
100-42-5	Styrene
60-51-5	Dimethoate
98-86-2	Acetophenone
108-88-3	Toluene
95-48-7	*o*-cresol
110-82-7	Cyclohexane
96-22-0	3-pentanone
108-95-2	Phenol
120-80-9	Catechol
65-85-0	Benzoic acid
591-78-6	2-hexanone
80-62-6	Methyl methacrylate
64-17-5	Ethanol
84-66-2	Diethylphthalate (DEP)
121-75-5	Malathion
85-68-7	Butyl benzyl phthalate (BBP)
131-11-3	Dimethylphthalate (DMP)
123-38-6	Propanal
117-81-7	Di-(2-ethylhexyl)-phthalate (DEHP)
628-63-7	Pentyl acetate
107-21-1	Ethylene glycol
117-84-0	DNOP
84-74-2	Dibutylphthalate (DBP)
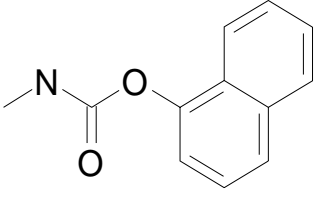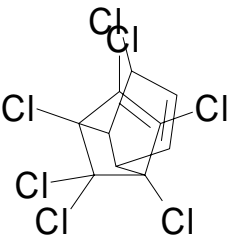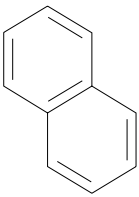
Table A-3. Summary of physical chemical properties and chemical structures for BIOWIN model calibrations.
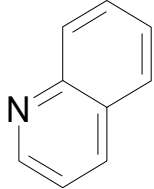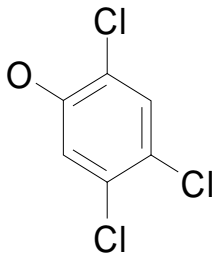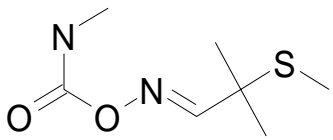
CAS	Name	MW (g/mol)	log Kow	VP (Pa)	Sw (mg/L)	Chemical Structure
71432	Benzene	78.11	2.13	1.16E+04	2.00E+03	
84662	Diethylphthalate (DEP)	222.24	2.42	3.39E-01	2.87E+02	
87865	Pentachlorophenol	266.34	5.12	1.44E-03	3.09E+00	

93765	2,4,5-trichlorophenoxyacetic acid	255.49	3.31	9.36E-04	8.16E+01	
108952	Phenol	94.11	1.46	4.31E+01	2.62E+04	
1912249	Atrazine	215.69	2.61	3.81E-03	2.14E+02	

| 85687 | Butyl benzyl phthalate (BBP) | 312.37 | 4.73 | 5.87E-03 | 9.49E-01 |

| 100414 | Ethylbenzene | 106.17 | 3.15 | 1.01E+03 | 2.29E+02 |

| 106445 | p-cresol | 108.14 | 1.94 | 1.65E+01 | 9.25E+03 |

| 58899 | γ-HCH (lindane) | 290.83 | 3.72 | 6.75E-02 | 4.04E+00 |

63252	Carbaryl	201.23	2.36	7.11E-03	4.16E+02

76448	Heptachlor	373.32	5.47	3.17E-02	2.76E-02

91203	Naphthalene	128.18	3.30	5.39E+00	1.42E+02

91225	Quinoline	129.16	2.03	7.19E+00	1.71E+03	
95954	2,4,5-trichlorophenol	197.45	3.72	6.76E-01	1.14E+02	
116063	Aldicarb	190.26	1.13	6.44E-01	5.31E+03	

118741	Hexachlorobenzene	284.78	5.73	4.07E-04	1.92E-01
122349	Simazine	201.66	2.18	1.22E-03	5.90E+02
131113	Dimethylphthalate (DMP)	194.19	1.60	6.16E-01	2.01E+03
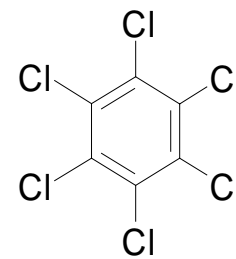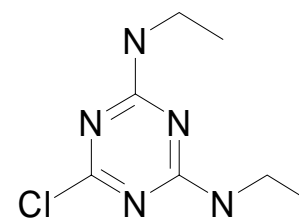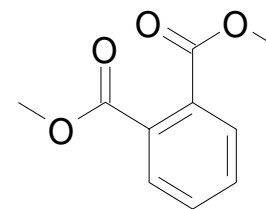
| 1563662 | Carbofuran | 221.26 | 2.32 | 7.39E-03 | 3.54E+02 |

| 1746016 | 2,3,7,8-TCDD | 321.98 | 6.80 | 2.60E-06 | 1.10E-03 |

| 1918009 | Dicamba | 221.04 | 2.21 | 7.05E-03 | 4.41E+02 |

| 50328 | Benzo[a]pyrene | 252.32 | 6.13 | 2.65E-06 | 1.04E-02 |

| 56553 | Benz[a]anthracene | 228.30 | 5.76 | 3.63E-05 | 2.91E-02 |

| 72435 | Methoxychlor | 345.66 | 5.08 | 5.56E-03 | 3.02E-01 |
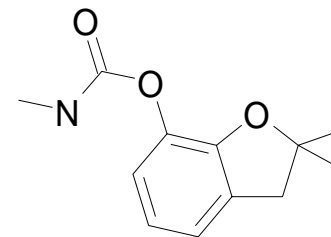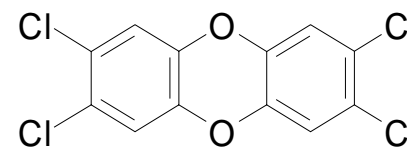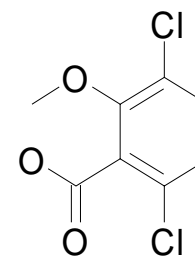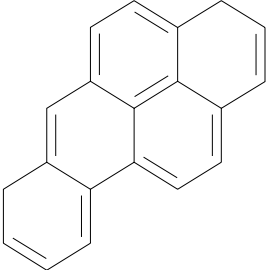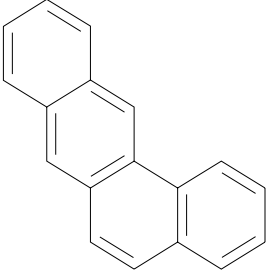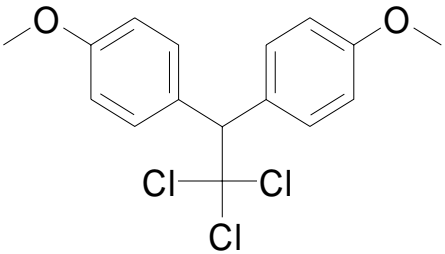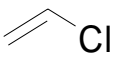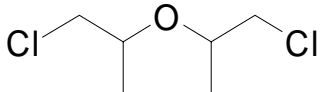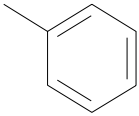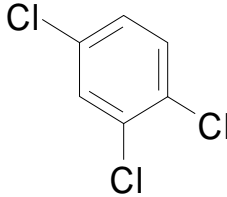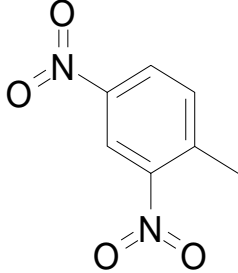
75014	Chloroethene (Vinyl chloride)	62.50	1.62	3.63E+05	5.63E+03	
108601	Bis(2-chloroisopropyl)ether	171.07	2.48	9.15E+01	4.63E+02	
108883	Toluene	92.14	2.73	3.16E+03	5.73E+02	
120821	1,2,4-trichlorobenzene	181.45	4.02	2.44E+01	2.00E+01	
121142	2,4-dinitrotoluene	182.14	1.98	9.59E-02	4.46E+02	

206440	Fluoranthene	202.26	5.16	4.17E-04	1.30E-01
7085190	Mecoprop	214.65	3.13	6.08E-02	1.94E+02
64175	Ethanol	46.07	-0.31	8.12E+03	7.92E+05
65850	Benzoic acid	122.12	1.87	3.97E-01	2.49E+03
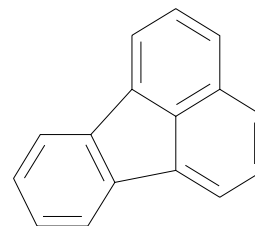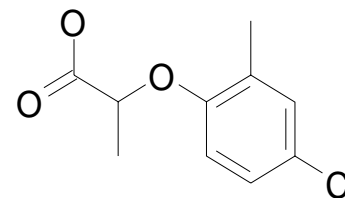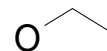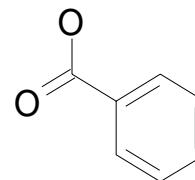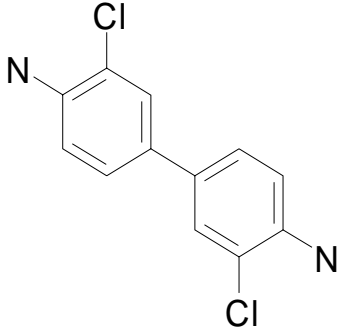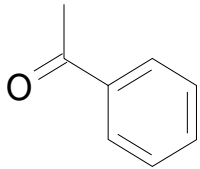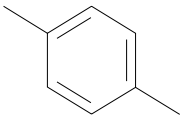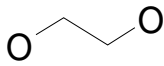
91941	3,3'-dichlorobenzidine	253.13	3.51	5.55E-04	2.29E+01	
98862	Acetophenone	120.15	1.58	4.35E+01	4.48E+03	
106423	*p*-xylene (Benzene, 1,4-dimethyl-)	106.17	3.15	9.16E+02	2.29E+02	
107211	Ethylene glycol	62.07	-1.36	1.23E+01	1.00E+06	
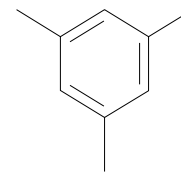
| 108678 | 1,3,5-trimethylbenzene | 120.20 | 3.42 | 2.68E+02 | 1.20E+02 |

| 120809 | Catechol | 110.11 | 0.88 | 1.52E-01 | 7.32E+04 |